Copyright © 2017 University of Birmingham. All rights reserved.

No parts of this publication may be produced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the prior written permission of University of Birmingham, Birmingham, UK.
Table of Contents

Preface

Papers (in Categories)

Advanced Applications ................................................................. 1

A local radial basis function collocation method (LRBFCM) for calculation of phononic band structures with scatterers of arbitrary geometry ............................................... 2
H. Zheng, Z. Yang, C. Zhang

Initial prestress optimisation of tensegrity structures based on artificial fish swarm algorithm . ................................................................. 6
R. Liang, Y. Feng, Y. Wang

Numerical modelling of geothermal reservoirs using the triple porosity-permeability approach ................................................................. 10
M.D. Aliyu, H.P. Chen

A model for simultaneous damage, healing and capillary flow in cementitious materials . . 14
T. Jefferson, R. Davies

Level set based topology optimisation using high-order reinitialisation methods and the discontinuous Galerkin method ....................................................... 18
T. Adams, S. Giani, W.M. Coombs

Analysis of a plate using EPR-based self-learning finite element method ............... 22
A. Nassr, A.A. Javadi

A numerical reduction scheme for multiple ion transport problems ..................... 26
B.L. Freeman, P.J. Cleall, T.D. Jefferson

A stable cut finite element method for multiple unilateral contact ...................... 30
P. Kerfriden, S. Claus

A new, meshless approach to fast solid dynamics: applications in metal plasticity .... 34

Simulations of sliding adhesive contact between microgear teeth in silicon-based mems work in a vacuum environment ......................................................... 38
N. Almuramady, F.M. Borodich

The optimisation of production well numbers in enhanced geothermal system .... 42
M. Samin, A. Faramarzi, I. Jefferson, O. Harireche
Biomechanics

Development of a 1D-0D cardiovascular model of pregnancy in humans
J.M. Carson, M.J. Lewis, D. Rassi, R.V. Loon

A semi implicit, locally conservative galerkin approach for modelling systemic blood
circulation
H.M. Hasan, P. Nithiarasu

Blood flow simulation using smooth particle hydrodynamics
M.K. AL-SAAD, S. Kulasegaram, S.P.A. Bordas

Numerical analysis of bone remodelling for equine 3rd metacarpal
K. Lewandowski, Ł. Kaczmarczyk, J.F. Marshall, C.J. Pearce

A polyconvex computational formulation for electro-activation in cardiac mechanics

Cell force identification
Ł. Kaczmarczyk, K. Lewandowski, M. Salmeron-Sanchez, C. Pearce

Contact and Error Estimation

Hyperdimensional offsets and polynomial Refinement and integration scheme for Harmonic
basis function finite elements
P.A.H. Gadoury, I.M. Gitman

Accuracy control and non-intrusive implementation of model order Reduction based on
greedy sampling for elasto-dynamics
X Du, A. Kundu, P. Kerfriden

Generalized finite elements for blow up solutions to reaction-diffusion equations
G. Estrada-Rodriguez, H. Gimperlein

Three-dimensional mortar contact formulation: an efficient and accurate numerical
implementation
Z. Ullah, Ł. Kaczmarczyk, C.J. Pearce

Efficiency analysis of patch size and type for error estimates based on implicit residual and
local dirichlet patch problems
P. Bonilla, A. Kundu, P. Kerfriden

A-priori error estimator based hierarchical $p$ adaptivity scheme for acoustic
X. Meng, J. Reboud, Ł. Kaczmarczyk

Failure, Fracture and Damage

Coupling enriched rbf and mfs for anti-plane shear cracks
F.M. Mukhtar, H.J. Al-Gahtani
Simulating evolution of fluid lag during hydraulic fracture propagation using finite element method .......................................................... 102
B. Chen, C. Li, B.R. Barboza

A non-ordinary state based peridynamics Implementation for anisotropic materials ..... 106
G. Hattori, J. Trevelyan

A constitutive model for elastic-plastic behaviour and delamination damage in fibre metal laminates .................................................. 110
A.S.M. Al-Azzawi, L.F. Kawashita, C.A. Featherston

Dynamic brittle fracture via material point method-a phase-field implementation ...... 114
E.G. Kakouris, S.P. Triantafyllou

Adaptive Hierarchical Refinement in Isogeometric Analysis for Cohesive Fracture ..... 118
L. Chen, R. De Borst

Higher order gradient continua: an isogeometric approach ............................ 122
I. Kolo, H. Askes, R. De Borst

Self-similarity of a brittle fracture phase field model ................................. 126
A.C. Hansen-Dörr, M. Kästner, R. De Borst

Explicit 3D crack modelling by the Cracking Particle .................................. 130
W. Ai, C.E. Augarde

An implicit implementation of non-ordinary state-based peridynamics .......... 134
N.A. Hashim, W.M. Coombs, G. Hattori, C.E. Augarde

A discontinuous Galerkin hp-adaptive finite element method for brittle crack propagation ................................................................. 138
R. Bird, W.M. Coombs, S. Giani

A finite element model for fault rupture ................................................... 142
S. Alizadeh Sabet, R. De Borst

Numerical analysis of flow parameters in hydraulic fracturing .................... 146
D. Mahdavian, A.A. Javadi

Fluid Mechanics and Fluid-Structure interaction ...................................... 150

Simulation of Aerodynamic Behaviour of a Road Vehicle in Turbulent Flow .... 151
A. Al-Saadi, A. Hassanpour, Y. Ghaffari Motlagh, T. Mahmud

Flow past a 3d elastic cantilever beam attached to a solid block .................... 155
M. Al Manthari, P. Nithiarasu

Aerodynamic improvement of the horizontal axis wind turbine by using winglets .... 159
A. Farhan, A. Hassanpour, A. Burns, Y. Ghaffari Motlagh
<table>
<thead>
<tr>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numerical investigation of particle-fluid flows: formulation, analysis and application</td>
<td>163</td>
</tr>
<tr>
<td>Y. Ghaffari Motlagh, A. Hassanpour, A. Bayly</td>
<td></td>
</tr>
<tr>
<td>Numerical simulation of two-phase flow with Eulerian model in a channel</td>
<td>167</td>
</tr>
<tr>
<td>B.R. Barboza, C. Li</td>
<td></td>
</tr>
<tr>
<td>CFD investigation of transitional separation bubble characteristics on Naca 63415 airfoil at low Reynolds numbers</td>
<td>170</td>
</tr>
<tr>
<td>I.F. Zidane, G. Swadener, K.M. Saqr, X.Ma, M.F. Shehadeh</td>
<td></td>
</tr>
<tr>
<td>Parallel performance of an open source fluid structure interaction application</td>
<td>174</td>
</tr>
<tr>
<td>S. Hewitt, L. Margetts, A. Revell</td>
<td></td>
</tr>
<tr>
<td>Geomechanics</td>
<td>178</td>
</tr>
<tr>
<td>Stability analysis of geometrically non-homogeneous stratified slopes</td>
<td>179</td>
</tr>
<tr>
<td>R. Sauffisseau, A. Ahangar Asr</td>
<td></td>
</tr>
<tr>
<td>An efficient large-scale DEM model initialization procedure</td>
<td>187</td>
</tr>
<tr>
<td>M.O. Ciantia, T.Shire</td>
<td></td>
</tr>
<tr>
<td>Energy dissipation in granular materials in triaxial tests</td>
<td>191</td>
</tr>
<tr>
<td>R.A. Mukwiri, Y. Ghaffari Motlagh, W.M. Coombs, C.E. Augarde</td>
<td></td>
</tr>
<tr>
<td>Numerical investigation of the bedding factors associated with the design of buried concrete pipes subjected to traffic loading</td>
<td>183</td>
</tr>
<tr>
<td>S. Alzabeebee, D.N. Chapman, A. Faramarzi</td>
<td></td>
</tr>
<tr>
<td>Enhancing efficiency of DEM modeling of particle breackage</td>
<td>195</td>
</tr>
<tr>
<td>M.O. Ciantia, N. Zhang, M. Arroyo</td>
<td></td>
</tr>
<tr>
<td>Numerical investigation into the effect of cavity size and location on stability of earth dams</td>
<td>199</td>
</tr>
<tr>
<td>H. Al-Ateya, A. Ahangar Asr</td>
<td></td>
</tr>
<tr>
<td>Layout optimization of soil reinforcement</td>
<td>203</td>
</tr>
<tr>
<td>J. González-Castejón, C. Smith</td>
<td></td>
</tr>
<tr>
<td>Dynamic response of improved seabed soil - caisson foundation under earthquake loading</td>
<td>207</td>
</tr>
<tr>
<td>E. Tatlıoğlu, M.B.C. Ülker, M. Ayşen Lav</td>
<td></td>
</tr>
<tr>
<td>The modelling of soil-tool interaction using the material point method</td>
<td>211</td>
</tr>
<tr>
<td>M. Cortis, W.M. Coombs, C.E. Augarde, S. Robinson, A. Brennan, M. Brown</td>
<td></td>
</tr>
<tr>
<td>Soil conditions and piping criteria during suction caisson installation in layered seabed strata</td>
<td>215</td>
</tr>
<tr>
<td>M. Mehravar, O. Harireche, A. Faramarzi, S. Dirar</td>
<td></td>
</tr>
<tr>
<td>Title</td>
<td>Page</td>
</tr>
<tr>
<td>----------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>Solids and Structures</td>
<td>219</td>
</tr>
<tr>
<td>Isogeometric analysis of small-scale plates with nonlinearity</td>
<td>220</td>
</tr>
<tr>
<td>H.X. Nguyen, T.P. Vo</td>
<td></td>
</tr>
<tr>
<td>Objective fixed-pole approach in geometrically exact 3d beams:</td>
<td>224</td>
</tr>
<tr>
<td>implementational aspects</td>
<td></td>
</tr>
<tr>
<td>M. Gaceša, G. Jelenic</td>
<td></td>
</tr>
<tr>
<td>An adapted artificial compressibility algorithm for nearly and truly</td>
<td>228</td>
</tr>
<tr>
<td>incompressible large strain solid dynamics</td>
<td></td>
</tr>
<tr>
<td>The point collocation method with a local maximum entropy approach</td>
<td>232</td>
</tr>
<tr>
<td>L. Fan, C.E. Augarde, W.M. Coombs</td>
<td></td>
</tr>
<tr>
<td>An accelerated black-box Fast Multipole Isogeometric Boundary</td>
<td>236</td>
</tr>
<tr>
<td>Element Method for 3D elasticity</td>
<td></td>
</tr>
<tr>
<td>J. Trevelyan, S. Li</td>
<td></td>
</tr>
<tr>
<td>On the implementation of gradient plasticity with the material</td>
<td>240</td>
</tr>
<tr>
<td>point method</td>
<td></td>
</tr>
<tr>
<td>T.J. Charlton, W.M. Coombs, C.E. Augarde</td>
<td></td>
</tr>
<tr>
<td>Rocking of single and dual rigid-block systems subject to</td>
<td>244</td>
</tr>
<tr>
<td>ground excitation: experimental and computational analysis of</td>
<td></td>
</tr>
<tr>
<td>overturning conditions</td>
<td></td>
</tr>
<tr>
<td>G. Jelenic, N. Ceh, N. Bicanic</td>
<td></td>
</tr>
<tr>
<td>Modelling mixed-mode rate-dependent delamination in layered</td>
<td>248</td>
</tr>
<tr>
<td>structures using geometrically nonlinear beam finite elements</td>
<td></td>
</tr>
<tr>
<td>L. Škec, G. Alfano, G. Jelenic</td>
<td></td>
</tr>
<tr>
<td>Multi-level Monte Carlo methods for large-scale eigenvalue problems</td>
<td>252</td>
</tr>
<tr>
<td>H.J.T. Unwin, N. Sime, G.N. Wells</td>
<td></td>
</tr>
<tr>
<td>Boundary representation and boundary condition imposition in the</td>
<td>256</td>
</tr>
<tr>
<td>material point method</td>
<td></td>
</tr>
<tr>
<td>Y. Bing, M. Cortis, T.J. Charlton, W.M. Coombs, C.E. Augarde</td>
<td></td>
</tr>
<tr>
<td>Isogeometric boundary element method based on adaptive hierarchical</td>
<td>260</td>
</tr>
<tr>
<td>refinement of Nurbs</td>
<td></td>
</tr>
<tr>
<td>H. Khaki, J. Trevelyan</td>
<td></td>
</tr>
<tr>
<td>Implicit MPM with second-order convected particle domain</td>
<td>264</td>
</tr>
<tr>
<td>interpolation</td>
<td></td>
</tr>
<tr>
<td>L. Wang, W.M. Coombs, C.E. Augarde, M. Brown</td>
<td></td>
</tr>
<tr>
<td>Prediction of burst pressure for steel pipes with gouge defect using</td>
<td>268</td>
</tr>
<tr>
<td>numerical modelling</td>
<td></td>
</tr>
<tr>
<td>A.H. Wordu, K.F. Tee</td>
<td></td>
</tr>
</tbody>
</table>
Progressive collapse of braced irregular steel structures located in regions with different seismic activity .......................................................... 272
A.H. Ebrahimi, P. Martinez-Vazquez, C. Baniotopoulos

Blast simulations and transient responses of long-span glass roof structures: a case of London’s railway station ................................................ 276
S. Kaewunruen, G. Pompeo, G. Bartoli

Recovery of strong equilibrium in plates revisited ........................................ 280
E.A.W. Maunder, J.P.M. De Almeida

Effective high-fidelity nonlinear analysis of metal sandwich panels using partitioned modelling ............................................................... 284
A.N. Nordas, L.P.F. Santos, B.A. Izzuddin, L. Macorini

Design-oriented mechanical models for local buckling assessment of sandwich panels with metal cores ..................................................... 288
L. Santos, A.N. Nordas, B.A. Izzuddin, L. Macorini

Realistic modelling of irregular floor slabs under extreme loading ................ 292
S. Grosman, B.A. Izzuddin

Debonding of cellular structures under shear deformation ......................... 296
A. Safar, H. Wyatt, L.A. Mihai

A modified applied element method using adaptive Gaussian springs for Elasto-plastic analysis of structures ........................................... 300
M. Abdul Latif, Y.T. Feng

Wave and Electromagnetics .................................................................... 304

Evaluation of highly oscillatory integrals in the Partition of Unity BEM for wave simulations in 2D .............................................................. 305

Boundary Elements and Mesh Refinements for the Wave Equation ........... 309
D. Stark, H. Gimperlein

Numerical simulations of semi–conductor plasmonic nanolasers ................ 313

Author index ......................................................................................... 317
Preface

We are delighted to present the Proceedings of the 25\textsuperscript{th} conference of the UK Association for Computational Mechanics (UKACM), formerly known as the UK Association for Computational Mechanics in Engineering (ACME). The organisation was founded in 1992 with the aim of promoting research in computational mechanics and various engineering applications and establishing formal links with similar organisations in Europe and the International Association of Computational Mechanics (IACM).

The 25\textsuperscript{th} UKACM Conference (UKACM 2017) aims to provide a forum for presenting and discussing research findings in many areas of mechanics, with an emphasis on interdisciplinary aspects. It extends the success of the previous 24 conferences which proved to be particularly useful events for bringing together researchers from different disciplines, and especially for providing young researchers with opportunities to present their work.

These Proceedings contain more than 70 papers presented at the UKACM 2017 Conference which was held at the School of Engineering, the University of Birmingham, from 12\textsuperscript{th} to 13\textsuperscript{th} April 2017. The Proceedings encompass a wide range of topics including solid and structural mechanics; failure, fracture and damage; geo-mechanics; fluid mechanics and biomechanics, to name but a few. UKACM 2017 was preceded by the UKACM School on 11\textsuperscript{th} April, where two lectures were delivered on the topics of train aerodynamics and very large-scale topology optimisation.

We would like to thank the many people who have contributed to this conference, especially all the authors, who meticulously prepared their papers and presented their original research, as well as the reviewers and the members of the scientific committee who carefully considered every paper ensuring the quality of these Proceedings. We would like to express our gratitude to the three invited keynote speakers; Professor Spencer Sherwin, Dr Fehmi Cirak and Professor Mike Hartnett; for their thought-provoking lectures and seminal scholarly contributions. We are grateful to the speakers of the UKACM School; Professor Chris Baker, Dr Hassan Hemida and Professor Michal Kočvara; for their excellent lectures on the very important topics covered in the School.

We are indebted to Professor Mark Sterling, Head of the School of Engineering, for his help, support and advice. Additionally, we would like to acknowledge the support provided by the College of Engineering and Physical Sciences, particularly Mr Martin Byrne and Mr Tony Rogers who have been instrumental in providing logistical support. Last but not least, we are thankful to the members of the local organising committee who worked tirelessly for the success of the UKACM 2017 conference.

Dr Asaad Faramarzi  
*The Conference Chairman and Co-Editor of the Proceedings of the 25\textsuperscript{th} UKACM Conference*

Dr Samir Dirar  
*Co-Editor of the Proceedings of the 25\textsuperscript{th} UKACM Conference*

Birmingham, April 2017
Advanced Application
A local radial basis function collocation method (LRBFCM) for calculation of phononic band structures with scatterers of arbitrary geometry

*H. Zheng¹, Z. Yang¹, Ch. Zhang²
¹Centre for Low Impact Buildings, Coventry University, CV1 5FB, United Kingdom
²Department of Civil Engineering, University of Siegen, D-57068 Siegen, Germany

*ac3471@coventry.ac.uk

ABSTRACT

The instability of the strong form meshless method is one of the key issues that limits its wider applications due to the difficulty in calculation of derivatives of field quantities on the domain boundaries. Based on our previous works, an improved local radial basis function collocation method (LRBFCM) is developed and applied to calculate phononic band structures in this work. The numerical results are validated by the finite element method and show that the developed strong form LRBFCM can greatly improve the instability problem associated with other methods.

Keywords: Phononic crystals; interface conditions; elastic wave propagation; band structures; eigenvalue problems; radial basis functions

1. Introduction

The global radial basis function (RBF) collocation method (GRBFCM) is a type of meshless method proposed in 1990s [1]. The full matrix formulation limits the wider applications of this method, and often causes numerical instability. In order to solve this problem, the finite difference scheme was introduced to the GRBFCM to generate a sparse system matrix, which is referred to as the RBF generated finite difference (RBF-FD) method [2-6]. As a variant of the RBF-FD method, the local RBF collocation method (LRBFCM) can greatly enhance the stability and the efficiency of the conventional GRBFCM [7, 8]. But the instability caused by the Neumann boundary conditions still exists. To overcome the instability, the least square method was introduced to the LRBFCM for the problem of phononic crystals [9, 10]. Nevertheless, the instability still exists and the application of LRBFCM for the phononic crystal is limited to simple cases such as a square lattice with square scatterers. In order to further solve the instability, the direct method, indirect method and fictitious node method were proposed in the LRBFCM for problems of phononic crystals [11] with higher stability.

In this work, we further improve the stability of LRBFCM for accurate calculation of band structures of phononic crystals with scatterers of arbitrary geometry, by proposal a new treatment of the interfacial boundary conditions between the . Examples are modelled using the LRBFCM and the results were validated by FEM models.

2. Numerical results

A square lattice with a star-shaped scatterer and its first Brillouin zone with 225 points are shown in Figure 1. 2585 degrees of freedom with 2454 nodes are used in the LRBFCM, as shown in Figure 2. An FE mesh with 2737 degrees of freedom and 1348 elements is also modeled in using COMSOL Multiphysics for comparison, as shown in Figure 3.
Figures 4 and 5 show the band structures of the aurum (Au) scatterers embedded in the epoxy (Ep) matrix from the FEM and LRBFCM, respectively, where the normalized frequency \( \omega a / (2\pi c) \) is introduced, with \( c_1 = \sqrt{\mu_1 / \rho_1} \). It can be seen that the present results are virtually identical with the FEM results. The same conclusion can be drawn from Figures 6 and 7 showing the band structures of an aluminium (Al) scatterers embedded in the epoxy matrix.
3. Comparison of computational time

The CPU times of the present LRBFCM and the FEM for the above numerical examples are given in Table 1. The lowest ten eigenvalues are compared and the errors are defined as

$$Errors = \frac{\sum |E_r - E_f|}{\sum |E_f|},$$

where $E_f$ is the result of the FEM and $E_r$ the result of the LRBFCM using an in-house Matlab code. All the simulations are run on the same laptop with Intel(R) Core(TM) i7-4510U, 2.00 GHz CPU and 8 GB RAM.

Table 1 shows that the performance of the present LRBFCM is much better than that of the FEM in general. The computing time required by the improved LRBFCM is much less than that required by the FEM, with more than 90% savings in all the cases considered here. The high efficiency of the present LRBFCM is attributed to the fact that it is based on a strong-form formulation of the partial differential equations and does not need any numerical integration for computing the system matrices.

4. Conclusions

In this paper, a new numerical technique based on the LRBFCM is developed. The LRBFCM is applied to the phononic crystals with a scatterer of arbitrary geometry. Numerical results show that the improved LRBFCM performs very well in calculations of the band structure of phononic crystals.
Table 1: Comparisons of computing time and accuracy for the phononic crystals

<table>
<thead>
<tr>
<th>Lattice form</th>
<th>Square</th>
<th>Triangular</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material properties</td>
<td>Au/Ep</td>
<td>Al/Ep</td>
</tr>
<tr>
<td>RBF Degrees of freedom</td>
<td>2585</td>
<td>2585</td>
</tr>
<tr>
<td>Time needed [s]</td>
<td>88.8</td>
<td>92.24</td>
</tr>
<tr>
<td>FEM Degrees of freedom</td>
<td>2055</td>
<td>2055</td>
</tr>
<tr>
<td>Time needed [s]</td>
<td>1003</td>
<td>1130</td>
</tr>
<tr>
<td>Comparison Errors</td>
<td>0.00698</td>
<td>0.00335</td>
</tr>
<tr>
<td>Time saving</td>
<td>91.14%</td>
<td>91.84%</td>
</tr>
</tbody>
</table>

References


INITIAL PRESTRESS OPTIMISATION OF TENSEGRITY STRUCTURES BASED ON ARTIFICIAL FISH SWARM ALGORITHM

*R. Liang¹ Y. T. Feng¹ and Y. Wang²

¹Zienkiewicz Centre for Computational Engineering, College of Engineering, Swansea University, Fabian Way, Swansea, SA1 8EN, UK
²State Key Laboratory of Geomechanics and Geotechnical Engineering, Institute of Rock and Soil Mechanics, Chinese Academy of Sciences, Wuhan, 430071, China

*744707@swansea.ac.uk

ABSTRACT

This work presents an optimisation scheme based on an artificial fish swarm algorithm (AFSA) for the determination of the geometric stability and initial prestress distribution of pin-jointed tensegrity structures without any external loading. By checking the positive definiteness of the stability matrix of tensegrity structures, the geometric stability condition can be established for a statically and kinematically indeterminate system, from which whether the system has a first-order infinitesimal mechanism or not can be checked [2]. Also, the definition of a tensegrity structure requires each element to be tension- or compression-type, which indicates that the prestress in the system needs to satisfy a feasible condition. An optimisation procedure is proposed to describe the geometric stability and feasible conditions, and a uniform distribution of the prestress is also taken into account. An artificial fish swarm algorithm [3] is employed to find the minimum value of the proposed 3-level optimisation problem. A tensegrity assembly consisting of twenty-four cables and six struts is investigated to demonstrate the efficiency and robustness of the proposed scheme.

Keywords: tensegrity structure; initial prestress; artificial fish swarm algorithm; optimisation modelling

1. Introduction

The first concern in designing a tensegrity structure is its geometry and topology. Most of existing fascinating works, however, are finished by imagination and intuition in the early years. In fact, tensegrity structures belong to statically indeterminate structures — their static equilibrium equations are not sufficient to uniquely determine the internal and reaction forces [1]. Like any other tensile structure, a tensegrity structure acquires the stiffness through the prestress or self-stress in it. Since the geometry of tensile structures also contributes to the stiffness, the prestress and geometry, or the “force” and “shape”, usually interact with each other. For a given geometry, the process of determining the prestress of a tensegrity structure is known as force-finding.

To know if the system is geometric stable, Calladine and Pellegrino [2] developed an automatic search algorithm based on the concept of a positive definite matrix. However, this algorithm is complicated, and the convergence cannot be guaranteed in a finite number of steps. Yuan and Dong [4] presented an integral feasible prestress algorithm which takes the advantage of the symmetry of the cable dome structures by sacrificing the generality. Xu [5] proposed a numerical scheme to study the force-finding procedure by establishing an optimisation model and applying simulated annealing algorithm (SAA) to solve the problem. In this work, an innovative optimisation model for the initial prestress distribution of pin-jointed assemblies is proposed, which accounts for the geometric stability, tension-compression feasibility as well as the uniformity of the prestress in the structure. A swarm intelligence method, artificial fish swarm algorithm [3] is employed to search for the extrema of the proposed 3-level optimisation problem.

2. Optimisation model
For a statically and kinematically indeterminate assembly, if the mechanism in the system can be stiffened by the self-stress or prestress, then this kind of mechanism is known as first-order infinitesimal mechanism [1]. As a result, this assembly is stable in the current geometry. The geometric stability of a system can be checked by studying its positive definiteness of the stability matrix [2]. One way to determine the definiteness of a matrix is to investigate its eigenvalues, that is, a matrix is positive definite only if all its eigenvalues are positive. Therefore to study the geometric stability of a system, one can perform a sign check of the eigenvalues of the stability matrix. Assume the number of the positive eigenvalues is \( n \), then a function \( f(\alpha_i) \) can be constructed as [5]

\[
f(\alpha_i) = m - n
\]  

where \( m \) is the dimension of the stability matrix, \( \alpha_i \) is the coefficient of the linear combination of all the existing states of prestress. Note that the states of prestress is a relative value, so the domain of \( \alpha_i \) is chosen to be \([0, 1]\) for simplification. In order to consider the negative definiteness situation, the domain is expanded to be \([-1, 1]\). It is clear to know that \( m \) is also the number of eigenvalues and the number of modes of mechanism. If \( f(\alpha_i) \) can be minimised to zero, the corresponding stability matrix is positive definite, and the assembly is geometric stable, or said to has a first-order infinitesimal mechanism.

The definition of a tensegrity structure requires all the components need to be in a specific stress state, compression (struts) or tension (cable). This requirement, also known as feasible condition, can be expressed by a function as

\[
g(\alpha_i) = p + q - Z
\]  

where \( Z \) is the number of members that satisfy the feasible condition, \( p \) and \( q \) are the number of components in tension and compression, respectively. In order to make sure all the elements meet the feasible requirement, function \( g(\alpha_i) \) need to vanish. Also, this can be done by minimising \( g(\alpha_i) \) to zero.

Moreover, to make a full use of the material, the prestress in a structure is expected to be uniformly distributed. The uniformity of the prestress can be measured by the following function as

\[
l(\alpha_i) = \sqrt{\sum_{i=0}^{b} (|t_i| - \bar{t})^2} \
\]

where \( t_i \) is the stress in element \( i \), \( \bar{t} = \frac{\sum_{i=0}^{b} |t_i|}{b} \) is the arithmetical mean value of the absolute value of prestress in all the members. A more uniform prestress distribution can be obtained when \( l(\alpha_i) \) is also minimised.

To combine the above three objective functions into one, and notice their different priorities, the total objective function can be defined as

\[
F(\alpha_i) = (p + q) f(\alpha_i) + g(\alpha_i) + l(\alpha_i)
\]  

and now the overall optimisation problem is

\[
\min(F(\alpha_i)), \quad s.t. \alpha_i \in [-1, 1]
\]  

3. Numerical example

A tensegrity structure with twelve joints and thirty members is shown in Figure 1. The members consist of twenty-four cables (black) and six struts (red). Since tensegrity structures are self-stressed and self-stable, the constraints are not necessary for its geometric stability except for the rigid body motion. In
this case the assembly has one mode of mechanism \((m = 1)\) and one state of self-stress \((s = 1)\), which means the prestress distribution is unique.

![Figure 1: A tensegrity structure with twenty-four cables and six struts](image)

When four joints of this assembly are fully fixed, shown in Figure 1 (b), it will have six states of self-stress \((s = 6)\) and zero mechanism \((m = 0)\), and accordingly this structure is statically indeterminate and kinematically determinate, and its geometrically stability is achieved automatically. However, the tension-compression feasibility and uniformity are still need to be investigated. The optimisation curves of the objective function of feasibility and uniformity conditions are obtained by applying artificial fish swarm algorithm (AFSA), which are shown in Figure 2 and 3.

Figure 2 clearly show that the objective function of feasible prestress, \(g(\alpha_i) = p + q - Z\), is minimised to zero, because after some iterations, the prestress in all the members of the tensegrity structure tend to satisfy the tension-compression requirement: twenty-four members are in tension while the rest six are in compression.

![Figure 2: Optimisation curve of \(g(\alpha_i)\)](image)

After the uniformity optimization being performed, the prestress distribution tends to be more uniform. Our results show he ratio \(\xi\) of the maximum to the minimum value of feasible prestress (absolute value) is \(\xi = \frac{1.1473}{0.00014924} \approx 7688\), while the ratio of that of uniform prestress is remarkably
reduced to $\xi = \frac{0.1012}{0.0125} \approx 8$, and the optimisation curve of $F(\alpha_i)$ is given in Figure 3.

![Figure 3: Optimisation curve of $F(\alpha_i)$](image)

**4. Conclusions**

A new optimisation model for the prestress distribution of tensegrity structures is proposed in this work. This model accounts for the geometric stability, tension-compression feasibility as well as the uniformity of the prestress in the structure. The artificial fish swarm algorithm is employed to search for the extrema of the objective function of the optimisation model. A numerical example is studied to present the efficiency and robustness of the proposed method.

**Acknowledgements**

The research is supported by National Natural Science Foundation of China (51579237 and 51309027), the Foundation of State Key Laboratory for Geomechanics and Deep Underground Engineering (SKLGDUEK 1110), and the Natural Science Foundation of Zhejiang Province, China (LY13E080009).

**References**


NUMERICAL MODELLING OF GEOTHERMAL RESERVOIRS USING THE TRIPLE POROSITY-PERMEABILITY APPROACH

Musa D. Aliyu¹ and Hua-Peng Chen¹*

¹Department of Engineering Science, University of Greenwich, Chatham Maritime, Kent, ME4 4TB, United Kingdom.

*Corresponding author: H.Chen@greenwich.ac.uk

ABSTRACT

Predicting long-term performance with the aid of modelling in deep heterogeneous subsurface media is of importance for problems such as geothermal energy mining, waste disposal reservoirs, hydrocarbon reservoirs, and supercritical carbon dioxide (CO₂) sequestration systems. In order to examine the nature of these systems, coupled process modelling is required in understanding the nature of interactions that occurs within the media and transport processes. However, the mathematical difficulty in representing the reservoir heterogeneity regarding dimensions, and other spatial distributions of fractures and faults, have to be addressed properly. To accomplish this task, this study proposes to introduce a concept of a triple porosity-permeability model so as to capture the presence of multiple pore media in deep geological formation for geothermal energy exploitations using the finite element methods (FEM). A numerical model is developed based on the Soultz deep geothermal reservoir experimentation data to predict long-term performance during an operational period of 30 years. The model is implemented as a fully coupled transient thermo-hydraulic processes in the simulation, and produced fluid temperature at the production wellbore and the temperature at the fracture-fault interface are observed. The results demonstrated that the prediction achieved using the proposed model is closer to the response experience in field measurements. Therefore, the proposed approach is computationally efficient and accurate in modelling porous media with multiple contiguous.

Keywords: Fractures; Faults; Triple porosity-permeability; thermo-hydraulic; multiple pore media

1. Introduction

The study of heat and fluid transport in naturally fractured reservoirs has recently received increased attention because of its importance to subsurface natural-resource recoveries such as geothermal reservoirs, hydrocarbon reservoirs, waste disposal, and carbon dioxide (CO₂) storage. For more than 50 years, several models have represented the understanding and modelling of heat and fluid transport processes in naturally fractured reservoirs [1]. Despite the advances, modelling the coupled processes of heat and fluid transport in naturally fractured reservoirs with multiple pore media (i.e. triple and tetra porosity-permeability) remains a mathematical and conceptual challenge.

This paper presents a triple porosity-permeability model of a deep geothermal reservoir that communicates via the matrix, fractures, and fault plane as in Soultz graben formation [2]. In order to achieve this goal, a three-dimensional (3-D) numerical model of a reservoir is developed using the proposed triple porosity-permeability model by employing coupled processes of heat and fluid transfer in a finite element solver. Thus, in this model, the heat and fluid transfer are initiated from the injection well that intersects a fracture plane. The fracture plane is then connected to a fault plane that serves as a communicator to the fracture that intersects the production well.

2. Model formulation

In this study, a triple porosity-permeability model is proposed, employing the transient interporosity and permeability flow approximation and the surfaces between the three media to generate a transient interporosity and permeability flow. The model proposes a multiple pore media that considers the interaction between the matrix, fractures, and fault together. However, the fault plane is assumed as a fracture plane that has a wider opening with different petrophysical properties.
The heat and fluid transport models are developed for this system using conservation equations for momentum and mass to generate the required field equations. For the transient flow of mass, the model is expressed as

$$\rho_i S_i \frac{\partial P_i}{\partial t} + \nabla \cdot \rho_i v_i = Qm_i, \text{ and } v_i = -\frac{\kappa_i}{\mu} \nabla P$$  \hspace{1cm} (1)

where the sub-index (i.e. \(i = m, f, F\)) \(i\) represents transport in the matrix (\(m\)), in the fractures (\(f\)), and in the fault (\(F\)). The parameters in equation (1) are defined as \(\rho\) density of fluid, \(S\) linearised storage, \(P\) pressure, \(Qm\) mass source/sink, \(v\) is Darcy’s velocity, \(\kappa\) is the permeability, and \(\mu\) the fluid viscosity. In this work, the permeability of the fractures and the fault are assumed to obey the cubic law of parallel plates and is expressed as

$$\kappa_{f,F} = \frac{b^2}{12} \text{ or } \kappa_{f,F} = \frac{b^3}{12w}$$  \hspace{1cm} (2)

where \(\kappa_{f,F}\) is the fracture-fault permeability, \(b\) is the fracture-fault aperture, and \(w\) is the fracture spacing. For the transient flow of heat, the model is given as

$$\left(\rho C_p\right)_i \frac{\partial T_i}{\partial t} + \rho L C_{p,L} v_i \cdot \nabla T_i + \nabla \cdot q_i = Q_i$$  \hspace{1cm} (3)

The variables \(\rho\) and \(C_p\) (i.e. \(\rho C_p\)) \(i\) are the effective densities and specific heat capacities, respectively, which is expressed as

$$\left(\rho C_p\right)_i = \phi_s \left(\rho L C_{p,L}\right) + \left(1 - \phi_s\right) \rho S C_{p,S}$$  \hspace{1cm} (4)

The parameter \(T_i\) is the temperature, \(C_{p,L}\) and \(C_{p,S}\) are the fluid and solid heat capacities, \(\rho S\) is the solid density, \(q_i\) is the heat flux that is derived from Fourier’s law, which is given as

$$q_i = -\lambda_s \nabla T_i, \text{ and } \lambda_s = \phi_s \lambda_L + \left(1 - \phi_s\right) \lambda_s$$  \hspace{1cm} (5)

where \(\lambda_s\) is the effective thermal conductivities, \(\phi_s\) is the solid volume fraction, \(\lambda_L\) and \(\lambda_s\) are solid and fluid thermal conductivities.

### 3. Model set-up and configurations

A numerical model is developed to represent a deep geothermal reservoir of 500 x 500 x 500 m\(^3\) at the Soultz formation. The model consists of a fractured-faulted reservoir located at -4550 m below natural ground level, and a doublet representing an injection and production wellbores. Each of the wellbores intersects an active fracture, and both fractures are connected to a fault plane as shown in Figure 1. The wellbores are 300 m away from each other, and the penetration depths are -4730 and -4810 m for the injection and production wells, respectively. The hydrological and thermal properties of the geothermal reservoir are reported in the literature [3]. The mesh consists of 134,548 domain elements, 8912 boundary elements, and 1232 edge elements as presented in Figure 1 Right.

Initially, at \(t = 0\), the temperature distribution is assumed as \(T_0 = T_{surf} - \alpha \times (-z)\), in which \(T_0\) is the initial temperature of the reservoir, \(\alpha\) is the geothermal gradient, equal to 0.038 K/m in this case, \(T_{surf}\) is the surface temperature, which is assumed here as 12°C, and \(z\) is the vertical depth in metres. For the hydraulic case the pore pressure distribution is hydrostatic at \(t = 0\). In the case of boundary conditions (B.C.s), a constant temperature of 40°C is employed at the injection wellbore.
Constant pressures of 10 MPa and -10 MPa are applied at the injection and production wellbores, respectively, and all other boundaries are thermally insulated.

4. Results and discussions

In this section, the results obtained from the triple porosity-permeability model of the geothermal reservoir are presented. Three sets of results are analysed here, and the first group presents the produced fluid temperature at the production wellbore at different times as shown in Figure 2. The breakthrough curve shows an early decline in the produced fluid at approximately 1.4 years of production, where a 12°C temperature drop takes place after 30 years of simulation.

The second set shows the temperature variation at the injection fracture-fault interface for the selected period in the simulation as presented in Figure 3. It shows the injection fluid movement along the interface of the fracture-fault; as can be seen, after one year of simulation the edges of the interface maintain the same temperatures as the initial reservoir temperature, while at the central interface it has undergone significant changes in the temperature. However, after 10, 20, and 30 years of simulation, the temperature at the edges has also experienced a decline similar to the central part due to the effect of a cold water front that contributes to the immediate drawdown. The last set of the results is presented in Figure 4; it shows the effect of cold water propagation after one year (i.e. Left) and 30 years (i.e. Right) on the surfaces of the fractures and faults, with arrows indicating the heat flow directions. It can be seen, that the heat flow changes direction with time.
5. Conclusions

In this study, a 3-D numerical model of a deep geothermal reservoir is developed using a triple porosity-permeability approach. The model is implemented using the finite element method that is computationally efficient for modelling coupled transient heat and fluid flow processes in a geothermal system. The produced fluid temperature at the production wellbore, the temperature variation at the injection fracture-fault interface, and the effect of cold water front propagation during the simulation period of 30 years are analysed. The proposed model is computationally efficient and accurate in predicting long-term reservoir performance.

Acknowledgement

The first author is thankful for the PhD scholarship funding received from both the University of Greenwich (United Kingdom) and Petroleum Technology Development Fund (PTDF) Nigeria.

References


A MODEL FOR SIMULTANEOUS DAMAGE, HEALING AND CAPILLARY FLOW IN CEMENTITIOUS MATERIALS

* Tony Jefferson¹ and Robert Davies¹

¹ Cardiff University, School of Engineering, Cardiff, CF24 3AA, UK

*JeffersonAD@cardiff.ac.uk

ABSTRACT

This extended abstract describes a damage-healing-transport model for self-healing cementitious materials. The model simulates the transport of healing agents in discrete cracks using capillary flow theory and addresses mechanical damage-healing behaviour with a new constitutive formulation. The main contribution of the work is a new model that allows continuous and simultaneous damage and healing to be simulated. The model is applied to the analysis of a notched cementitious beam experiment in which healing agent was supplied via embedded glass capillary tubes filled with cyanoacrylate. The experiment exhibited simultaneous damage and healing and thus provided a useful set of data to validate the model. The comparisons between the experimental data and numerical predictions show that the model is able to represent the physical behaviour with good accuracy.

Keywords: Self-healing; constitutive; damage; cracking; cementitious

1. Introduction

Damage and healing processes can never be entirely decoupled, although many numerical models that simulate damage and healing are built on restrictive assumptions. These have included; healing always takes place under zero-strain conditions; healing and damage are never concurrent; healed material cannot re-damage; and healed material can only re-damage once [1-4]. There are many real damage-healing scenarios that are consistent with some of these assumptions. For example, if damage in a structure occurred as the result of an extreme short-term loading event and this was subsequently healed, then a single-time healing model would be appropriate. Conversely, damage from cyclic transient actions can result in multiple occurrences of damage and healing. In general, simultaneous damage and healing tends to occur when damage and healing rates are similar. This type of behaviour was observed in tests conducted at Cardiff University on concrete samples with inbuilt vascular networks containing cyanoacrylate [5].

Recent work has been undertaken on developing models to simulate the transport processes associated with self-healing, both in damaged continua [6-7] and in specimens with discrete cracks [8].

The processes that drive the transportation of healing agents and the mechanisms that govern mechanical self-healing are strongly coupled. Therefore, a comprehensive damage-healing model should include the transportation of healing agents and be able to simulate simultaneous (and multiple) damage and healing events. This extended abstract provides an outline description of a new coupled model for simulating continuous, or multiple event, damage-healing behaviour.

2. Capillary flow model

The capillary flow model employed in the current work is described in Gardner et al [8]. The model simulates flow in tortuous cracks of varying cross-section. It accounts for stick-slip behaviour, frictional resistance at the moving front and wall slip. The model has been shown to simulate the flow of capillary agents in discrete cracks in concrete with good accuracy. The flow rate at the meniscus is given by equation (1):
\[
\dot{z} = \left( p_{r0}(1 - \beta_s) - \rho g z \sin(\varphi) \right) \left( \frac{2 \beta_m}{b( z )} + \eta \right)
\]

(1)

where \( \eta = A(z) \int^z_0 \left[ \frac{b(x) \beta_w}{2} + \frac{k(x)}{\mu} \right] A(x) dx \) and in which the superior dot denotes the time derivative, \( z \) is the capillary rise height; \( b(x) \) is the channel (crack) opening; \( \beta_w, \beta_s \) and \( \beta_m \) are the wall, stick-slip and meniscus correction parameters respectively; \( \varphi \) is the capillary inclination angle; \( \rho \) is the density of liquid; \( g \) is the gravitational acceleration; \( \mu \) is the dynamic viscosity; \( t \) is the capillary rise time (s); effective permeability term \( k = b^2/12 \), and \( \alpha \) is the inclination of the capillary wall.

3. Damage-healing model

The damage-healing model presented here is described for a ‘crack-plane’, which is defined as the mid-surface of a narrow band of material that contains a macro-crack or a number of micro-cracks. The model relates the crack-plane traction vector \( \tau \mathbf{e} \) to the relative displacement vector \( u \mathbf{e} \), for which the damage-healing constitutive relationship is as follows:

\[
\mathbf{\tilde{t}} = (1 - \omega) \mathbf{k}^e \mathbf{\hat{u}} + h \mathbf{k}^h (\mathbf{\hat{u}} - \mathbf{\tilde{u}}_h)
\]

(2)

in which \( \omega \in [0,1] \) is the damage parameter, \( h \in [0,\omega] \) is the proportion of healed material and \( \mathbf{\tilde{u}}_h \) is the permanent healing displacement that ensures that the healing material forms in a stress-free state.

\( \mathbf{k}^e \) and \( \mathbf{k}^h \) are the elastic constitutive matrices for the original and healed material respectively. The inelastic component of \( \mathbf{\hat{u}} \) is computed from equation (3).

\[
\mathbf{\hat{u}} = \mathbf{\tilde{u}} - \left( \mathbf{k}^e \right)^{-1} \mathbf{\tilde{t}}
\]

(3)

The normal component of \( \mathbf{\hat{u}} \) is taken as the crack width and is denoted by the scalar \( u_f \). During step-by-step finite element computations, the damage may increase by \( \Delta \omega \) over time period \( t \) to \( t + \Delta t \). The equivalent discrete crack width, for an element with embedded discontinuity, is then computed and the flow of the healing agent calculated using the capillary flow model described in Section 2. The volume of healing agent arriving during the time interval is equal to \( \Delta v (= \Delta a \cdot u_f) \). There may be a delay between the occurrence of damage and the time of arrival of the healing agent, thus the flow must be tracked. Once the agent has arrived at a particular location it may take some time to cure. In the present work we assume, as in the work of Mergheim & Steinmann [3], that the characteristic healing of the agent follows an exponential function but in this work we have also allow for the possibility of a delay to the start of curing. The resulting curing function (equation 4) gives the volume of cured material \( \Delta V_c \) at time \( t \) assuming a volume of agent \( \Delta v \) arrived at time \( t_a \).

\[
\Delta V_c = \Delta v \cdot (1 - e^{-\frac{(t - t_a - \Delta t_r)}{\tau_h}})
\]

(4)

in which \( \Delta t_r \) is cure delay time and \( \tau_h \) is the characteristic curing time parameter. \( <> \) is a McCauley bracket defined as \(<x>=0 \text{ if } x \leq 0 \text{ and } =x \text{ if } x > 0 \).

At any one place during any one time increment, new healing material may arrive, healed material may damage and damaged material may re-heal. To account for these factors the relative area of curing and cured material \( a \) at a particular point is given by:

\[
a = a + \Delta a_c - \Delta a_{redam} + \Delta a_{rec}
\]

(5)
in which $\Delta a_{c}$ is the increment of (relative) area of virgin filled crack, $\Delta a_{redam}$ is the incremental area of re-damaged material and $\Delta a_{rec}$ is the incremental area of re-filled cracks; noting that $a = v / u_p$.

The total relative proportion of healed material is then computed from equation (6).

$$h = h \cdot e^{-\frac{\Delta a_{h}}{\tau_h}} + a \left( 1 - e^{-\frac{\Delta a_{h}}{\tau_h}} \right)$$

(6)

A much fuller description of the model, including details of the damage model, a description of the element with strong discontinuity, the method used to track the increments of material arriving and curing, the function used to compute $\delta_h$ and the computational details of the coupled non-linear solution procedure will be provided in a forthcoming journal paper.

4. Example

The model has been applied to the simulation of a set of experimental specimens tested in Cardiff by Joseph et al. [5]. The testing arrangement employed in this experimental study is shown in Figure 1.
5. **Discussion and concluding remarks**

The single simulation presented in the previous section does not provide a complete validation of the model but it does serve as a first indication of the effectiveness of the model. The full study on this model includes simulations of a number of control and self-healing samples loaded at different rates. Based on the results obtained to date, the authors believe that the model presented here is able to simulate the type of continuous and simultaneous damage-healing behaviour described in the introductory section of this paper with good accuracy.

**References**


Level set based topology optimisation using high-order reinitialisation methods and the discontinuous Galerkin method

*Thomas Adams, Stefano Giani and William M. Coombs

School of Engineering and Computing Sciences, University of Durham, South Road, Durham, DH1 3LE, UK.

*thomas.d.adams@durham.ac.uk

ABSTRACT

This paper extends the work presented in [1], which presented a topology optimisation approach using the level set method (LSM) and the discontinuous Galerkin symmetric interior penalty (SIPG) method, by applying a SIPG discretisation to a number of level set reinitialisation methods. This allows the reinitialisations methods to more accurately capture the topology during reinitialisation, and thus reduce the errors introduced by such methods during the optimisation process. Currently existing methods of level set reinitialisation include an elliptic PDE-based method [2], and a hyperbolic PDE-based method [3], as well as others. This paper presents SIPG solutions to these aforementioned PDE-based reinitialisation methods.

Key Words: topology optimisation; level set methods; level set reinitialisation methods; discontinuous Galerkin method.

1. Introduction

The topology optimisation method in [1] used a level set function (LSF), which is a function one dimension higher than the problem domain, to determine the location of a structural boundary. The LSF, and thus the structural boundary, can be evolved such that it becomes the minima of some objective functional by solving a Hamilton-Jacobi equation in pseudo-time often called the level set evolution equation. This equation was simplified based on the assumption that the gradient of the LSF will always be approximately equal to unity, an assumption which can be satisfied for all pseudo-time through the frequent use of level set reinitialisation techniques.

There are two main reasons why frequent reinitialisation, and therefore such a simplification, is generally not considered advantageous: the added computational expense of solving the reinitialisation problem, and the introduction of errors which occur when the boundary moves during reinitialisation. This work is an attempt to reduce the effects of these two problems by using the SIPG method to solve the reinitialisation problem, which due to their synergy with $hp$-adaptivity, are able to exploit higher order elements to more accurately capture the original position of the interface as well as optimise the number of degrees of freedom for the problem. Not to mention further speed increases will be available through the ease with which the method can be parallelised.

2. Level set methods

The LSM [4] is a numerical technique for computing and analysing moving boundaries. The LSM uses a LSF, $\phi$, to implicitly define a problem’s internal boundaries. It does this by defining the internal boundaries of the problem by the intersection of the LSF with the $\phi = 0$ plane. This can be stated mathematically as follows

$$
\begin{align*}
\phi &> 0 \quad \text{in } \Omega, \\
\phi &= 0 \quad \text{in } \Gamma \text{ and} \\
\phi &< 0 \quad \text{in } D/\Omega,
\end{align*}
$$

(1)
where $\Gamma$ is the interface between the subdomains $\Omega$ and $D/\Omega$. This is shown graphically in Figure 1.

![Graphical representation of the level set function.](image)

(a) The problem domain with internal boundary, $\Gamma$. (b) The LSF intersecting the problem domain.

Figure 1: Graphical representation of the level set function.

3. Level set reinitialisation

As discussed in [4], it can be beneficial to ensure that the LSF is always close to being a signed distance function (SDF), i.e one which satisfies equation (2). For certain problems evolving the LSF can cause it to become excessively distorted and as such reinitialisation methods were developed to allow the LSF to be rebuilt into an SDF during the evolution process without moving the current position of the interface. For the topology optimisation method presented in [1], it is assumed that the LSF will always be an SDF and therefore it is imperative that a reinitialisation method is capable of ensuring that this is the case.

The aim of level set reinitialisation then is, for a given interface described by a LSF, $\phi^0$, to find a new LSF, $\phi^n$, which satisfies the following conditions

$$|\nabla \phi^n| = 1 \quad (2)$$

and

$$\phi^n = 0 \text{ on } \Gamma(\phi^0) \quad (3)$$

3.1. Elliptic PDE-based reinitialisation

The elliptic PDE-based reinitialisation method initially proposed by Basting and Kuzmin [2], is a method whereby the reinitialised LSF is the solution to a minimisation problem where the cost functional is given by the least squares solution to (2). The boundary condition described by (3) is then enforced weakly through the addition of an immersed boundary term. This problem can be stated

$$\min \left( \frac{1}{2} \int_\Omega (|\nabla \phi| - 1)^2 \, dx + \frac{\alpha}{2} \int_{\Gamma(\phi^0)} \phi^2 \, ds \right) . \quad (4)$$

A continuous Galerkin (CG) solution is presented in [2]. Equation (6) presents the LHS of the SIPG solution. The first two terms of (6) will be the only terms present in the LHS of the CG solution. The SIPG solution presented below includes three extra surface integrals on the LHS which is congruent with the analysis of SIPG solutions to elliptic problems presented in [5]. The third term in (6) comes from an integration by parts; whilst in CG this term will be equal to zero everywhere except the Neumann boundary, the SIPG discretisation is carried out over each element separately and with no requirement of equality at shared nodes. For this reason it is necessary to compute this term over the skeleton of the mesh using the the average and jump operators written as $\{\cdot\}$ and $[\cdot]$ respectively. The inclusion of these operators makes the solution non-symmetric with respect to the level set and test functions. The fourth
term in (6) is added to make the LHS symmetric, which is necessary to ensure optimal convergence. Finally, the last term added in (6) is a penalty term, which penalises the jump in the solution and thus weakly enforces interelement continuity. Similarly the only term present in the RHS of the CG solution is the first term in (7) with the second term once again coming from the integration by parts. As the RHS is both a vector and using a previous solution there is no reason to include the symmetry or penalty terms. Thus using the SIPG method in space and a fixed point iteration method, the solution to (4) can be stated

\[ K\phi^{k+1} = F(\phi^k), \]  

where the matrix \( K = (k_{ij}) \), has elements given by

\[ k_{ij} = \int_\Omega \nabla v_i \cdot \nabla v_j \, dx + \alpha \int_{\Gamma(\phi^0)} v_i v_j \, ds - \alpha \int_S [\nabla v_i] \cdot [\nabla v_j] \, ds - \mu \int_S \| v_i \| \cdot \| v_j \| \, ds, \]  

(6)

and the column vector \( F = (f_j) \), has elements given by

\[ f_j = \int_\Omega \nabla \phi^0 \cdot \nabla v_j \, dx - \int_S \left( \frac{\| \nabla \phi^0 \|}{\| \nabla \phi^0 \|} \right) \cdot \| v_j \| \, ds, \]  

(7)

where \( S \) denotes the union of element edges, \( v \) is the test function, \( \alpha \) is a large positive constant which determines the extent to which the Dirichlet boundary condition is adhered to, and \( \mu \) is a penalty parameter which determines the extent to which continuity is enforced.

### 3.2. Hyperbolic PDE-based reinitialisation

The hyperbolic PDE-based reinitialisation method initially proposed by Sussman et al. [3] involves finding the steady state solution to the following PDE

\[ \frac{\partial \phi}{\partial \tau} = \text{sign}(\phi^0) (1 - |\nabla \phi|), \]  

(8)

where \( \tau \) is psuedo-time.

Since there is no integration by parts required the resulting SIPG discretisation requires only the addition of the penalty term in order to weakly enforce continuity. In order to find a unique solution it is necessary to include a Dirichlet boundary condition on the interface, \( \Gamma \). This is achieved weakly by the inclusion of an immersed boundary term, the same one as used in the elliptic reinitialisation method. In order to ensure stability, (8) is solved implicitly using a Newton–Raphson method leading to a solution as follows

\[ \phi^{k+1} = \phi^k - \frac{\partial R(\phi^k)}{\partial \phi}^{-1} R(\phi^k), \]  

(9)

where \( R = (r_j) \) is the residual vector, with elements given by

\[ r_j(\phi^k) = \int_\Omega \text{sign}(\phi^0)(1 - |\nabla \phi^k|) v_j \, dx - \mu \int_S \| \nabla \phi^k \| \cdot \| v_j \| \, ds - \alpha \int_{\Gamma(\phi^0)} \phi^k v_j \, ds, \]  

(10)

and \( \frac{\partial R(\phi^k)}{\partial \phi} = (J_{ij}) \), is the Jacobian matrix of the residual, with elements given by

\[ J_{ij}(\phi^k) = -\int_\Omega \text{sign}(\phi^0) \left( \frac{\nabla \phi^k}{|\nabla \phi^k|} \cdot \nabla v_i \right) v_j \, dx - \mu \int_S \| v_i \| \cdot \| v_j \| \, ds - \alpha \int_{\Gamma(\phi^0)} v_i v_j \, ds. \]  

(11)
4. Numerical results

A simple example problem is presented below in which an initial LSF defined by

$$\phi^0(x, y) = -((x - 0.5)^2 + (y - 0.5)^2 - 0.15), \quad (12)$$

which is projected onto 1m x 1m domain discretised by a mesh of 50 x 50 linear, piecewise continuous, square elements, is reinitialised using the two methods. The initial configuration can be seen in Figure 2(a). One iteration of the hyperbolic and elliptic methods are computed to achieve the reinitialised LSFs shown in Figure 2(b) and 2(c) respectively.

![Initial Level Set Function](image1)

(a) Initial Level Set Function, $\phi^0$.

![After one hyperbolic iteration](image2)

(b) After one hyperbolic iteration, $\phi^n_{hyp}$.

![After one elliptic iteration](image3)

(c) After one elliptic iteration, $\phi^n_{ellip}$.

Figure 2: Graphical representation of the level set function before and after reinitialisation.

<table>
<thead>
<tr>
<th>Method</th>
<th>Average Error (%)</th>
<th>$\epsilon_{interface}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hyperbolic</td>
<td>0.14</td>
<td>6.03e-3</td>
</tr>
<tr>
<td>Elliptic</td>
<td>0.05</td>
<td>5.49e-3</td>
</tr>
</tbody>
</table>

Table 1: Average error and interface movement error after one iteration.

Table 1 shows that just one iteration of both the elliptic and hyperbolic reinitialisation methods yield a reasonable approximation of an SDF. The average error is a measure of the average difference between the gradient and unity for each element in the mesh, which is less than 1% for both of the methods. The measure of movement of the interface is quantified by evaluating the integral, $\epsilon_{interface} = \int_{\Gamma(\phi^0)} (\phi^n)^2 ds$.

5. Conclusions

SIPG solutions to two level set reinitialisation methods have been presented. Preliminary results show promise in achieving the aims of developing a discontinuous reinitialisation method which is efficient and accurate. Combining this with earlier work presenting a SIPG, level set based topology optimisation method, will result in a fully discontinuous topology optimisation method which will be able to exploit the advantages associated with discontinuous Galerkin methods.

Acknowledgements

The first author acknowledges financial support during the completion of this work by a UK Engineering and Physical Sciences Research Council (EPSRC) grant.

References

Analysis of a plate using EPR-based self-learning finite element method

*Ali Nassr¹, Akbar A. Javadi¹

¹Department of Engineering, University of Exeter, North Park Road, Exeter, EX4 4QF

*Adnn201@exeter.ac.uk

Abstract

A constitutive model that accurately represents the material behaviour under various loading conditions is essential to solving complex boundary value problems. In the last decade the self-learning simulation (SelfSim) method has been introduced that uses a neural network (ANN) to train and generate a constitutive model. Although the methodology has been used successfully, the drawbacks of using ANN remain unsolved. This paper presents an alternative data mining technique, called EPR, that has been utilised in the SelfSim framework to overcome these drawbacks. The framework has been coded as an automation process in Matlab. The application of the developed methodology is illustrated through analysis of a square plate under plane stress conditions using the EPR-based self-learning FEM. The results show that the proposed method is very effective in capturing and representing the constitutive behaviour of the plate with high reliability.

Key Words: finite element method, self-learning simulation, evolutionary polynomial regression

1. Introduction

The self-learning simulation is an extension of the autoprogessive algorithm originally introduced by Ghaboussi et al. [1]. Hashash et al. [2] proposed a self-learning simulation methodology, also called inverse analysis technique. This methodology employs the auto-progressive algorithm that extracts material’s constitutive behaviour (stress-strain relationship) using global load-displacement measurements. The self-learning finite element method utilizes a neural network (ANN) based constitutive model to extract the materials behaviour [2]. Although there has been valuable research on the self-learning FEM using ANN, and demonstration of the advantages that ANN offers in constitutive modelling, however, it is generally known that ANNs also suffer from a number of drawbacks. For example, the number of neurons, number of hidden layers, transfer function, etc. must be determined a priori, requiring a time-consuming trial and error procedure. In addition, it generates a complex model to represent a phenomenon that is not easily accessible to the user [3–4]. Recently, the evolutionary polynomial regression (EPR) has been used to address the shortcomings of ANN in the framework of self-learning FEM for modelling of material behaviour [5]. This paper presents the application of the EPR-based self-learning methodology for analysis of a square plate under plane stress conditions. The advantages of the proposed methodology over the ANN-based approach are highlighted.

2. Evolutionary polynomial regression (EPR)

Evolutionary polynomial regression (EPR) is a new hybrid technique based on evolutionary computing, aimed to search for polynomial structures representing the behaviour of a system [6]. EPR is a combination of a genetic algorithm (GA) to search for symbolic structures describing the behaviour of the system and least square (LS) regression which is used to estimate the constants values [6]. A typical formulation of EPR expression can be stated as:

\[ y = \sum_{j=1}^{m} F(X, f(X), a_j) + a_0 \quad (1) \]

where \( y \) is the estimated output of the system; \( a_j \) is a constant value; \( F \) is a function constructed by the process; \( X \) is the matrix of input variables; \( f \) is a function defined by the user; and \( m \) is the number of terms of the expression excluding bias \( a_0 \). The accuracy of the developed EPR models is calculated at each stage based on the coefficient of determination (CoD) i.e., the fitness function as:
\[ CoD = 1 - \frac{\sum_n(Y_a - Y_b)^2}{\sum_d(Y_a - \bar{Y}_a)^2} \]  

(2)

where \( Y_a \) is the actual output value; \( Y_p \) is the EPR predicted value and \( N \) is the number of data points on which the CoD is computed.

3. Methodology

The methodology of incorporating EPR in finite element analysis was first presented by Javadi and Rezania [3]. They showed that a properly trained EPR on experimental data can be implemented in a finite element model with more simplicity compared with a conventional constitutive model [3]. However, this approach of training EPR needs a large number of experiments which is costly and may not be available in all cases. Therefore, training EPR within the self-learning FEM seems to be much more efficient. The implementation of EPR-based self-learning model in finite element analysis provides the material stiffness matrix, also called Jacobian matrix \( J \), as:

\[ J = \frac{\partial (d\sigma)}{\partial (d\varepsilon)} \]  

(3)

The framework of the self-learning FEM consists of two steps. In step 1, the applied load and constrained boundary conditions are implemented and the boundary forces and displacements are measured for each loading increment. Two finite elements analyses are considered in parallel (FEA and FEB) and an EPR model which represents the stress-strain relationship is trained. The FE model (A) simulates the structure and applies the forces while in parallel, the FE model (B) applies the corresponding displacements. The stresses and strains are determined at each integration point for both FE models. The methodology assumes that the stresses of FE (A) and strains of FE (B) are accurate and hence they are used to train the EPR model. Each cycle of self-learning that accomplishes the entire applied load is called a pass. The linking of the FE code (ABAQUS) with EPR was done via Matlab environment in a fully automated iterative loop. The flowchart of the EPR-based self-learning FEM is shown in Figure 1.
4. Numerical example: square plate under a biaxial loading

A 2D plane stress square plate subjected to a biaxial loading is considered. The geometry of the plate, boundary conditions and loading are shown in Figure 2. Due to the symmetry, only a quarter of the plate is simulated. The experimental measurements are generated synthetically by using a non-linear elastic model implemented in the FE engine (ABAQUS) via its user subroutine UMAT facility [4]. The applied stresses are (17.5Pa) and (25Pa) along the x and y axes and the corresponding strains are (5%) and (10%) respectively. These values represent loading along the principal axes only (shear strains and shear stresses are zero) which are not enough to train the EPR-based self-learning model. Consequently, a strategy is applied to generate more data with non-zero shear stresses and strains. This strategy has been utilised by several researchers to generate more data when the material being analysed is isotropic [4,7]. The pressures and the corresponding displacements on the edges of the plate (the monitoring points) are considered as the experimental measurements and used in the self-learning process. Two finite element models, FEA and FEB, are created and the self-learning process is initialized first with an elastic modulus of 500 Pa and Poisson’s ratio 0.3. The total stress-strain strategy is employed in which the values of strains and stresses are used as input and output respectively as: 

$\sigma_x = f(\varepsilon_x, \varepsilon_y, \varepsilon_{xy}), \sigma_y = f(\varepsilon_x, \varepsilon_y, \varepsilon_{xy}), \sigma_{xy} = f(\varepsilon_x, \varepsilon_y, \varepsilon_{xy}).$

After training, in each run, three EPR models with the highest CoD values are chosen and Jacobian matrix is calculated from the partial derivation of these models and implemented in ABAQUS at every loading step through its UMAT.

During the self-learning process, the EPR model gradually learns and captures the material behaviour within a single pass. Figure 3 shows the convergence between the FEA and FEB in the self-learning process. The results show an excellent convergence between both FE analyses until the softening behaviour occurred when FEA was stopped.

To verify the capability of the EPR based self-learning model, a comparison between actual data and EPR model applied on FEB is shown in Figure 4. The results show an excellent agreement between the
EPR-based FE analysis and the actual data and demonstrate the excellent ability of the developed EPR-based self-learning model to capture the nonlinear behaviour of the plate.

Fig. 4 Comparison between actual data and EPR-based self-learning model

5. Conclusion

This paper presented the development and application of an EPR-based self-learning FE model as an efficient approach for learning the constitutive behaviour of materials. The main advantage of using EPR in the self-learning FEM is that it provides transparent and structure equations representing the constitutive behaviour of material which can be readily implemented in FE code. In the self-learning FEM, there is no need to check yielding, to compute the gradients of plastic potential curve, to update the yield surface, etc. The developed automated framework of EPR based SelfSim reduces the overall computational time, simplifies the training and allows the methodology to be applied to more complex material behaviour. The results generally show very good predictions of EPR in capturing and representing the nonlinear behaviour within a single pass of the self-learning algorithm. However, it should be noted that in finite element (A), the model stopped at the onset of softening behaviour (where the gradient of the stress-strain curve becomes slightly negative), although the predicted behaviour is very accurate up to that point. Developing the EPR-based self-learning algorithm to describe the softening behaviour of materials is the subject of current investigations by the authors. It should also be noted that, the trained EPR model (like any other data mining technique), is good at interpolation but not so good at extrapolation. Therefore, any attempt to use EPR models developed using the self-learning finite element method outside the range of the training data may not be accurate.

References

A NUMERICAL REDUCTION SCHEME FOR MULTIPLE ION TRANSPORT PROBLEMS

*B.L. Freeman1, P.J. Cleall1 and A.D. Jefferson1

1 School of Engineering, Queen’s Buildings, Cardiff University, The Parade, Cardiff, CF24 3AA

*freemanbl@cardiff.ac.uk

ABSTRACT

Transport models have a wide range of applications in porous media ranging from contaminant transport problems to describing the self-healing behaviour of cementitious materials. The computational cost associated with these models can however be large for certain chemical systems. There is a need then to address this and to develop models with a lower computational demand whilst maintaining suitable accuracy. The model presented here utilises a numerical approach to reduce the number of coupled equations to be solved simultaneously thereby improving the efficiency. The accuracy of the reduction scheme is tested against an example problem concerning the diffusion of four chemical species through a concrete specimen. It was found that the computational cost was greatly reduced and a good level of accuracy maintained.

Keywords: Reactive Transport; Porous Media; Reduction of Problem Size; Numerical Simulation

1. Introduction

Transport models are often coupled models which consider the advection, dispersion and in some cases reaction of chemical ions, moisture flow, heat transfer and often mechanical behaviour of the porous medium, through the appropriate mass and energy balance equations. The computational cost of solving these equations can become quite large. According to Cleall et al [3] this is driven by three main areas, the domain size, time scale and complexity of the analysis; where the complexity of the analysis is dependent on the number of variables and degree of coupling between them, the non-linearity of the system and the number of processes considered. A number of authors deal with this problem by using an operator splitting scheme, changing the numerical treatment of the problem from a GIA (Global Implicit Approach) to SIA or SNIA (Sequential Iterative Approach or Sequential Non-iterative Approach); calculating the transport and reaction of the solutes separately in a step-wise manner, as opposed to simultaneously [2,11,12]. SNIA methods however may introduce splitting errors [7,8]. SIA methods iterate between the two to avoid this but may require small time steps in order to converge [7,8]. For this reason many authors have instead proposed reduction schemes for the GIA method [6–9]; the approach being one of reformulating the system of equations, decoupling a number of the governing PDE’s and eliminating a number of local equations (ODE’s or AE’s). However, a number of these schemes have limitations including the assumption that the diffusion coefficients are the same for all species [7,8] as their affect can be negligible when mechanical dispersion is large although this is not always the case [10].

The model presented here takes a numerical approach to reducing the number of transport equations to be solved. To do this an indicator species is chosen, for which the governing equation of mass balance is solved, taking into account the advection, dispersion and reaction of the solute. The transport of the remaining species is then calculated as a function of the transport of the indicator species at the end of each time step, with the reactions then being calculated on a point-wise basis. The reduction technique is then applied to an example problem and the results compared to those of a full (non-reduced) model.
2. Problem Reduction Scheme and Key Theory

In this section the mass balance of the chemical species as well as their reactions will be presented before describing the reduction scheme considered. The full description of both the theoretical formulation and the reduction schemes can be seen in [5]. The governing mass balance equation for the transport of a chemical ion is given by:

\[
\frac{\partial c}{\partial t} + \nabla \cdot (\rho_w c \nu_w) + \nabla \cdot J_d = -\dot{m}_c
\]  

(1)

where \( c \) is the chemical concentration, \( \nu_w \) is the pore water velocity, \( \dot{m}_c \) is the source/sink due to chemical reaction, \( J_d \) is the dispersive flux, made up of the mechanical dispersion and molecular diffusion, and \( \rho_w \) is the liquid phase density given as \( \rho_w = n \rho_w S_w \) where \( n \) is the porosity, \( \rho_w \) is the water density and \( S_w \) is the degree of saturation of the liquid phase. The superior dot denotes the time derivative. The reactions considered here are of the non-equilibrium chloride binding with the Freundlich type description given by:

\[
\dot{\rho}_p = -\frac{(S_p - \mu \gamma)}{\tau}
\]  

(2)

where \( \rho_p \) is the sorbed mass density, \( S_p \) is the degree of salt saturation, \( \mu \) and \( \gamma \) are rate parameters and \( \tau \) is a characteristic time. The pore water velocity is governed by generalised Darcy’s law and the dispersive flux is governed by Fick’s law.

The rate of transport of an ion depends upon the pore water velocity, diffusion coefficient and concentration gradient. The differential transport rates of different ions therefore must depend on the diffusion coefficients and concentration gradients. The reduction scheme considered here takes the ratios of concentration gradient and diffusion coefficient, of the species under consideration to the indicator species, and uses them to scale the transport of an indicator species over a time step. The equation is given as:

\[
c_{rs}^{t+1} = c_{rs}^t + \left( \frac{c^0_s - c^p_s}{c^0_{ind} - c^p_{ind}} \right) \frac{D_s}{D_{ind}} \Delta c_{ind}
\]  

(3)

where \( c_{rs} \) is the concentration of a chemical species, \( D_s \) and \( D_{ind} \) are the diffusion coefficients where the \( s \) and \( ind \) subscripts represent a species and an indicator respectively, \( \Delta c_{ind} \) is the change of the indicator species over a time step and \( c^0 \) and \( c^p \) refer to the initial and boundary concentrations respectively.

3. Problem Reduction Example

The example considered here is of the chemical diffusion of four chemical species through a mortar specimen as reported in [1], based on experimental results in [4]. The chemical species considered are \( \text{Na}^+ \), \( \text{OH}^- \), \( \text{K}^+ \) and \( \text{Cl}^- \), and the chloride binding onto the cement matrix is considered through the non-equilibrium binding isotherm given by (2). Following [1] it was also assumed that as chlorine ions are bound to the cement matrix, hydroxide ions were released thereby maintaining charge neutrality. The initial and boundary coefficients along with the diffusion coefficients are given in Table 1. The problem geometry can be seen in Figure 1. The full details of the material and reaction parameters can be found in [1,5]. The chosen indicator species here was \( \text{Na}^+ \).

<table>
<thead>
<tr>
<th>Chemical Species</th>
<th>Initial Conc. (kg/kg)</th>
<th>Boundary Conc. (kg/kg)</th>
<th>( D_{ind} ) (10^-10 m^2/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Na}^+ )</td>
<td>0.000299</td>
<td>0.01352</td>
<td>1.33</td>
</tr>
<tr>
<td>( \text{OH}^- )</td>
<td>0.001105</td>
<td>0.00188</td>
<td>5.3</td>
</tr>
<tr>
<td>( \text{K}^+ )</td>
<td>0.002028</td>
<td>0.00319</td>
<td>1.96</td>
</tr>
<tr>
<td>( \text{Cl}^- )</td>
<td>0.0</td>
<td>0.01954</td>
<td>2.1</td>
</tr>
</tbody>
</table>
The concentration and total chloride content (Tcc) profiles after 12hrs as predicted by (1) and the reduced model can be seen below in Figure 2.

As can be seen from the profiles above, the predictions of the reduced model are very close to those of the full (non-reduced) model. The biggest difference can be seen in the OH$^-$ profile with the difference being in the peak concentration where the hydroxide ions are being released due to the chloride adsorption. In order to determine the efficiency of the reduction scheme an investigation into the computational cost was made; the geometry was divided into a finite element mesh consisting of 42
nodes and 20 bilinear quadrilateral elements. The analysis was performed on a laptop with an Intel Core i5-3230M @2.60GHz and 5.88GB useable RAM. The CPU time of the time step loop was measured for a number of runs and an average taken. The averaged CPU times were 620.1s and 293.9s for the full and reduced models respectively, equating to a reduction of 52.6%.

4. Conclusions

A numerically based problem reduction scheme has been presented here that has successfully reduced the computational cost of the simulation of an example problem whilst still accurately predicting the chemical behaviour. The reduction in cost was achieved through reducing the number of governing mass balance equations to be solved from four to one.

References

A stable cut finite element method for multiple unilateral contact

*P. Kerfriden*¹ and S. Claus¹

¹School of Engineering, Cardiff University, Queen’s Buildings, The Parade, Cardiff, CF24 3AA

*pierre.kerfriden@gmail.com*

ABSTRACT

This paper presents a novel CutFEM-LaTIn algorithm to solve multiple unilateral contact problems over geometries that do not conform with the finite element mesh. We show that our method is (i) stable, independently of the interface locations (ii) optimally convergent with mesh refinement and (iii) efficient from an algorithmic point of view.

Key Words: cut finite elements, contact, multiple materials, LaTIn

1. Introduction

Since the pioneer work presented in [5], several research teams have successfully developed stable XFEM schemes for unilateral contact (see e.g. [10, 6, 1]). However, it is extremely challenging to make sure that these methods are optimally convergent with mesh refinement. As far as we are aware, this has only been achieved recently in [4, 3]. In this paper, we propose an alternative to the latter contributions that is based on an extension of the CutFEM [7, 2] technology for embedded interface problems, coupled with the LaTIn mixed formulation of contact [9, 5, 8, 6]. We show that the formulation is always stable, and that our high-performance computing implementation allows us to perform 3D computations involving arbitrarily complex intersections of solids, potentially leading to field singularities. Moreover, we show optimal convergence with mesh refinement of the background grid. Incidentally, our work is also a stabilisation of the LaTIn hybrid-mixed formulation. In this respect, our method is an alternative to the two previous non-locking LaTIn formulations based on (i) a local coarsening of trace meshes (see e.g [9, 8]) and (ii) a relaxation of interface kinematic conditions together with the addition of penalty terms, as presented in [6]. Our approach is algorithmically quite advanced. We therefore choose, in this short contribution, to focus on the most novel aspects of it, which is the discrete non-conforming and non-locking mixed LaTIn formulation of contact, enriched and further stabilised with tools of the CutFEM technology. This scheme is developed in section 2, whilst section 3 contains some representative examples and short conclusions.

2. Finite Element Formulation

2.1. Domain Discretisation

We consider a domain $\Omega$ divided into $n_d$ non-overlapping subdomains $\Omega^i$. We partition the boundary of domain $\Omega$, $\partial \Omega$, into a Dirichlet $\partial \Omega_D$ (body is clamped) and a Neumann part $\partial \Omega_N$ (tractions are imposed). Furthermore, each subdomain $\Omega^i$ is considered to be covered by a linear elastic body $i$. We assume that if two elastic bodies share an interface $\Gamma^{i,j} = \partial \Omega^i \cap \partial \Omega^j$ these two bodies are expected to come into contact. For example, in Figure 1a, we employ contact conditions on the interfaces $\Gamma^{1,2}$, $\Gamma^{1,3}$ and $\Gamma^{2,3}$. We introduce a non-conforming finite element discretisation of the domains as follows. Firstly, let $\mathcal{T}_h$ denote a tessellation of domain $\Omega$ independent of the interface locations $\Gamma^{i,j}$. Secondly, we introduce the following mesh subsets of our background mesh $\mathcal{T}_h$. For each subdomain $\Omega^i$, we introduce a so-called fictitious domain $\Omega^i = \{K \in \mathcal{T}_h : K \cap \Omega^i \neq \emptyset\}$. In a similar fashion, we define the set of elements intersected by an interface $\Gamma^{i} = \bigcup_{(k,l) \notin \Gamma^{i}} \mathcal{T}_h \cap \Gamma^{i}$ as $\mathcal{G}^i := \{K \in \mathcal{T}_h : K \cap \Gamma^{i} \neq \emptyset\}$. We also define the following two subsets of faces between two elements $\mathcal{F}(K, K') = K \cap K'$; the set of element faces associated with $\mathcal{G}^i$, namely $\mathcal{F}^i_G := \{F \in \mathcal{F}(K, K') : K \in \mathcal{G}^i \text{ or } K' \in \mathcal{G}^i\}$, which we call ghost penalty faces, and the set of intersected faces $\mathcal{F}^i_I := \{F \in \mathcal{F}(K, K') : K \in \mathcal{G}^i \text{ or } K' \in \mathcal{G}^i\}$ (see Figure 1b).
2.2. Discrete hybrid-mixed formulation of the contact problem

Let $\mathcal{U}_h^i$ denote the vector valued space of continuous piecewise linear polynomials defined on the fictitious domain $\hat{\Omega}_h^i$. Our weak formulation of linear elasticity reads: For all $\delta u_h^i \in \mathcal{U}_h^i$ such that for all $\delta u_h^i \in \mathcal{U}_h^i$,

$$a(u_h^i, \delta u_h^i) + a_b(u_h^i, \delta u_h^i) + j(u_h^i, \delta u_h^i) = l(\delta u_h^i).$$  \hspace{1cm} (1)

The terms of $a(u_h^i, \delta u_h^i)$ and $l(\delta u_h^i)$ are given by

$$a(u_h^i, \delta u_h^i) = \int_{\Omega_h^i} \sigma(u_h^i) : \epsilon(\delta u_h^i) \, d\Omega - \int_{\Gamma_h^{i,j}} (\sigma(u_h^i) \cdot n_{i,j}) \delta u_h^i \, d\Gamma,$$

$$l(\delta u_h^i) = \int_{\Omega_h^i} f \cdot \delta u_h^i \, d\Omega,$$ \hspace{1cm} (2)

where $\sigma(u) = \lambda \epsilon(u) + 2\mu \underbrace{\epsilon(u)}_{= \epsilon(u) \text{ is the Cauchy-stress tensor}}, \epsilon(u) = \frac{1}{2} \left( \nabla u + \nabla u^T \right)$ is the strain tensor, $n_{i,j}$ is the normal on $\Gamma_h^{i,j}$ pointing from $\Omega_h^i$ to $\Omega_h^j$, $\lambda$ and $\mu$ are the two Lamé coefficients, i.e.

$$\lambda = \frac{E}{1 + \nu(1 - 2\nu)}, \quad \mu = \frac{E\nu}{1 + \nu},$$

with $E$ the Young’s modulus and $\nu = 0.3$ the Poisson’s ratio. $\Omega_h^i$ and $\Gamma_h^{i,j}$ denote piecewise polynomial approximations of exact geometrical sets. The terms $a_b(u_h^i, \delta u_h^i)$ and $l_b(\delta u_h^i)$ weakly enforce Dirichlet conditions using Nitsche’s method and Neumann boundary conditions

$$a_b(u_h^i, \delta u_h^i) = - \int_{\partial \Omega_D} (\sigma(u_h^i) \cdot n_{i,j}) \delta u_h^i \, d\Gamma - \int_{\partial \Omega_D} (\sigma(\delta u_h^i) \cdot n_{i,j}) u_h^i \, d\Gamma + \int_{\partial \Omega_D} \frac{aE^i}{h} u_h^i \cdot \delta u_h^i \, d\Gamma,$$

$$l_b(\delta u_h^i) = - \int_{\partial \Omega_D} (\sigma(\delta u_h^i) \cdot n_{i,j}) g \, d\Gamma + \int_{\partial \Omega_D} \frac{aE^i}{h} g \cdot \delta u_h^i + \int_{\partial \Omega_N} T \delta u_h^i \, d\Gamma,$$ \hspace{1cm} (3)

where $T$ is a prescribed surface load, $g$ is a prescribed displacement and $\alpha > 0$ is the Nitsche penalty parameter. The term $j(u_h^i, \delta u_h^i)$ regularises the solution in the interface region and is given by

$$j(u_h^i, \delta u_h^i) = \sum_{F \in \mathcal{F}_G} \frac{1}{E^i} \int_{F} \gamma_F \left[ (\sigma(u_h^i) \cdot n_F) \cdots (\sigma(\delta u_h^i) \cdot n_F) \right] \, ds.$$ \hspace{1cm} (4)

We call $j(u_h^i, \delta u_h^i)$ ghost penalty stabilisation ([2]). Here, $\left[ x \cdot n_F \right]$ denotes the normal jump of the quantity $x$ over the face, $F$, defined as $\left[ x \cdot n_F \right] = x|_K \cdot n_F - x|_{K'} \cdot n_F$, where $n_F$ denotes a unit normal to the
At contact interfaces $\Gamma^{i,j}_h$, we introduce interface force $F^i_h$ and interface displacement $W^i_h$ satisfying
\[
\int_{\Gamma^{i,j}_h} F^i_h \cdot \delta u^i_h \, d\Gamma = \int_{\Gamma^{i,j}_h} \left(D(u^i_h) \cdot n^{i,j}_i\right) \cdot \delta u^i_h \, d\Gamma, \quad \text{and} \quad W^i_h = u^i_h \quad \text{at} \Gamma^{i,j}_h. \tag{5}
\]

Now, let $Q_h(G^i) := \left\{ \psi \in C^0(G^i); \forall \psi\vert_K \in P_1(K)^d, \forall K \in G^i \right\}$ denote the space of continuous piecewise linear polynomials on the band of intersected elements. Then, we determine the interface fields as follows. Find $F^i_h \in Q_h(G^i)$ and $W^i_h \in Q_h(G^i)$, such that for all $\delta F^i_h \in Q_h(G^i)$ and for all $\delta W^i_h \in Q_h(G^i)$
\[
\int_{\Gamma^{i,j}_h} (F^i_h - F^j_h) \cdot \delta F^i_h \, d\Gamma + J_F(F^i_h, \delta F^i_h) = 0, \tag{6}
\]
\[
\int_{\Gamma^{i,j}_h} (W^i_h - W^j_h) \cdot \delta W^i_h \, d\Gamma + J_F(W^i_h, \delta W^i_h) = 0,
\]
where
\[
J_F(F^i_h, \delta F^i_h) = \sum_{F \in F^i_h} \gamma H h^2 \int_F \left[ \nabla F^i_h \cdot \sigma_F \right] \cdot \left[ \nabla \delta F^i_h \cdot \sigma_F \right] \, ds \tag{7}
\]
regularises the interface fields with a penalty parameter $\gamma H > 0$. Heart quantities $F^i_\partial, W^i_\partial$ are required to fulfill contact at a set of quadrature points along the interface $\Gamma^{i,j}_h$
\[
(W^i_\partial - W^j_\partial) \cdot n^{i,j}_i \geq 0; \quad F^i_\partial \cdot n^{i,j}_i \leq 0; \quad ((W^j_\partial - W^i_\partial) \cdot n^{i,j}_i) \cdot (F^i_\partial \cdot n^{i,j}_i) = 0. \tag{8}
\]
and the system is closed by requiring that the fluctuation of the heart quantities around $F^i_h$ and $W^i_h$ satisfy a Robin condition, which reads as
\[
(F^i_h - F^j_h) - \beta (W^i_h - W^j_h) = 0, \tag{9}
\]
where $\beta$ is an algorithmic parameter that is homogeneous to a stiffness (we set it equal to the LaTIn search direction parameter for reasons not detailed here). We can finally solve the nonlinear coupled system of equations (1,5,6,8) for $u^i_h, F^i_h, W^i_h, F^i_\partial, W^i_\partial$, using an extension of the LaTIn iterative algorithm [9] whereby the local stage is “non-localised” by two-scale continuity condition (6).

3. Results

![Image](image-url)

(a) $\sigma_{yy}$

(b) Convergence rates.

Figure 2: Convergence rates and energy norm error for two inclusions with $E_1 = E_2 = E_3 = 1$.

The structure illustrated in Figure 2 is made of two interacting inclusions within a square matrix. The square matrix is meshed using a regular grid of triangles (Figure 1a). The matrix is compressed in the vertical direction. We plot the vertical compressive component of the stress. We also show the convergence rate together with the element size $h$. The convergence rate is optimum in both $H^1$ and energy semi-norm. Figure 3 shows the versatility of the method and the stability of the implementation in 3D.

32
4. Conclusions

We have presented a novel non-conforming finite element formulation for multiple linear elastic bodies in contact. We have demonstrated that our discretisation scheme is stable independent of how the contact interfaces intersect our fixed regular background mesh and that the contact problem solution converges optimally with mesh refinement. The next stage of our investigations is to extend the approach to the context of large displacements, whereby the contact region is an unknown of the problem.

Acknowledgements

We acknowledge the support provided by the Welsh Government and Higher Education Funding Council for Wales through the Sêr Cymru National Research Network in Advanced Engineering and Materials.

References

A new, meshless approach to fast solid dynamics: applications in metal plasticity


1Cardiff University, the Parade, Cardiff, CF24 3AA
2Swansea University, Bay Campus, Swansea, SA1 8EN
3University of Greenwich, London, SE10 9LS

*GretoG@cardiff.ac.uk

ABSTRACT

This paper summarises numerical results obtained by adapting to metal plasticity a mixed formulation originally devised for nearly incompressible hyperelasticity. The formulation is mixed in the sense that momentum and a number of strain definitions, instead of displacements, act as the main unknowns. This opens up the possibility of applying stabilisation techniques common in computational fluid dynamics (CFD) to solid dynamics. Coupled with meshless discretisation, it eliminates shortcomings occurring with finite elements in fast explicit codes. Two applications, under different loading conditions, are examined to show the suitability of the method in a new setting.

Key Words: Fast Dynamics; Conservation laws; SPH; Metal Plasticity; ECAE

1. Introduction

Recent developments in computational fast solid dynamics [1, 3] call for the representation of body motion and deformation via a system of first order, mixed-formulation conservation laws. The partial differential equations that appear in the system do not present the displacement as the main unknown to be recovered, but yield a set of different quantities (vectorial velocity, tensorial deformation gradient and cofactor of the deformation, scalar Jacobian of the deformation), depending on the number of conservation laws being considered. This choice will be driven on the one side, by the need to reproduce certain features of material behaviour (near or full incompressibility) while guaranteeing polyconvexity to the strain energy function and, on the opposite side, by speed of computation.

Problems currently affecting the widely employed, displacement-based, low order finite element analysis include lower order of convergence for derived variables; excessive element distortion under large deformations, requiring periodic remeshing; locking behaviour in bending scenarios; non-physical pressure instabilities, and high-frequency noise due to Newmark-type time integrators.

Mixed conservation laws have already been proven [1, 3] to reach second order of accuracy for stresses and strains. A novel computational framework has been devised to tackle the other issues. Under a total Lagrangian perspective, it combines the use of Smooth Particle Hydrodynamics (SPH), a meshless space discretisation technique, with an explicit, two-stage, total variation diminishing Runge-Kutta (TVD-RK) temporal scheme.

Until now, mixed formulation testing efforts have mostly focussed on nearly incompressible hyperelasticity [1, 3], where many of the aforementioned finite elements shortcomings take place. This work aims to demonstrate its feasibility in the field of metal plasticity, and will do so by presenting two test cases. The first example will consist of a high-velocity impact scenario. In the other application, an external load, continuously applied throughout the simulation, will induce severe plastic deformation on a metal piece. Stability will thus be demonstrated not only for impact dynamics, but also in the challenging conditions determined by the introduction of external energy at every time step.

The overall numerical framework, the system of conservation laws it is tasked to solve, and the material model employed are briefly described in section 2. The two metal plasticity applications are presented in section 3, while some conclusive remarks are offered in section 4.
2. Conservation laws, and their discretisation

In this work, \( p \) will indicate the linear momentum of a material point \( X \) occupying position \( x \) at time \( t \) in a deformable, continuum body, \( F \) will be the deformation gradient tensor, \( H \) the matrix of cofactors of \( F \), \( J \) the Jacobian of \( F \), \( P \) the first Piola-Kirchhoff stress tensor, \( \rho_0 \) the material density, \( b \) the body forces per unit mass, and \( t \) the surface traction forces per unit area. The gradient operator referring to initial spatial coordinates will be expressed as \( \nabla_0 \). The system of conservation laws that describes the motion and deformation processes then is:

\[
\frac{\partial p}{\partial t} - \nabla_0 \cdot P(F, J, H) = \rho_0 b; \quad \frac{\partial F}{\partial t} - \frac{1}{\rho_0} \nabla_0 p = 0; \quad \frac{\partial J}{\partial t} - \frac{1}{\rho_0} \nabla_0 \cdot (H^T p) = 0; \quad \frac{\partial H}{\partial t} - \frac{1}{\rho_0} \nabla_0 \times (p \times F) = 0
\]  

System (1) is solved for \( p, F, J, H \) at time \( t \). It is a set of hyperbolic differential equations close in structure to the ones used in fluid dynamics. This allows to employ well-established techniques from CFD in order to add artificial dissipation, and hence stabilise, the \( p \) and \( J \) equations. With regards to the material model, it is noted that a prerequisite for the validity of an elastic constitutive relation is the polyconvexity condition, which states that a one-to-one relationship has to exist between the stress \( P \) and strain measures \( F, J, H \). A stretch-based, polyconvex, hyperelastic energy function will be defined as:

\[
\Psi(\lambda_1, \lambda_2, \lambda_3) = \mu[(\ln \lambda_1)^2 + (\ln \lambda_2)^2 + (\ln \lambda_3)^2] + (\lambda/2)(\ln J)^2
\]  

where \( \mu \) and \( \lambda \) are the Lamé constants, and \( \lambda_1, \lambda_2, \lambda_3 \) are the principal stretches. In the plastic domain, (2) will be coupled to von Mises models with isotropic hardening. SPH spatial discretisation of (1) is derived from its corresponding weak form. Physical quantities of interest in SPH are known at a certain characteristic length. The spatially semi-discretised system then assumes the form:

\[
\begin{aligned}
\frac{\partial p_a}{\partial t} &= t_a + b_a - \sum_{b \in \Lambda_a} V_b (p_b \nabla_0 W_a(x_b) - p_a \nabla_0 W_b(x_a)) + D^{JST}(p_a) \\
\frac{\partial F_a}{\partial t} &= \sum_{b \in \Lambda_a} \frac{V_b}{\rho_0} (p_b - p_a) \otimes \nabla_0 W_b(x_a) \\
\frac{\partial J_a}{\partial t} &= H_a \cdot \sum_{b \in \Lambda_a} \frac{V_b}{\rho_0} (p_b - p_a) \otimes \nabla_0 W_b(x_a) + D^{JST}(J_a) \\
\frac{\partial H_a}{\partial t} &= F_a \times \sum_{b \in \Lambda_a} \frac{V_b}{\rho_0} (p_b - p_a) \otimes \nabla_0 W_b(x_a)
\end{aligned}
\]

In (3), \( \nabla_0 \) stands for corrected SPH gradient operator [3], and JST terms \( D^{JST}(U_a) \) depend on the Laplacian of Laplacian of kernel \( W(X) \) and on local wave speed \( c_p(X) \).

An explicit, two-stage TVD Runge-Kutta integrator scheme is used to advance the solution at particle \( a \) from instant \( t^n \) to \( t^{n+1} \), as in (4):

\[
U_a^n = U_a^n + \Delta t R_a(U_a^n, t^n); \quad U_a^* = U_a^n + \Delta t R_a(U_a^n, t^{n+1}); \quad U_a^{n+1} = (1/2)(U_a^n + U_a^*)
\]  

From the CFL condition, \( \Delta t = \alpha_{cfl} \frac{h}{\max_a(c_p)} \), with \( \alpha_{cfl} \) a constant, and \( h \) the characteristic length.
3. Applications in metal plasticity

High-velocity impact. A common benchmark test for plastic deformation at high-speed is the classical Taylor bar impact problem [5]. The original test was performed on an aluminium cylinder, but work-hardening effects, essential in order to derive an acceptably realistic plastic flow model, are better demonstrated with copper. Elastic behaviour is governed by (2), coupled with a standard von Mises plastic yield model with linear isotropic hardening. The material has the following properties: Young’s modulus $E = 117$ GPa, Poisson ratio $\nu = 0.35$, yield stress $\tau_0 = 0.4$ GPa, hardening modulus $H = 0.1$ GPa and density $\rho = 8930$ kg/m$^3$. The bar has initial height $h_0 = 32$ mm and radius $r_0 = 3.2$ mm, and is discretised in a set of 4131 particles arranged in a regular pattern, each being assigned a spherical subvolume $k$ with radius $r_k = 0.32$ mm. The impact is frictionless and takes place at an initial speed $v_0 = -227$ m/s on a rigid, normal wall. Due to extensive plastic dissipation, the JST stabilising term is set to a very low value. Fig. 1 shows results of the Taylor bar simulation performed by JST-SPH:

![Taylor bar simulation results](image)

Figure 1: JST-SPH Taylor bar problem. Initial configuration on the left. Other pictures show the cross sectional shape of the bar, and the plastic strain contour plot at various instants in the simulation. 4131 particles, $E = 117$ GPa, $\nu = 0.35$, $\tau_0 = 0.4$ GPa, $H = 0.1$ GPa, $\rho = 8930$ kg/m$^3$, $v_0 = -227$ m/s.

In Figure 1, as expected [5], the plastic front is shown to remain close to the bottom wall in the early stages of the simulation (red contour regions). It then slowly climbs up, as more kinetic energy dissipates into plastic strain. In Table 1, the radius of the bottom surface at $t_f = 80$ $\mu$s is compared to results of identical tests performed using different numerical techniques [1].

<table>
<thead>
<tr>
<th>numerical method</th>
<th>final radius (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>standard finite elements, hexahedra [1]</td>
<td>6.95</td>
</tr>
<tr>
<td>standard finite elements, tetrahedra [1]</td>
<td>5.55</td>
</tr>
<tr>
<td>mixed JST finite volumes, vertex-centred [1]</td>
<td>6.98</td>
</tr>
<tr>
<td>mixed JST-SPH</td>
<td>$6.66 + r_k = 6.98$</td>
</tr>
</tbody>
</table>

As can be seen from Table 1, mixed formulation techniques, being locking-free, avoid the excessively rigid response of the structure of FEM displ.-based analyses. More to note, SPH particles station at the centre of their assigned subvolumes of radius $r_k$. Results in table 1 account for $r_k$ in the JST-SPH case.

Severe plastic deformation process. Numerous metallurgic techniques exploit in various, specific manners the mechanics of plastic deformation, in order to attain smaller grain size – and thus better material standards – for metals and alloys. Among them, Equal Channel Angular Extrusion (ECAE) [4] can guarantee high levels of shear strain for relatively low levels of external pressure, making it suitable for mass production. In the present setting, the ECAE process will be simulated in its 2-turns, 90°-channel variant. The test will showcase the robustness of the JST-SPH numerical setup, and indeed the overall adequacy of the CFD-inspired mixed formulation implementations, under a demanding dynamical regime of continuous introduction of external energy, and subsequent extremely large distortions. The analysis
is performed in plane strain conditions, and focuses on a bar made of commercially pure aluminium (Al1100, $E = 69$ GPa, $\nu = 0.33$, $\rho = 2800$ kg/m$^3$, width $l = 8$ mm) passing through a channel carved into a rigid die, of the same width of the bar. The right-angled corners are rounded, with 1.5 mm and 1 mm external and internal fillet radii. Contact between bar and die is assumed lubricated, and hence simulated frictionless. The JST term was set to a very low value, given the presence of plastic dissipation. The hyperelastic-plastic material model used obeys to (2) and to the plastic isotropic hardening law:

$$\tau_{pl} = 159(0.02 + \varepsilon_{pl})^{0.27} \text{ MPa}$$  \hspace{1cm} (5)

Eq. (5) is solved for $\varepsilon_{pl}$ numerically by employing the Newton-Raphson method. Fig. 2 captures graphically the deformation process of the billet at various instants in time.

![Figure 2: JST-SPH ECAE plane strain simulation: plastic strain at various stages of the process. The billet being extruded is made of Al1100, with $E = 69$ GPa, $\nu = 0.33$, $\rho = 2800$ kg/m$^3$ and plastic properties determined by (5); it is discretised with 400 particles and subjected to a velocity of $v = -1$ m/s.](image)

There is substantial agreement of Figure 2 with data presented in [4]. The meshless nature of JST-SPH eliminates the excessive element distortions associated with the presence of a mesh in case the strains are too high. A total Lagrangian point of view can then be adopted, which is able to follow the path of the material particles in time, and thus permits to gain a better understanding of the physics of deformation.

### 4. Conclusions

The JST-SPH mixed methodology has proved to be a valid tool for computing plastic deformations in dynamic regimes. It has been shown that there is good agreement between results the previous section and data for the same tests found in literature. The Taylor bar impact case provides an ideal application for JST-SPH, since SPH performs particularly well in high velocity, large deformation settings. On the other hand, the ECAE test confirmed the robustness of JST-SPH. In fact, the total Lagrangian framework was able to withstand the high local gradients of stresses, strains and displacements, while the presence of a constant loading in time did not lead to any kind of instability. Introduction of friction, and thus contact, to the model may constitute a natural step forward in research. More realistic impact and fracture analyses could also be worth considering, to further check the soundness of the method.

### References


Simulations of sliding adhesive contact between microgear teeth in silicon-based MEMS work in a vacuum environment

* Nabeel Almuramady¹,², Feodor M. Borodich¹

¹School of Engineering, Cardiff University, Cardiff, Wales, UK, CF24 3AA
²College of Engineering, University of Al-Qadisiyah, Al-Qadisiyah, Iraq

*AlmuramadyNS@cardiff.ac.uk

ABSTRACT

Sliding friction and adhesive contact interactions between microgear silicon-based MEMS teeth working in a clean and vacuum environment have been modelled using a multiscale hierarchical elastic structure. Here the results of numerical simulations based on the use of multiscale block model are presented. The tooth is modelled as a bulk silicon-based MEMS surface covered by roughness having two subscales specified by the character of interactions: atomic subscale level and adhesive subscale. Friction over completely meshing teeth surfaces is estimated by calculation of the total energy dissipated during sliding. The dissipation is caused by the different physical and chemical mechanisms. Due to the vacuum environment, these mechanisms reduced to the energy lost by the dissociation of chemical and van der Waals bonds, and by the elastic interlocking between the asperities located on the meshing micro-tooth surfaces. It is argued that due to the Polonsky-Keer effect, there is no plastic deformation of the MEMS tooth surface asperities because the asperity sizes are within the validity of this effect. The adhesion layer is defined employing ideas of the Maugis approximation. The adhesion force of each nanoasperity has assumed to be equal to the pull-off force in the Boussinesq-Kendall model corrected by the Borodich no-slip coefficient. The simulations show that MEMS with the clean silicon surfaces of teeth cannot work due to stiction between surfaces, while friction between tooth surfaces functionalised by carbon-based layer is much smaller. If the functionalised coating is worn away then stiction may occur.

Keywords: MEMS; microgear wear; adhesion; sliding contact; stiction.

1. Introduction

Micro-Electro-Mechanical Systems (MEMS) have been used in the wide variety of industrial and space applications [1]. However, there are various challenges that may lead to device failure, in particular, these related to the stiction, adhesion and friction between various micro/nano components of MEMS that are used to transfer the load and torque [2]. Stiction is defined as the unintentional adhesion (the static friction) that highly restricts the movements of the micro/nano elements. This phenomenon may significantly reduce the MEMS reliability [3]. Microgear is one the most important torque transmitter in MEMS. When it work there is contact between the teeth. Cold welding (cohesion) between micromachined device surfaces could occur when these surfaces are clean and work in the vacuum environment [2, 4]. If the MEMS teeth are clean and work in a vacuum then there is a high probability of sticking with each other and as a result for this cold welding occurred in the contact zone, which lead finally to structure collapse. Here stiction has defined as the unintentional adhesion between the teeth that does not allow MEMS to work at all. Surface functionalisation is one of the successful solutions to reduce cohesion and, therefore, to eliminate stiction [1]. The dimension of the meshing microgear as was taken as in [5]. Figure 1 shows a micro-pinion that is meshing with micro-gear. The gap between surfaces of microgears meshing teeth, which is different at each time step, is calculated using Hertz line contact theory.
In this study, the term ‘scale’ is defined as the term that reflects validity of different physical-chemical mechanisms of interactions between surfaces. The multiscale hierarchical model of an asperity [6] is modified and employed in order to simulate the work of multi-asperity rough surfaces of MEMS microgear teeth as shown in Figure 2. $W_{\text{adhesive}}$ is the width of the adhesive subscale where the van der Waals interactions likely occur.

Due to the nanoscale dimensions of the asperities of the microgear tooth, it does not have the microscale roughness. In addition, the asperities do not have plastic deformations due to the Polonsky and Keer effect [7]. Thus, the present model has two nanoscales: atomic scale as the first subscale of nanoasperity and adhesive nanoscale as another subscale. The latter subscale reflects the dimensions where the van der Waals interactions are significant.

2. **Friction force**

The friction force and the coefficient of friction are estimated over the whole meshing surfaces of the teeth. The dry friction force ($F_f$) is calculated through the energy dissipated ($U_{\text{diss}}$) during relative sliding distance ($x$) between two meshed micro-tooth elastic rough surfaces.

$$F_f = \frac{U_{\text{diss}}}{x}$$

This energy lost is due to dissociation of chemical and van der Waals bonds, and the energy lost through elastic deformation of nanoasperity during the contact.

$$U_{\text{diss}} = U_{\text{totalchem}} + U_{\text{totalvdW}} + U_{\text{elastic}}$$

Then it follows from (1) and (2) that the friction force $F_f$ and the coefficient of friction $\mu$ can be calculated respectively using the following expressions.
\[ F_f = \frac{U_{\text{Total chemical}} + U_{\text{Total vdW}} + U_{\text{elastic}}}{x} \]  \hspace{1cm} (3)

\[ \mu = \mu_{\text{chemical}} + \mu_{\text{vdW}} + \mu_{\text{elastic}} \] \hspace{1cm} (4)

The total energy loss through the different mechanisms between the counterpart’s surfaces has been shown in Figure 3 and the coefficient of friction (COF) for non-functionalised teeth surfaces has been shown in Figure 4.

Thus, as it has been mentioned, due to the vacuum environment, the energy lost the mechanisms may be reduced to the dissociation of chemical and van der Waals bonds, and the energy lost through the elastic interlocking between the asperities located on the meshing micro-tooth surfaces.

3. Adhesion force

The force of adhesion for one nano-asperity is assumed as the pull-off force according to Boussinesq-Kendall model, corrected with non-slip coefficient \((C_{NS})\) introduced by Borodich [8]. Let \(F_{\text{adh1}}\) be the adhesion force of one asperity and \(n\) be the number of asperities in contact. Then one has

\[ F_{\text{adh}} = nF_{\text{adh1}} \] \hspace{1cm} (5), (6)

Where \(w_{12}\) is the surface energy. For silicon, the Hamaker constant \(A_{12} = 1.1 \times 10^{-18} J\) [9] and the separation distance between atoms \(D_0 = 1.49 \text{ Å}\) respectively. The half width \(a\) of the silicon adhesive asperity is 97.5 nm. The contact modulus can be calculated by substitution the corresponding values of Young’s modulus \(E = 161 \text{ GPa}\), and the Poisson’s ratio \(\nu = 0.23\) [5, 9].

In small scale devices that having sliding interfaces such as gear MEMS, wear considerably decreases their lifetime and reliability, and stiction will stop them from working at all. Applying specific carbon-based layers, such as Octadecyltrichlorosilane self-assembly monolayer (OTS-SAM), that functionalise the micro-tooth surfaces (see Figure 5), may reduce friction and the probability of stiction and friction.

![Figure 3: Total energy loss](image1)

![Figure 4: COF for non-functionalised teeth surfaces](image2)

![Figure 3: FunctionaliSed coating layer covered the counterpart’s microgear MEMS teeth](image3)
Indeed, it has found that the friction between the tooth surfaces functionalised by this carbon-based layer is much smaller. Then, with operation, stiction will start to occur when the coating is worn away.

![Figure 4: Comparison of the COF before and after the functionalisation of the teeth surface by OTS-SAM layer](image)

4. Conclusions

A new approach to modelling of friction and adhesion between the silicon-based microgears MEMS working in a vacuum environment is described. In this approach, for the first time roughness has characterised as multi-block structures covering the entire micro-tooth surface. Each block has represented by a multiscale hierarchical asperity that consists of two different scales: atomic subscale, where the chemical interactions are significant, and adhesive subscale, where the van der Waals interactions are likely occur. The total energy dissipated due to interlocking of nano subscale asperity, dissociation of chemical and van der Waals bonds has been calculated. Simulations have shown that the probability of stiction is very high if the gear surfaces are not functionalised. In contrast, the tooth surfaces having functionalised monolayer carbon-based coatings are much less prone to stiction. The wear of the functionalised coating leads to increase the probability of stiction between surfaces.

Acknowledgements

The authors are grateful to the Leverhulme Trust for financial support of their collaboration within the framework of the CARBTRIB International Network. In addition, the Iraqi Ministry of Higher Education and Scientific Research and University of Al-Qadisiyah are gratefully acknowledged for supporting the studies of one of the authors (Nabeel Almuramady) at Cardiff University.

References

THE OPTIMISATION OF PRODUCTION WELL NUMBERS IN ENHANCED GEOTHERMAL SYSTEM

*Maleaha Samin ¹, Asaad Faramarzi ¹, Ian Jefferson ¹ and Ouahid Harireche ²

¹School of Engineering, University of Birmingham, Edgbaston, Birmingham, B15 2TT
²Department of Civil Engineering, Islamic University of Madina, Madina

*MYS172@bham.ac.uk

ABSTRACT

The number of production wells in an Enhanced Geothermal System (EGS) plays a very crucial role in the long term performance and commercial feasibility of the system. The relationship between influential parameters such as flow rate and the distance between wells has a complex nature and requires a comprehensive study. Therefore, in this study a series of numerical simulations are carried out using a coupled heat-flow finite element model to study the performance of multi-well EGS. Different scenarios are considered for the number of production wells, kept at a constant distance to the production wells, to determine their optimum arrangement. The results show that the accumulative thermal power for the thermal breakthrough of the production wells has the highest thermal production with the five production wells. Naturally, the cost increases with increasing the number of production wells; therefore, a design efficiency indicator was proposed to select the optimum efficient design for the multi-wells EGS reservoir. The results show that the triplet wells reservoir (two production wells with a single injection well) is the most efficient design with respect to both power and cost.

Keywords: EGS; Geothermal reservoir; COMSOL Multiphysics; Production well; Thermal breakthrough

1. Introduction

Hot subsurface rocks contain a huge thermal storage capacity that can be used as an economical source of renewable energy. For example, the subsurface temperature of the United States at a depth of 5 km can rise to 350 °C and up to 1200 °C at 40 km [4]. However, this huge capacity of energy source is not yet commercially viable due to inefficient methods of extraction of heat resources [2]. Several studies have used numerical analysis and in particular finite element to optimise the design of Enhanced Geothermal System (EGS) reservoirs with the aim to find maximum thermal power with heat extraction efficiency [3]. In the present research, a finite element model of a typical reservoir is developed to investigate the efficiency of an EGS reservoir with respect to the numbers of production wells. Multiphysics finite element (FE) solver (COMSOL) is used to investigate the optimum productivity of EGS for different number of production wells under the effect of fully coupled Thermo-Hydro (TH) processes due to its efficiency in coupling Multiphysics with FE method.

2. Finite Element (FE) model development

In this study, the developed FE model describes the reservoir as a fully saturated porous medium with isotropic permeability equivalent to the fractured zone and rock matrix combined. The fluid properties and the initial and boundary conditions are same as those discussed in [3]. In general, thermal-hydraulic-mechanical and chemical (THMC) coupled processes take place during the heat extraction from an EGS [7]. However, heat transfer and fluid flow (TH) are the most effective coupled processes affecting heat extraction [3]. The 3D transient model presented in this paper is developed to predict the long term performance of multi-well EGS taking into consideration the full coupling of TH process. The governing equations of this model are as follows [3]:

Fluid flow: mass conservation is applied to the hydraulic process and is governed by Darcy’s Law for fluid flow in a porous medium:
\[
\frac{\partial}{\partial t} (\phi \rho_r) + \nabla (\rho_r \mathbf{u}) = Q_f
\]
(1)

\[
\mathbf{u} = \frac{k}{\mu} \nabla p
\]
(2)

Where, \( \phi \) is the rock porosity (dimensionless), \( \rho_r \) is the rock density (kg/m\(^3\)), \( \mathbf{u} \) represents the Darcy’s velocity (m/s), \( k \) is the equivalent permeability of the rock matrix (m\(^2\)), \( \mu \) is the fluid dynamic viscosity (Pa.s), \( Q_f \) is the fluid source/sink term and \( p \) is the pressure (MPa).

Heat transfer: energy conservation is applied to the conductive and convective heat flux as follows:

\[
\left( \rho c_p \right)_{\text{eff}} \frac{\partial T}{\partial t} + \rho_w c_p \dot{w} \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = Q
\]
(3)

\[
\mathbf{q} = -k_{\text{eff}} \nabla T
\]
(4)

\[
\left( \rho c_p \right)_{\text{eff}} \mathbf{q} = \phi \rho_w c_p \dot{w} + (1 - \phi) \rho_r c_p
\]
(5)

\[
k_{\text{eff}} = k_w + (1 - \phi) k_r
\]
(6)

Where, \( \rho \) and \( \rho_w \) are the equivalent and fluid density respectively (kg/m\(^3\)), \( c_p, c_p, c_p \) are the equivalent, fluid and rock matrix heat capacity at constant pressure (J/(kg. o C)), \( (\rho c_p)_{\text{eff}} \) is the equivalent volumetric heat capacity at constant pressure, \( k_{\text{eff}}, k_w \) and \( k_r \) are the equivalent, fluid and rock matrix thermal conductivity (W/(m. 0 C)), \( Q \) is the heat source/sink term and \( \mathbf{q} \) is the conductivity heat flux in the rock matrix.

3. Model geometry

A 3D numerical model of EGS reservoir was developed using six scenarios for the number of production wells within the reservoir with a single injection well at the centre of the proposed reservoir. A cylindrical model of 500 m diameter and 500 m height was selected for the fractured reservoir, centred at a depth of 4000 m. The cylinder shape is applied to reduce the boundary impacts on the different scenarios of the number of production wells. The position of the production wells was selected so that there was a distance of 100 m to the boundary. The initial and boundary conditions are presented in [3]. In the present study, the number of production wells was optimised. Production wells are located at an equal distance to the injection well. In addition, other design parameters are also assumed to remain constant for all scenarios such as the injection and production pressure of a value of 5 MPa.

4. Long term performance criteria

Predicting the thermal breakthrough, which is the time that the cold water front reaches the production well [5], of an EGS reservoir should be considered during the analysis of geothermal reservoirs [1]. At the thermal breakthrough of an EGS the efficiency of the power plant will be very low [3] and consequently the reservoir will become abandoned. Thus, the thermal breakthrough has been set out as an objective of the reservoir long term performance [1]. It is calculated through the thermal drawdown of the EGS reservoir, i.e. equation 7, and the thermal breakthrough is assumed to happen when 10% of the thermal drawdown of the reservoir is reached [1].

\[
TD = \frac{T_p - T_o}{T_{inj} - T_o}
\]
(7)

Where, \( TD \) is the thermal drawdown, \( T_p, T_o \) and \( T_{inj} \) are the production, initial and injected fluid temperatures (°C). In addition, the high drilling cost (\( P_d \)) was a further objective has been considered to optimise the number of production wells, this has been emphasised by [6] for a doublet reservoir design (one production and injection wells).
5. Results and discussions

A comprehensive study was carried out to optimise the number of the production wells in a multi-well EGS reservoir. Six different EGS design simulations were conducted to find the optimum number of the production wells with the optimum accumulative thermal production power ($\sum W_{hp}$) at the thermal breakthrough of production wells. The parameters that were investigated include thermal drawdown, thermal power and the total cost of well drilling. The first set of results show of the thermal evolution of the six design scenarios after ten years of heat mining in Figure 1. The cooling boundary around the injection well has been expanded in different ranges within the six scenarios. Also, the fluid flow path differs based on the number of production wells. Cooling fronts of the reservoir for the 2, 3, 4, 5, 6 and 7 production numbers are represented in Figure 1(A), 1(B), 1(C), 1(D), 1(E) and 1(F) respectively.

![Figures 1(A) to 1(F)](image)

Figure 1: Thermal evolution of the reservoirs for different design scenarios of production numbers: (A) 2 wells, (B) 3 wells, (C) 4 wells, (D) 5 wells and (E) 6 wells.

The second sets of results analysed in the present study represents the productivity and the economy analysis of the above six scenarios. The accumulation of the production thermal power ($\sum W_{hp}$) dramatically increased with the increase of the production well numbers to five, the maximum value, and then the productivity declines with six and seven production well scenarios, as shown in Figure 2 (a). Thus, increasing the number of production wells results in decreasing the fluid flow rate and the velocity in the production wells and hence the productivity increases. However, once the number of the production wells increases more than five wells, the productivity decreases due to the interaction between the flow path areas of the production wells. In comparison, the total drilling cost increases linearly with an increase in the number of production wells. However, design with five production wells produces the optimum accumulative thermal power after 10 years of heat mining, but the cost of the design, which can be seen by the dash line in Figure 2 (a), is very high. Hence, to find the optimum design an equation is proposed to be used as an indicator of the design efficiency for different scenarios at the thermal breakthrough of the production well.

$$ DeI = \frac{\sum W_{hp}}{P_d} $$

(8)

Where $DeI$ is the design efficiency indicator (Mw/unit drilling cost), $\sum W_{hp}$ is the accumulative of thermal power at the breakthrough of the production well (Mw) and $P_d$ is the total cost of drilling. Figure 2 (b) represents the design efficiency indicator of each scenario. From Figure 2 (b), it can be concluded that the first scenario (two production wells) is the most efficient design.
Although the accumulative thermal power of five production wells is 1.5 times the thermal power of two production wells, the cost is about twice. However, DeI shows that the two production wells reservoir is a more efficient design as shown by the DeI value of 50 Mw/unit price.

6. Conclusions

A numerical study was conducted to investigate the impact of the number of production wells on the performance of EGS and in particular the thermal breakthrough of the system. The results show that for a typical EGS the accumulative thermal power will increase up to five production wells and after that will start to gradually decline. However, once the cost is added to the model, the results indicate that the system with one injection and two production wells is the most efficient design.

References


Biomechanics
DEVELOPMENT OF A 1D-0D CARDIOVASCULAR MODEL OF PREGNANCY IN HUMANS

*Jason M. Carson¹, Michael J. Lewis¹, Dareyoush Rassi² and Raoul Van Loon¹

¹College of Engineering, Swansea University, Bay Campus, Fabian Way, Swansea, SA1 8EN
²College of Human and Health Sciences, Swansea University, Singleton Park, Swansea, SA2 8PP

*485621@swansea.ac.uk

ABSTRACT

In this work a model of the cardiovascular system during human pregnancy is presented. The female cardiovascular system undergoes significant changes including an increase of up to 50% blood volume and a significant decrease in total peripheral resistance. By various adaptations the mean pressures do not significantly change in a healthy pregnancy. The closed loop model presented simulates the cardiovascular system in the supine position and includes: 456 1D vessels from the systemic and pulmonary systems; venous valves; a heart model with three types of interaction; and an external pressure on the inferior vena cava from the gravid uterus, which increases over the course of pregnancy. Data collected from various studies is used to tune and validate the model. The model produced mean uterine arterial blood flow is consistent with published measurements.

Key Words: 1D-0D; Cardiovascular Model; Pregnancy; Closed Loop; Implicit Scheme

1. Introduction

The human female cardiovascular system undergoes significant adaptation during pregnancy, including: up to 50% increase in blood volume, up to 50% cardiac output (CO), significant decrease in total peripheral resistance (TPR) [1], remodelling of vessels [2] (particularly near uterus and ovaries), and substantial increases in blood flow to the uterus, ovaries and kidneys. Even with these adaptations the mean blood pressures tend to remain relatively consistent, often decreasing during the first or second trimester, and increasing to normal pressures by full term [1]. Given the extensive adaptation, there are many problems associated with pregnancy, such as hypotension (low blood pressure), hypertension (high blood pressure), pre-eclampsia (symptoms include high blood pressure), placental insufficiency (high resistance from underdeveloped placenta).

In this work the cardiovascular network chosen is based on [3] (with a number of changes and additions), while the valve model is from [4]. The closed loop model includes: 456 1D vessels; generic 0D vascular beds, with more specialised 0D vascular beds for the liver and coronaries; 0D heart model with three types of interaction; 339 0D venous valves. An external pressure, which increases during pregnancy and simulates the effect of the gravid uterus, is applied to the inferior vena cava. The system of equations are solved by the globally implicit enhanced trapezoidal rule method (ETM) by [5]. In that paper the ETM was rigorously compared with published benchmark problems and was shown to correctly determine the intensity and speed of shock waves.

The main aim of this work is to further understand the mechanisms involved in adaptation during pregnancy, and to eventually improve understanding of how various health issues may arise as a result of pregnancy. Measured data sets from various studies [6, 7, 8, 9] are used in order to tune and validate the model.
2. Governing Equations

The governing equations describing 1D blood flow in compliant vessels are the conservation of mass and conservation of momentum

\[
\begin{aligned}
\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} &= 0, \quad \text{(mass)}, \\
\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \frac{Q^2}{A} \right) + \frac{A}{\rho} \frac{\partial P}{\partial x} + \frac{\xi \mu Q}{\rho A} &= 0, \quad \text{(momentum)};
\end{aligned}
\]  

(1)

together with the following constitutive law

\[
P - P_{\text{ext}} - P_0 = \frac{2\rho c_0^2}{b} \left[ \left( \frac{A}{A_0} \right)^{a_1} - \left( \frac{A}{A_0} \right)^{a_2} \right] + \frac{\Gamma}{A_0 \sqrt{A}} \frac{\partial A}{\partial P} \frac{\partial P}{\partial t},
\]  

(2)

where \( P, P_0 \) and \( P_{\text{ext}} \) are the hydrostatic, reference and external pressures respectively. \( A \) and \( A_0 \) are the cross sectional area at the hydrostatic and reference pressures, respectively. \( Q \) is the volumetric flow rate, \( \rho \) and \( \mu \) are the density and viscosity of blood. \( \xi \) is the viscous friction constant, while \( \Gamma \) is the wall viscous coefficient. \( c_0 \) is the reference wave speed, \( b \) is a scaling term as in [3], and \( a_1 = \frac{b}{2}, \ a_2 = -\frac{3}{2} + \frac{3}{b} \).

3. Methodology

Many of the model components, such as: 1D vessel properties, vascular beds, valve models, and heart model; are from [3]. The model has an addition of the utero-ovarian system which supplies blood to the uterus, placenta and ovaries, and vessels in this system remodel over the course of pregnancy. Figure 1 shows the systemic arterial 1(b) and systemic venous 1(a) trees. While Figure 2 shows the utero-ovarian system used in the model. The governing equations including the 1D equations (1) and (2), and all 0D models are solved implicitly using the ETM scheme [5]. The data used to aid tuning the model are from [6, 7, 8, 9] and include heart rate (HR), systolic and diastolic pressures, stroke volume (SV), left ventricular ejection time (LVET), and variables which can be calculated from these such as total peripheral resistance (TPR), pulse pressure (PP) and cardiac output (CO). Note that in the model the
initially defined TPR is a maximum, as the model has variable resistances in vascular beds, decreasing when pressure is above reference (diastolic pressure) and increasing when model pressure is below the reference pressure. Moreover, in the model the blood volume of the system is defined at the beginning (via initial pressures), therefore during simulation blood volume is added to the system in the venules in order to achieve expected cardiac outputs. In the model the effect of the gravid uterus is simulated by applying external pressure to the inferior vena cava, increasing over the duration of pregnancy.

Figure 2: One side of the utero-ovarian system used in this work

4. Results and Discussion

Waveforms of the left uterine artery for non-pregnant and pregnant cases is show in Figure 3(a). Mean flow in the left uterine artery for the non-pregnant case in the model is 47.1 ml/min, for trimester one 90.2 ml/min, for trimester two 421.4 ml/min, while for trimester three is 534.5 ml/min. These are consistent with literature, which indicate 20 – 40 ml/min for non-pregnant and 450 – 800 ml/min in singleton pregnancies [2]. Velocity waveforms (found by dividing flow by area) in the uterine artery are also in good agreement with published Doppler measurements [10].

Figure 3: (a) Comparison of Uterine artery waveforms for non-pregnant and pregnant cases. (b-c) Comparison of model outputs with standard deviations of measured data as background colours (trimester 0 is non-pregnant case).

Figures 3(b) and 3(c) show a comparison of standard deviation of all participants (background colours) with model output (both scaled by the maximum values of measured data) for TPR, CO, LVET, and PP. The majority of model variables are within the standard deviation of the measured data. The estimated total peripheral resistance for the model is calculated using

\[ TPR_{model} = \frac{\text{mean}(\text{Aortic Root Pressure})}{\text{Cardiac Output}} \]  

as the vascular bed resistance in the model vary by over 20% during a cardiac cycle. The total peripheral resistance estimation of the model captures most of the features of the measured data although the model gives higher estimations. Although the measured data (average of all participants) has an increase in TPR from second to third trimesters, while the mean TPR in the model decreases. This deviation could arise
from the vascular bed resistance model [5] (and possibly vascular compliance) which adapts vascular resistance based on arterial blood pressure in that region, as the blood pressure increases the resistance decreases and vice versa. Thus as the volume of blood increases (while the compliance may not increase by an equal amount), the pressures in the model for the 3rd trimesters are higher and may cause reduced average vascular resistance. The pulse pressure in the model is generally higher than the measured data for the pregnancy models, which could indicate an under-estimated compliance in the model. The left ventricular ejection time is generally underestimated by the model, however it does show the general behaviour of decreasing over the course of pregnancy. For the non-pregnant case the LVET is still within the normal range given in literature, albeit outside the standard deviation of the measured data.

5. Conclusions

The pregnancy model presented produces expected blood flow volume to the utero-placenta system, while generally capturing the behaviour of measured data from various studies. Model gives good agreement with the non-pregnant group data, and gives a good representation of the pregnant group data at various stages of pregnancy. The model tends to underestimate the compliance for the pregnancy cases, which may indicate an improvement of the constitutive law is necessary to account for the various remodelling of vessels. Future work involves the significant challenge of implementing the model in the upright (standing) position, for which various auto-regulation mechanisms are required to maintain venous return.

References


A SEMI IMPLICIT, LOCALLY CONSERVATIVE GALERKIN APPROACH FOR MODELLING SYSTEMIC BLOOD CIRCULATION

Hayder M. Hasan\textsuperscript{1} and P. Nithiarasu\textsuperscript{1*}

\textsuperscript{1}Zienkiewicz Centre for Computational Engineering
College of Engineering, Swansea University, Swansea SA2 8PP, United Kingdom

\textsuperscript{*}P.Nithiarasu@Swansea.ac.uk

ABSTRACT

A stabilised semi-implicit, locally conservative Galerkin method (SILCG) is proposed for predicting blood flow characteristics in a 1D human arterial network. The new method enforces flux continuity at the element interface and solves the system of equations element by element. While the accuracy of Continuous Galerkin (CG) method is matched by the LCG method, the matrix size never exceeds the element matrix size resulting in a significant simplification to the solution procedure. Unlike the CG method in which the Newton method becomes slower with larger matrices, SILCG method for systemic circulation requires a maximum matrix size of 4 x 4 per element. This allows us to employ the classic version of Newton iteration, which has a quadratic convergence rate. Although standard Newton method requires evaluation of both Jacobian matrix and the residual at every single iteration, which may be expensive for large scale problems. The results shows that, the number of iterations in SILCG are considerably lower as a result of small matrix size. Also, the numerical experiments show that Jacobian matrix can be limited to one factorization per time step, which makes the SILCG even faster.

Key Words: systematic circulation-1D modelling-semi implicit locally conservative Galerkin (SILCG)-Newton method

1. Introduction

Modelling of blood flow problem has been intensively investigated using explicit and implicit schemes [1, 2, 3, 4]. Explicit solvers are accurate but admit smaller time steps. The implicit methods on the other hand, admits larger time steps but the iterative solution for the non linear matrix can be quite expensive, making the implicit methods often inefficient [5]. However, implicit scheme may be more efficient at dealing with linear system of equations. In general, time step size is often compromised by the accuracy for any implicit scheme. So, we attempt to obtain good accuracy in comparison with explicit method and relaxing time step restrictions by introducing the semi implicit locally conservative Galerkin method (SILCG). As SILCG uses only element matrix (i.e. 4 x 4), this removes the poor global convergence from Newton methods that often are associated with large scale problems [6]. This issue is the basic motivation behind the quasi Newton methods like Broydn approach where Jacobian matrix is approximated rather than solved at every iteration. Although this speeds up the calculations, it also produces more error leading to less accurate approximation. Moreover, many current methods use finite difference approximations for obtaining Jacobian matrix. Due to small matrix size, SILCG employs the finite element procedure to construct Jacobian matrix every time step. All these advantages of the SILCG method are briefly explained below.

2. Numerical Formulations

The governing equations for the problem are the mass and momentum equations which may be written in a compact form as [1, 2]

\[ \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} - S = 0 \]  

where
\[
\mathbf{U} = \begin{bmatrix} A \\ u \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} A u \\ u^2 + \frac{p}{\rho} \end{bmatrix} \quad \text{and} \quad \mathbf{S} = \begin{bmatrix} 0 \\ -\frac{8\sigma \mu u}{A} \end{bmatrix}
\]

\( A \) and \( u \) are the main variables while pressure is linked to the area by the correlation \( p = p_{\text{ext}} + \beta (\sqrt{A} - \sqrt{A_0}) \). The parameters, \( \rho, \mu, p_{\text{ext}} \) and \( A_0 \) are fluid density, fluid viscosity, the pressure from the surrounding tissues and the area at zero transmural pressure respectively. And, \( \beta \) accounts for the material properties of the elastic vessel and given as \( \beta = \frac{\sqrt{\pi h E}}{A_0 (1-\sigma^2)} \), where \( h \) is the vessel wall thickness, \( E \) is Young’s modulus and \( \sigma \) is the Poisson’s ratio, assumed to be 0.5 (i.e. the vessel wall is incompressible) (see [2] for more details). As the convection is significant here, an upwinding procedure is often required to obtain a descent solution, so the discrete form in time can be presented by using Taylor expansion as

\[
\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} = \left\{ \mathbf{S} - \partial_x \mathbf{F} - \frac{\Delta t}{2} \left[ \partial_x (\mathbf{B} \mathbf{S} - \mathbf{B} \partial_x \mathbf{F}) - \mathbf{C} \partial_x \mathbf{F} - \mathbf{CS} \right] \right\}^{n+1}
\]

where \( \mathbf{B} = \frac{\partial \mathbf{F}}{\partial \mathbf{U}} \) and \( \mathbf{C} = \frac{\partial \mathbf{S}}{\partial \mathbf{U}} \) are two Jacobian matrices. The finite elements discretisation procedures are applied to the to above equation according to [7] by adopting linear shape functions, which results in fully discrete SILCG form as

\[
[M]_e \Delta \mathbf{U}^n_e = \Delta t \left[ [\mathbf{K}] (\mathbf{F}^{n+1}) + [\mathbf{L}] (\mathbf{S}^{n+1}) + \{f_i\}^n \right]_e
\]

where the subscript \( e \) refers to an element and all matrix details (i.e. \( M, K \) and \( L \)) can be found in [2]. The flux \( f_i^e \) is used to transfer information between elements, and this flux must be evaluated at \( n \) time for maintaining flux continuity. Apparently, this restricts time step as this leads to semi implicit method as the name suggests. However, as stated before, the proposed simplified approach shows good agreement with the established explicit LCG [1, 2]. To solve the resulting system of equations (i.e. Eq.3), we adopt the Newton method [8, 9], i.e.

\[
\mathbf{U}^{k+1} = \mathbf{U}^k + \delta \mathbf{U}^k
\]

where \( \mathbf{U} \) can be either \( A \) or \( u \) (i.e. the main variables). The update \( \delta \mathbf{U}^k \) is estimated via Newton iteration, i.e.

\[
\mathbf{J} \left( \mathbf{U}^k \right) \delta \mathbf{U}^k = -\mathbf{R} \left( \mathbf{U}^k \right)
\]

where \( \mathbf{J} \left( \mathbf{U}^k \right) \) is a 4 x 4 Jacobian matrix while \( \mathbf{R} \left( \mathbf{U}^k \right) \) is the residual vector. Eq.5 has to be solved every single iteration until convergence (original Newton solver).

We use characteristic system at the boundaries and an initial pressure wave is enforced from the left ventricle (see [1, 2] for full details). Note that, these boundaries are evaluated from the previous time step, which means an additional restriction on the time step. So, time step for the current approach is experimentally chosen (i.e. maximum possible time step). Note that, the only other time step limitation appears due to the edge fluxes that are assumed to be from the previous time step (see discussion below Eq.3). In the next section, the agreement of the current approach with the established explicit LCG, along with speed of calculations is investigated.

3. Results

The governing equations are solved over 63 arterial segments as shown in Figure 1. All properties corresponding to the network can be found in [1, 2]. We plot the pressure and flow at three different locations along the aorta, where the monitoring points are set at the middle of each segment (segments numbers are: 9, 35 and 47 respectively) as shown in Figure 2. The time step is set as 0.3 ms, while spatial
step is taken as 0.5 cm and a total of 3151 elements are used. The corresponding maximum CFL number is 1.104. We have developed a new numerical approach that removes convergence issues associated with large matrices and allows us to use the basic version of Newton method. The classical Newton method in which the matrix $J(U^k)$ is solved at every single iteration if the first approach we used. In the second approach (legend SILCG 2) the matrix solution is obtained at every time step regardless of number of iterations. As expected the second case is much faster. The CPU time used by the first case was 512 s and the second case was 161 s per cardiac cycle respectively. Figure 2 clearly demonstrates that both cases are accurate when compared against the explicit method given by [1, 2]. In addition, the cost of calculations is highlighted in Figure 3 for both cases. As seen, both cases have almost identical convergence properties where the tolerance used is $10^{-4}$. The fitted line (green centred) shows that the maximum value of iterations/elements ratio is less than 0.5.

Figure 1: Configuration of the arterial tree for the current model [1].

Figure 2: Pressure and flow variation along the aorta.
4. Conclusions

A SILCG method has been developed for a human circulatory system. The solution is obtained by using Newton method in which the governing equations have been solved over 63 arterial segments. The flux continuity is ensured by enforcing fluxes over elements edges. The proposed approach shows implementation simplicity in dealing the non linear system and resolves the poor convergence issues by solving the system element by element. This makes Newton solver robust and easy to use. The accuracy is comparable to that of the well established explicit LCG method as the approach relaxes the explicit time step restriction. Further examination is required in order to determine the actual time step limit of the proposed method.

References


BLOOD FLOW SIMULATION USING SMOOTH PARTICLE HYDRODYNAMICS

Mohammed K. AL-SAAD¹², Sivakumar Kulasegaram³ and Stephane P.A. Bordas⁴

¹School of Engineering, Cardiff University
Cardiff University, Queen’s Buildings, the Parade, CARDIFF CF24AA,
²Collage of Engineering, BasraUniversity
Karmat Ali, Basra, IRAQ
³School of Engineering, Cardiff University
Cardiff University, Queen’s Buildings, the Parade, CARDIFF CF24AA,
⁴School of Engineering, Cardiff University
Cardiff University, Queen’s Buildings, the Parade, CARDIFF CF24AA,

SUMMARY

To understand the characteristics of blood flow, it is important to identify the key parameters that influence the flow of blood. The characterisation of blood flow will also enable us to understand the flow parameters associated with physiological conditions such as atherosclerosis. Thrombosis plays a crucial role in atherosclerosis and it also helps to stop bleeding when a blood vessel is injured. This article focuses on using a meshless particle-based Lagrangian numerical technique, named the smoothed particles hydrodynamic (SPH) method, to study the flow behaviour of blood and to explore the flow conditions that induces the formation of thrombus in a blood vessel. Due to its simplicity and effectiveness, the SPH method is employed here to simulate the process of thrombogenesis for various blood flow parameters. In the present SPH simulation, blood is modelled by particles that have the characteristics of plasma and of platelets. To simulate the coagulation of platelets which forms thrombus, the adhesion and aggregation processes of the platelets are modelled by an effective inter-particle attraction force model. With these models, the motion of platelets in flowing blood, and their adhesion and aggregation are effectively coupled with viscous blood flow. In this study, the adhesion and aggregation of blood particles are analysed on a (straight tube vessel) under various low Reynolds number scenarios. The results are compared with the experimental results, and a good agreement is found between the simulated and experimental results.

Keywords: smooth particle hydrodynamics (SPH); blood flow; thrombus; arteries

1 INTRODUCTION

A thrombus is considered to be one of the most important causes of many diseases in human body. On the other hand, A blood clot anchored to a damaged vascular wall can stop bleeding or it can prevent atherosclerosis in arteries. The danger is that a thrombus can affect the blood flow in the vessels and this can cause potentially deadly accidents, such as cardiac infarction (or heart attack) or ischemic stroke when the damage occurs in the coronary or the carotid arteries, respectively. The formation of a thrombus depends on platelet flow; for example, the transport to denuded subendothelium, formation of membrane tethers, adhesion to the subendothelium, and aggregation. Many experimental studies have provided information on the biochemical effects of fluid forces on thrombogenesis. In recent years, due to the availability of vast computational power, research on computer simulation of thrombosis has become a field of deep interest. Although fluids can be simulated in either the Eulerian or Lagrangian method, the Lagrangian method is considered to be more suitable for this type of simulation due to their obvious advantages in tracking movement of particles similar to platelets[1]. The purpose of this study is to analyse flow parameters that influence the formation of thrombosis inside arteries. A Lagrangian smooth particles hydrodynamics (SPH) is used for numerical simulations of the blood flow consisting plasma and platelets.
2 NUMERICAL METHODOLOGY

The governing equations for solving incompressible or weakly compressible isothermal fluid flow using SPH are mass and momentum conservation equations given by,

$$\frac{1}{\rho} \frac{Dp}{Dt} + \nabla \cdot \mathbf{v} = 0; \quad \frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v} + \mathbf{F} \tag{1}, \tag{2}$$

Where \(\rho\), \(t\), \(v\), and \(p\) represent the density, time, kinematic viscosity, velocity and pressure of the fluid particles and, \(\mathbf{F}\) represents the external force acting on fluid particles. The fluid pressure for weakly compressible SPH formulation is obtained by an equation of state as presented in [2]. The numerical procedure to calculate fluid velocity is derived from the momentum equation (2) as,

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \left( -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v}^n + \mathbf{F} \right) \Delta t \tag{3}$$

Where superscript \(n\) and \(n + 1\) refer to current and next time steps, respectively, and \(\Delta t\) is the numerical time step. The position and density of the fluid can be updated respectively at every time step by,

$$\mathbf{x}^{n+1} = \mathbf{x} + \mathbf{v}^{n+1} \Delta t, \tag{4}$$

and (from the continuity equation (1)),

$$\rho^{n+1} = \rho^n - \rho^n (\nabla \cdot \mathbf{v}^{n+1}) \Delta t. \tag{5}$$

The pressure is then estimated from the updated density.

3 MODELLING PLATELET MOTION

The platelets tend to adhere and aggregate when the blood vessel is damaged. This can lead to formation of a primary thrombus. Inside the primary thrombus the neighbour platelets link together, which are then bound by vWF fibrinogen in plasma and collagen in the sub-endothelial tissue [3]. This process takes place by making a link between neighbouring platelets and bound by vWF fibrinogen in plasma and collagen in the sub-endothelial tissue. To numerically model such platelet motion, an algorithm based on a penalty or spring force mechanism [4] is adopted. This model dictates the interactions between platelets and plasma inside the blood vessel. When the platelets are within a distance \(d_{ad}\) from the damaged area, the platelets are attracted towards the damaged wall by an adhesive force given by eq. (6). The platelets adhering to the wall are then activated and attract other platelets which are within a distance of \(d_{ag}\) from them. This attractive force is called an aggregation force which is given by eq. (7). The aggregation force takes the same form as that of the adhesive force but has a different spring constant.

$$\mathbf{F}_{ad} = \begin{cases} K_{ad}(|\mathbf{r}_{ij}| - r_0)n_{ij} & (|\mathbf{r}_{ij}| \leq d_{ad}) \\ 0 & (|\mathbf{r}_{ij}| > d_{ad}) \end{cases}; \mathbf{F}_{ag} = \begin{cases} K_{ag}(|\mathbf{r}_{ij}| - r_0)n_{ij} & (|\mathbf{r}_{ij}| \leq d_{ag}) \\ 0 & (|\mathbf{r}_{ij}| > d_{ag}) \end{cases} \tag{6}, \tag{7}$$

In the above equations \(\mathbf{F}_{ad}, \mathbf{F}_{ag}\) are the adhesive and aggregate forces and \(K_{ad}, K_{ag}\) are the corresponding spring constants. The \(\mathbf{r}_{ij}\) here is distance between activated platelet and vessel wall (or other non-activated platelets), \(r_0\) is the original or natural length of the spring and \(n_{ij}\) is a unit vector linking platelet and damaged wall (or linking activated platelet and other surrounding platelets). These two forces are introduced in equation (2) for platelet particles which are influenced by adhesion and aggregation.

4 BLOOD FLOW MODEL

In this work, the blood flow simulations were performed inside a straight blood vessel with constant velocity of blood flow (i.e. 100, 500 and 700 \(\mu\)m/s), which were defined at the inlet entrance of the tube. The total length of the vessel \((L)\) and the width between two walls \((D)\) are respectively 500 \(\mu\)m and 50 \(\mu\)m. The dimensions of the damaged wall \((L_o)\) is 30 \(\mu\)m (refer to the length of the wall damage) and the distance from the inlet to the damaged wall \((L_o)\) is 40 \(\mu\)m (see
Four layers of boundary dummy particles were also used. The initial distance between particles is 1.0 μm. The density $\rho$ and kinematic viscosity $\nu$ of the plasma and platelets, were set as $\rho = 1 \times 10^3 \text{kg/m}^3$ and $\nu = 1 \times 10^{-6} \text{m}^2/\text{s}$. The boundary conditions were: a uniform velocity at the inlet, zero pressure at the outlet and, non-slip condition at the walls enforced by dummy boundary particles. The amount of the platelet particles used is approximately 0.336% of the plasma to resemble normal physiological condition. The time step was set to $5 \times 10^{-7}$ s to ensure the stability of numerical integration scheme. In the reported numerical simulations, the spring constants $K_{ad}$ and the $K_{ag}$ are $9.0 \times 10^9 \text{N/m}$ and $4.5 \times 10^9 \text{N/m}$ respectively, while $d_{ad} = 2 \mu\text{m}$, $d_{ag} = 4 \mu\text{m}$, and $r_o = 2.0 \mu\text{m}$.

## 5 RESULTS

The purpose of this study is to demonstrate the formation of thrombus in 3-dimensions and to investigate the applicability of SPH in modelling such process. The corrected SPH is used to improve the accuracy [5] of the simulation. Normally, a thrombus is formed by adhesion and aggregation of platelets which are transported by the blood flow in different geometries of arteries or vessels, where the growth rate of thrombus formation varies with the stenosis and the flow rate of blood. Figure 1 illustrates the formation of thrombus at two different stages of the flow. In these figures, for clarity, here plasma has been hidden while platelet particles show by two different colours to the activated and non-activated platelets. The platelets particles denote by light and dark spheres for non-activated and activated particles respectively. The platelets are activated when they are within $d_{ad}$ distance from the damaged region and form a primary thrombus. During the course of time, a primary thrombus is developed to cover the whole damage area by forming several layers of platelets. When thrombus grows to a certain volume, part of the thrombus is separated and transported downstream by the blood flow. Figure 1 depict the growth of thrombus at different times for varies velocities. From the figures below, various stages of thrombus growth on the damaged area of the wall are clearly evident. It can be noted from Fig. 1 the primary thrombus grows to a substantial volume. It transpires from Fig. 2 that the growth rate of thrombus gradually increases with blood velocity until approximately 500 μm/s. Beyond 500 μm/s, the thrombus growth rate drops to a lower level as in 700 μm/s. It is interesting to observe that the volume of the primary thrombus is affected by the flow rate. From this figure, it can be concluded that the higher the flow rate the thinner the thrombus growth would be. The results are consistent with experimental observations reported in[6].

![Figure 1: The platelet aggregation in the time 10s at (a) $V=500 \mu\text{m}/\text{s}$; (b)$V=700 \mu\text{m}/\text{s}$](image)
6 DISCUSSION

The influence of changing hemodynamics on the platelet transport and thrombus formation was investigated using SPH. The formation and subsequent behaviour of thrombus at various blood flow rates were analysed by numerical simulations. It is evident from the results above that the blood flow rate plays a crucial role in the build-up and separation of thrombus. The results show that the growth rate of the thrombus, its thickness, and formation vary according to the blood flow rate. These results are consistent with the observations reported in [6].

7 CONCLUSIONS

This work has focused on the simulation of the thrombogenesis process in 3-D using the SPH method by considering platelet aggregation and the influence of blood flow rates on thrombus growth. In the numerical simulations, blood inside a straight tube vessel is discretised by particles which are assumed to have the characteristics of blood constituents, such as plasma and platelets. The potential of SPH method to simulate thrombogenesis process is demonstrated via numerical examples. This study also demonstrates the ability and accuracy of the SPH method in modelling blood flow with different velocities.

REFERENCES


NUMERICAL ANALYSIS OF BONE REMODELLING FOR EQUINE 3rd METACARPAL

*Karol Lewandowski¹,², Łukasz Kaczmarczyk¹, John F. Marshall² and Chris J. Pearce¹

¹School of Engineering, The University of Glasgow, Glasgow, UK, G12 8LT
²School of Veterinary Medicine, The University of Glasgow, Glasgow, UK, G61 1QH

*k.lewandowski.1@research.gla.ac.uk

ABSTRACT

The aim of this study was to realistically simulate density growth in the equine 3rd metacarpal bone (MCIII), the most frequently fractured lower limb bone in the Racehorse. A well-established open system thermodynamics approach was adopted into a hierarchical approximation framework. This allowed for an efficient construction of multigrid iterative solvers and solving large problems in 3D including entire bones with their complicated structure. The coupled nonlinear governing equations of mass and linear momentum conservation were implemented in finite element code MOFEM, where tangent stiffness matrix was acquired automatically by using ADOL-C library. Its performance was demonstrated with classical benchmark problems. In order to accurately represent geometry, the final numerical model of the equine bone was generated by processing CT scan images. Furthermore, simplified boundary conditions corresponding to peak forces at mid-stance of a gallop were applied to the bone surface. The obtained density pattern was validated by comparison with the CT scanning data from a cadaver racehorse metacarpal bone. It was shown that the method has the potential to accurately model the effect of loading on bone and could be applied to future studies in order to prevent fatal injuries.

Key Words: finite element analysis; hierarchical approximation; bone remodelling; racehorse; 3rd metacarpal

1. Introduction

Bones are able to adapt their local density when subjected to mechanical loading. They can change their morphology within days as a result of continuous microstructural tissue turnover and regeneration. Such an adaptation process results in densification of the bone in regions of high loading levels and in resorption of the material in regions of low loading levels. This process is especially essential for racing horses. Due to their intensive training, high tissue accumulation in the distal condyle of metacarpal bones results in the suppression of bone regeneration. This often leads to fatigue fracture, the most commonly reported in the UK during both racing and training [1]. Moving forward, the objective of our study is to develop an efficient diagnostic tool that could help to estimate the risk of fatal injuries by means of finite elements analysis. This paper presents the application of open system thermodynamics approach for functional adaptation in response to external loading. This well-established method was embedded into hierarchical approximation framework of finite element code MOFEM [2]. Derivation of the balance equations was briefly summarised. Application of automatic differentiation with ADOL-C library simplified the derivation of stress tensors and tangent stiffness matrix. Next, a computational solution of a simple one-dimensional problem was presented. It proved that basic functional adaptation assumptions were fulfilled with this approach. Subsequently, three-dimensional model of entire bone was generated, the analysis of which yielded a density pattern at equilibrium state that was then compared with CT scan data from a horse in training for quantitative validation.

2. Modelling of density growth

2.1. Governing equations

When investigating biological material, density can change in time as opposed to classical mechanics wherein the material density ρ is conserved within a given body. Following Kuhl and Steinmann [3]
it is assumed that its evolution is driven by the free energy $\psi_0$ as described by the biological equilibrium equation:

$$\frac{\partial \rho_n}{\partial t} = R_0,$$

where $R_0 = c \left[ \frac{\rho_0}{\rho_n} \right]^{-m} \psi_0 - \psi_0^*$ (1)

which represents the balance of mass with $R_0$ - mass source that accounts for density changes. The constant $c$ characterizes the speed of adaptation, $n$ and $m$ are two characteristic exponents, $\rho_0$ is the reference density and $\psi_0^*$ is the reference free energy, also known as the biological stimulus. To complete the model, an equation of the mass specific free energy density was introduced as the elastic free energy of Neo-Hookean type $\psi_{\text{neo}}$, weighted by the relative density:

$$\psi_0 = \left[ \frac{\rho_0}{\rho_n} \right] \psi_{\text{neo}}^*, \quad \text{where } \psi_{\text{neo}}^* = \frac{\mu}{2} (\text{tr}(C) - 3) - \mu \ln(J) + \frac{\lambda}{2} \ln J^2,$$

with $J^2 = \det(C)$ (2)

For porous materials, the exponent $n$ typically varies between $1 \leq n < 3.5$. Specifically the MCIII bone exponent $n$ was based on mechanical testing by Les (1994) [4]. Although bones undergo only small deformations, theory for adaptation was generalised into finite strains. Therefore, free energy was parametrised in terms of right Cauchy-Green deformation tensor $C = F^T F$, where $F$ is a deformation gradient ($F = \nabla u$). Moreover, $\lambda$ and $\mu$ are the two Lamé parameters. The free energy equation (2) defines the Piola stress $P$ that enters the conservation of momentum equation as:

$$\text{Div}(P) = 0$$

With both balance equations at hand, residuals for non-linear solver can be calculated. In this study, tangent stiffness matrix was derived with ADOL-C automatic differentiation - first by deriving 2nd Piola stress tensor $S$ from $\partial \psi / \partial C$ and then calculating the derivative $\partial S / \partial C$. Calculations with ADOL-C were in agreement with analytical solutions. As the evolution of the density $\rho_n^{n+1}$ at time $t^{n+1}$ is governed by the balance of mass (1), an implicit Euler backward scheme was used for time discretization. Summarised algorithm is shown in the table below.

<table>
<thead>
<tr>
<th>Loop over all time steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nonlinear solver iteration</td>
</tr>
<tr>
<td>Loop over all elements</td>
</tr>
<tr>
<td>Loop over all integration points</td>
</tr>
<tr>
<td>evaluate balance of mass and momentum</td>
</tr>
<tr>
<td>evaluate residuals and their partial derivatives</td>
</tr>
<tr>
<td>evaluate $R^n, R^\nu, K^{\nu \nu}, K^{\nu \nu}, K^{\nu \nu}$</td>
</tr>
<tr>
<td>global residuals and iteration matrices</td>
</tr>
<tr>
<td>biological equilibrium</td>
</tr>
</tbody>
</table>

Table 1: Computational algorithm for monolithic solution approach.

2.2. Benchmark problem

To depict the features of open system thermodynamics approach, a simple homogeneous bar of unit size is presented here. The following parameters were used: elasticity modulus $E = 1$, Poisson’s ratio of $\nu = 0$. The reference density was chosen to be $\rho_0 = 1$ and energy stimulus was $\psi_0 = 1$. To ensure uniqueness and stability of the solution, exponents of growth were $m = 3$ and $n = 2$. Time integration was performed with time steps of $\Delta t = 0.1$. The specimen was axially loaded by multiple step loading function as illustrated in Figure 1 below. The corresponding deformation proves the non-linearity of the problem. The time dependent nature of the balance of mass was visualised. Curves of primary unknowns demonstrated the relaxation towards biological equilibrium, the state when density converged to a final value for particular loading magnitude.
Figure 1: One-dimensional model problem. Evolution of density $\rho_0$, displacements $u$ and energy values $\psi$ and relative energy $\left[\rho_0/\rho^*\right]^{-m} \psi$.

3. Numerical example

Proposed density growth model was subsequently applied to a subject-specific three-dimensional, full-scale model of equine MCIII bone derived from CT scanning. Initial density distribution was homogeneous in this study. However, developed code has a capability of mapping density data into finite element mesh. Segmented geometry was discretised into 7255 high quality (shape ratio $> 0.3$) quadratic tetrahedrons. $2^{nd}$ order geometry elements were used for high-detail representation as shown in Figure 2. Boundary conditions have been simplified to two representative forces (5 kN each) spanning over a small area based on pressure film studies by Brama (2001) [5]. They are often considered as an equivalent of peak force at the mid-stance of a horse gait. Furthermore, degrees of freedom at the proximal end were fixed. In reality, metacarpal bone articulates with proximal phalanx bone, which will be the subject of future contact mechanics studies. The analysis was divided into 100 time steps with the constant time step size of $\Delta t = 0.5$ [d]. External forces were applied by linearly increasing their magnitude within first 5 time steps and held constant thereafter. Material and model parameters (Table 2) were adopted based on previous studies of human bones [6]. Higher stiffness of equine bones derived from mechanical testing studies [4] was also taken into account. Results of the analysis are presented in Figure 2b where density maps at four different points in time (0, 10, 20, 30) [d] are visualised. Great densification occurred just after reaching maximum level of the loading, particularly in the proximity of applied forces, where the high levels of strain energy were expected. In the areas not affected by the loading, material degradation can be observed. After time 30 density levels on entire bone became saturated, biological equilibrium was achieved, hence no changes appeared thereafter. At this point, density was measured in the region of the sagittal grooves as demonstrated in Figure 2c, the most frequent site of a fracture initiation in MCIII bone. Simultaneously, the density of bone in the same region of a horse in training was derived from the CT scan using quantitative computed tomography with appropriate (dipotassium phosphate) phantoms.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$</td>
<td>Poisson ratio</td>
<td>0.3 [-]</td>
</tr>
<tr>
<td>$\rho_0'$</td>
<td>Initial density</td>
<td>1.0 [g/cm$^3$]</td>
</tr>
<tr>
<td>$\psi_0'$</td>
<td>Target energy</td>
<td>0.0275 [MPa] Waffenschmidt (2012) [6]</td>
</tr>
<tr>
<td>$c$</td>
<td>Density growth velocity</td>
<td>5.0 [d/cm$^3$]</td>
</tr>
<tr>
<td>$m$</td>
<td>Algorithmic exponent</td>
<td>3.35 [-]</td>
</tr>
</tbody>
</table>

Table 2: Material parameters used for the simulations.
Figure 2: a) Geometry of the distal end of the MCIII bone and finite element mesh with applied concentrated forces. b) Density evolution in the proximal tibia at four different points in time. c) Variation of bone mineral density in the region of interest derived from FEM and CT.

Subsequently, both resultant data were compared and found to be in satisfying agreement.

4. Conclusions

Despite certain limitations of this study, it showed that a reasonable agreement with experimental data can be achieved. Using the theory of open systems thermodynamics allowed to simulate natural behaviour of hard biological tissues. It is believed that results can be greatly refined by improving many aspects of this approach, like more accurate boundary conditions and taking anisotropy of density growth into account. The proposed computational method may have a great potential to identify the risk of fracture related to changes in bone mineral density.

Acknowledgements

The authors are particularly grateful to the staff of the Small Animal Hospital, where the CT scans of the equine metacarpal bone were performed. Lord Kelvin Adam Smith PhD Scholarship is acknowledged for providing financial support.

References


A POLYCONVEX COMPUTATIONAL FORMULATION FOR ELECTRO-ACTIVATION IN CARDIAC MECHANICS

Emilio García-Blanco, Antonio J. Gil, Rogelio Ortigosa and Chun Hean Lee

Zienkiewicz Centre for Computational Engineering, College of Engineering, Swansea University, SA1 8EN

\{840559 ; a.j.gil ; r.ortigosa ; c.h.lee\}@swansea.ac.uk

ABSTRACT

Cardiovascular diseases, such as heart infarction or dysrhythmia, represent the main cause of death in the world and its prevalence is more significant in developed countries. This is one of the reasons behind the increasing scientific interest over the last decade in the computational modelling of the complex physical phenomena occurring in the human heart, as computational tools can facilitate a better understanding of the mechanisms driving the behaviour of the system from both physiological and pathological standpoints.

The computational modelling of the heart requires the solution of two coupled Partial Differential Equations (PDEs), namely the conservation of linear momentum and the evolution of the uprisings electric potential. Two models can be used capturing the influence of the latter on the mechanics of the heart, namely active stress or active strain. The second PDE is a reaction diffusion type equation governing the evolution of the electric potential. The complexity of this equation resides on its source term, which embeds the cellular ion exchange. Two models have been used in this work for this source term, namely the Minimal model and the Ten-Tusscher model. From the discretisation standpoint, following the work of Gil and Ortigosa in the context of nonlinear electro-elasticity, this work presents a novel mixed Finite Element formulation which overcomes drawbacks inherent to classical displacement-based formulations, namely volumetric and shear locking, spurious pressure oscillations, etc. A numerical example is presented in order to assess the robustness and accuracy of the proposed formulation.

Key Words: cardiac electromechanics; mixed formulations; polyconvexity; finite elements

1. Introduction

Computational modelling is playing an increasingly relevant role in the area of cardiovascular medicine by, for example, providing augmented simulation-based diagnosis tools for patients or innovative surgery techniques for clinicians. Computational modelling must take into account the complex chemo-electro-mechanical coupled phenomena (modelled by means of phenomenological models) taking place across a wide range of scales in the human heart. However, reliability of the results obtained can be compromised even if these phenomena are perfectly characterised. Specifically, the challenges associated with this specific problem (nearly incompressibility of the human heart, strongly anisotropic behaviour, etc.) demand robustness and accuracy from the numerical formulation. The latter features can be seriously compromised specially for low order displacement-based Finite Element formulations, which surprisingly, are very commonly used among researchers in this area. The objective of this paper is to present a novel mixed Finite Element formulation which does not compromise accuracy or robustness.

2. Heart Mechanics

The complex anatomy of the cardiac tissue consists of two sets of helicoidal muscle bands that allow ventricles to contract sequentially. The conservation of linear momentum determines the equilibrium configuration of these bands, and is expressed as

$$\nabla_0 \cdot P + b_0 = 0,$$

where $b_0$ represents a body force and $P$, the first Piola-Kirchhoff stress tensor, related to the strain energy of the cardiac tissue $\Psi$, embedding its mechanical constitutive behaviour. The later must account for the anisotropic structure of the heart tissue, consisting of muscle cells embedded in collagen layers oriented
in preferred directions denoted as \( \{ f_0, s_0, n_0 \} \) (in the material or Lagrangian setting) as shown in Figure 1. Therefore, it is customary to additively decompose the strain energy \( \Psi \) into isotropic and anisotropic contributions. The isotropic contribution is further additively decomposed into an isochoric term \( \Psi^\text{iso}(F) \) (with \( F = \nabla_0 x \) the deformation gradient tensor) and a purely volumetric term \( U(J) \) (with \( J = \det F \)). Finally, the anisotropic contribution, namely \( \Psi^\text{ani} \), must depend on invariants of \( F \) (or more appropriately \( C \) to guarantee material frame indifference) and on the fibres \( \{ f_0, s_0 \} \), namely

\[
\Psi(F) = \Psi^\text{iso}(F) + U(J) + \Psi^\text{ani}(F, f_0, s_0) .
\]

(2)

**Isotropic contribution \hspace{1cm} Anisotropic contribution**

![Figure 1: Internal anisotropic structure of the cardiac walls. Representation of the preferred directions in the spatial or Eulerian setting \( \{ f, s, n \} \), with \( \{ f, s, n \} = \{ F f_0, F s_0, F n_0 \} \).](Image)

For example, let us consider the classical invariant-based representation of the strain energy proposed by Holzapfel [5]. For this energy, each of the terms introduced in equation (2) are

\[
\Psi^\text{iso}(F) = \frac{a}{2b} e^{b \cdot \langle F^{-3} \rangle} ; \hspace{1cm} U(J) = \frac{k}{2} (J - 1)^2 ;
\]

\[
\Psi^\text{ani}(F, f_0, s_0) = \frac{af}{2bf} \left( e^{bf_0} (F f_0 F f_0^{-1})^2 - 1 \right) + \frac{as}{2bs} \left( e^{bs} (F s_0 F s_0^{-1})^2 - 1 \right) + \frac{af s}{2bf s} \left( e^{bf s} (F f_0 F s_0)^2 - 1 \right) .
\]

(3)

(4)

where \( \langle \bullet \rangle \) denotes the Macaulay brackets. In order to ensure that the strain energy leads to a physically meaningful behaviour, this must satisfy certain convexity criteria which guarantee the ellipticity condition. The latter is automatically satisfied by polyconvex [6] energy functionals. The strain energy \( \Psi^\text{ani}(F) \) is polyconvex if can be written as

\[
\Psi(\nabla_0 x) = W(F, H, J) ; \hspace{1cm} H = \frac{1}{2} F \times F ,
\]

(5)

where \( W \) represents a convex multi-variable functional with respect to the extended set \( \{ F, H, J \} \) and with the tensor cross product operation \( \times \) between two second order tensors \( A \) and \( B \) defined as \( (A \times B)_{ij} = E_{ikmn} A_{kj} B_{mn} \) [3], with \( E \) the third order Levi-Civita tensor. It would be possible to prove that for the energy functional in (3), only the last term in \( \Psi^\text{ani} \) is non-elliptic and hence, non-polyconvex. However, loss of ellipticity induced by this sole invariant has not been investigated yet for the physiological range of deformations.

The incorporation of the electrical contribution into the constitutive model can be carried out following two approaches. In the first, denoted as active stress, a stress term along the fibres \( T_A(\phi) F f_0 \otimes f_0 \) [1] is added to the passive mechanical contribution of \( P \). In the second, denoted as active strain, a multiplicative decomposition of \( F \) into its elastic \( F^E \) and active \( F^A \) contributions is carried out as \( F = F^E F^A \). The first Piola-Kirchhoff stress tensor for both active stress and active strain is computed as

\[
P = \frac{\partial \Psi(F)}{\partial F} + T_A F f_0 \otimes f_0 ; \hspace{1cm} P = \frac{\partial \Psi(F^E(F^A))}{\partial F} = \frac{\partial \Psi(F^E)}{\partial F^E}(F^A)^{-T} ,
\]

(6)

respectively, where \( F^A \) depends upon the stretches \( \{ \gamma_f, \gamma_s, \gamma_n \} \) along the anisotropy directions as \( F^A = I + \gamma_f f_0 \otimes f_0 + \gamma_s s_0 \otimes s_0 + \gamma_n n_0 \otimes n_0 \). Evolution equations for \( \{ \gamma_f, \gamma_s, \gamma_n \} \) and \( T_A \) can be found in [2] and [1], respectively.
3. Cardiac Action Potential

Heart fibres contract as a result of the electrical stimuli initiated in the sinoatrial node and propagated over the entire tissue. This electric wave, known as cardiac action potential, alters the polarity of the cell membrane and generates a wide range of ion interchanges, leading to the eventual contraction of the cardiomyocytes. The evolution of the intermembrane electric potential $\phi$ is governed by a reaction diffusion type equation by means of the monodomain model approach as

$$\phi - \nabla_0 \cdot D \nabla_0 \phi - f_\phi = 0; \quad D = d_{\text{iso}} C^{-1} + d_{\text{aniso}} f_0 \otimes f_\phi,$$

where the source term $f_\phi$ depends upon the choice of ionic model. This consists of a set of ordinary differential equations (ODEs) for the gate variables $w$ and several ion concentrations $c$ (Figure 2), treated as internal variables (see equations (8)$_b$ and (8)$_c$). Two models are considered: the exhaustive Ten Tusscher model and the computationally fast and synthetic Bueno-Orovio model, also known as Minimal model. The set of ODEs enables to compute the several ion currents or intensities $I$, which together with $I_{\text{stim}}$ allows to compute the expression for the source term $f_\phi$ as

$$f_\phi(\phi, w, c) := \sum I(\phi, w, c) + I_{\text{stim}}: \quad \dot{w} = g(\phi, w, c); \quad \dot{c} = h(\phi, w, c).$$

Figure 2: Left: voltage variation on a cell. Right: arrhythmic waves by Bueno-Orovio and Ten Tusscher models.

4. Numerical Solution

Following the work of Gil and Ortigosa [3, 4], a new robust and accurate mixed formulation is presented for the numerical simulation of an idealised set of ventricles. In this formulation, displacement $u$, electric potential $\phi$, pressure $p$ and a set of additional fields are part of the unknowns of the problem. The latter include a set of variables $L$, comprising of $\{F, H, J, A\}$ (where $A$ represents a vector field) and its associated set of work conjugates $\Sigma_L$, comprising of $\{\Sigma_F, \Sigma_H, \Sigma_J, \Sigma_A\}$. The proposed formulation includes an extended set of weak forms, including the governing equations of the coupled electromechanical problem, the compatibility and the constitutive equations. The governing equations are expressed as

$$T_\phi := \int_{\Omega_0} \delta \phi \frac{\partial \phi}{\partial t} d\Omega_0 + \int_{\Omega_0} \nabla_0 \delta \phi \cdot \Sigma_A \phi d\Omega_0 - \int_{\partial\Omega_0} \delta \phi N \cdot D \nabla_0 \phi d\Gamma - \int_{\Omega_0} \delta \phi f_\phi d\Omega_0 = 0;$$

$$T_u := \int_{\Omega_0} \nabla_0 \delta u : P d\Omega_0 + \int_{\Omega_0} \delta u \cdot b_0 d\Omega_0 - \int_{\partial\Omega_0} \delta u \cdot t_0 d\Gamma = 0;$$

$$T_p := \int_{\Omega_0} \delta p (J - 1) d\Omega_0 = 0,$$

where $t_0$ represents a surface traction. Moreover, $P$ is expressed for both active strain and stress approaches in terms of the work conjugates as

$$P := \Sigma_F + \Sigma_H \times F_x + (\Sigma_J + p) H_x; \quad P := \Sigma_F + \Sigma_H \times F_x + (\Sigma_J + p) H_x + T_A F_x f_0 \otimes f_0,$$

where $\{F_x, H_x\}$ represent the kinematically admissible strain measures, namely $\{F_x, H_x\} = \{\nabla_0 x, \frac{1}{2} \nabla_0 x \times \nabla_0 x\}$. The weak form of the compatibility and constitutive equations are written as

$$T_{\Sigma_L} := \int_{\Omega_0} \delta \Sigma_L \cdot (L_x - L) d\Omega_0 = 0; \quad T_L := \int_{\Omega_0} \delta L \cdot \left( \frac{\partial W}{\partial L} - \Sigma_L \right) d\Omega_0 = 0,$$

65
where $L_x$ represents the set $\{F_x, H_x, J_x, \nabla \phi\}$. A consistent linearisation of the above set of weak forms has been carried out in this work, leading to quadratic convergence of the Newton-Raphson algorithm. For the Finite Element discretisation of the above set of weak forms, the following functional spaces have been chosen for the different fields included in the formulation: continuous quadratic interpolation of $u$ and $\phi$, constant interpolation of $p$, piecewise (discontinuous) linear interpolation of the conjugate pairs $\{F, \Sigma_F\}$, $\{H, \Sigma_H\}$ and $\{A, \Sigma_A\}$ and constant interpolation of $J$ and $\Sigma_J$. A static condensation procedure has been carried out to condense out all those discontinuously interpolated fields. Therefore, the resulting formulation has a computational cost comparable to that of a $u$-$p$-$\phi$ formulation. As an example, the new formulation has been tested for the analysis of a set of idealised ventricles (Figure 3).

![Simulation of a heartbeat with a 61,320 dofs mesh using the presented mixed-variable formulation and adaptive time-step ($\Delta t_{\text{min}} = 10^{-4} \text{s}, \Delta t_{\text{max}} = 10^{-2} \text{s}$). From left to right: $A_{yz}, F_{yz}, H_{yz}$ and $\phi$ for $t = 0.025 \text{s}$.](image)

As a result, the two-way electromechanical coupling has been successfully implemented and our simulated heartbeat, although modelled in an idealised geometry, shows a convincing reproduction of both deformation and electric wave propagation. The computing time is kept at a reasonable level thanks to the implementation of adaptive time-step and coarser meshes without compromising the accuracy.

5. Conclusions and Further Work

These results evidence a better capture of deformation and pressure fields in comparison with existing computational methodologies [1, 2], even though coarser meshes were considered. However, the utilisation of subjected to availability real human ventricle meshes remains an unresolved task in this paper that will be fulfilled in forthcoming works, pursuing the perfect match of both virtual and real hearts.

References


Cell force identification

Łukasz Kaczmarczyk\(^1\), Karol Lewandowski\(^1\), Manuel Salmeron-Sanchez\(^1\) and Chris Pearce\(^1\)

\(^1\)School of Engineering, University of Glasgow, Glasgow, Scotland

*łukasz.kaczmarczyk@glasgow.ac.uk

ABSTRACT

This paper presents a method for identification of cell forces. We propose both a local and non-local method. The former assumes rotation free field of surface tractions, while the latter introduces an intrinsic length scale parameter, such that cells can locally apply a moment on the material surface. This paper focuses attention on a numerical aspect of force identification without investigating, at this stage, the true nature of that forces.

Key Words: Force identification, Finite elements

1. Introduction

The forces exerted by living cells on a surface can be identified experimentally by observing displacements in the material. These displacements can, for example, be measured by tracking beads embedded in a flexible gel substrate on which the cells are cultured.

This work builds on a substantial number of papers on force identification, and in particular the calculation of forces exerted by cells. For example [1], where a semi-analytical approach is used, applying the fundamental solution to construct an objective function which is minimised to find cell tractions. In [1], the solution space is transformed using a Fourier transform so that the problem can be solved efficiently. In this paper, a similar approach to the one proposed in [2] is used, overcoming the limitations of the method proposed in [1], where here finite element method can be used. Such an approach enables heterogeneous materials, nonlinear behaviour and complex geometries to be taken into account.

In the following, we analyse the displacements observed on an arbitrary surface, inside or on a body, which in general will be different from the surface where tractions are applied. In the particular problem considered here, a body is covered by a transparent thin, but stiff gel layer. Below that layer is a large volume of soft gel. The movement of beads is recorded at the interface of the two layers. No assumption is made on the homogeneity of the material and the solution scheme presented could be applied to a nonlinear material response which evolves in time, see Figure 1.
2. Local rotation-free formulation

The problem of force identification can be mathematically described by a constrained minimisation problem, as follows

\[
\begin{aligned}
\min J(u, \rho) &= \frac{1}{2} (u - u_d, S(u - u_d))_{S_u} + \frac{\epsilon_p}{2} (\rho, \rho)_{S_{\rho}} \\
\text{div}[\sigma(u)] &= 0 \quad \text{in } V \\
n \cdot \sigma(u) &= \rho \quad \text{on } S_{\rho},
\end{aligned}
\]

(1)

where \( u \) are unknown displacements in the body, \( u_d \) are observed displacements on the surface \( S_u \) and \( \rho \) are unknown tractions on the given surface \( S_{\rho} \). Note that expressions of the form \((u, v)_V\) and \((u, v)_{S_u}\) are scalar products of functions \( u \) and \( v \) in the volume \( V \) and on the surface \( S_u \) respectively. The second and third equations are constraints, expressing linear momentum conservation and balance of internal material forces with externally applied cell forces \( \rho \). Operator \( S \) in the first term in equation (1) is a penalty controlling how well displacements in the body \( u \) satisfy measured displacements \( u_d \). For simplicity, \( S \) can be understood as a diagonal matrix scaled by a penalty parameter \( \epsilon_p \). The second term in the objective function controls tractions \( \rho \) and is required to ensure that the problem is well posed. Applying the standard Lagrange multiplier method, we get

\[
\begin{aligned}
\min J(u, \rho, \Upsilon) &= \frac{1}{2} (u - u_d, S(u - u_d))_{S_u} + \frac{\epsilon_p}{2} (\rho, \rho)_{S_{\rho}} + (\Upsilon, \text{div}[\sigma])_V \\
n \cdot \sigma(u) &= \rho \quad \text{on } S_{\rho},
\end{aligned}
\]

(2)

where \( \Upsilon \) is the Lagrange multiplier. Differentiating the first equation by parts and using the second constraint, leads to:

\[
J(u, \rho, \Upsilon) = \frac{1}{2} (u - u_d, S(u - u_d))_{S_u} + \frac{\epsilon_p}{2} (\rho, \rho)_{S_{\rho}} + (\Upsilon, \text{div}[\sigma])_V - (\Upsilon, \rho)_{S_{\rho}}.
\]

(3)

where the Neumann boundary condition is enforced in a weak sense. Expressing the material relationship as follows

\[
\sigma = \mathcal{A} (\text{grad}[u])^s
\]

(4)

and using the symmetry of operator \( \mathcal{A} \), we get

\[
J(u, \rho, \Upsilon) = \frac{1}{2} (u - u_d, S(u - u_d))_{S_u} + \frac{\epsilon_p}{2} (\rho, \rho)_{S_{\rho}} + (\Sigma, \text{grad}[u])_V - (\Upsilon, \rho)_{S_{\rho}}
\]

(5)

were \( \Sigma = \mathcal{A} (\text{grad}[\Upsilon])^s \). Finding the minimum of (5), we get the Euler equations in the following form

\[
\begin{aligned}
(\delta u, \delta u)_{S_u} + (\Sigma, \text{grad}[\delta u])_V &= 0 \\
(\sigma, \text{grad}[\delta \Upsilon])_V - (\rho, \delta \Upsilon)_{S_{\rho}} &= 0 \\
(\epsilon_p \rho, \delta \rho)_{S_{\rho}} - (\Upsilon, \delta \rho)_{S_{\rho}} &= 0
\end{aligned}
\]

(6)

Applying finite element discretization, the above equations are expressed as a system of linear algebraic equations, suitable for computer analysis

\[
\begin{bmatrix}
S & K_{\Upsilon u} & 0 \\
K_{\Upsilon u} & 0 & -B^T \\
0 & -B & D
\end{bmatrix}
\begin{bmatrix}
u \\
\Upsilon \\
\rho
\end{bmatrix}
= \begin{bmatrix}
Su_d \\
0 \\
0
\end{bmatrix}
\]

(7)

The field of Lagrange multipliers \( \Upsilon \) can be interpreted here as displacements in the body resulting from displacements given on the surface \( S_u \), without surface tractions present. Swapping first two rows, we finally get

\[
\begin{bmatrix}
K_{\Upsilon u} & 0 & -B^T \\
S & K_{\Upsilon u} & 0 \\
0 & -B & D
\end{bmatrix}
\begin{bmatrix}
u \\
\Upsilon \\
\rho
\end{bmatrix}
= \begin{bmatrix}
0 \\
Su_d \\
0
\end{bmatrix}
\]

(8)
The $\epsilon_u$ and $\epsilon_\rho$ are model parameters. As a rule of thumb, $\epsilon_u$ is large, and $\epsilon_\rho$ is small. Since the body only experiences forces due to the cells attached to the body surface $S_\rho$, it is not subject to rigid body motion. It is assumed that forces are generated by cells, considered here as 2D objects and, as a result, only tangential forces can be produced by those forces if the surface is planar. For non-planar surfaces additional force normal to the surface are present, and the magnitude of this force could be calculated purely from geometrical considerations. Thus, additional physical equations are not needed.

Assuming that straight and pre-stressed fibres within cells generate the forces exerted by the cell on the substrate, it can inferred that the force field is rotation-free. Therefore, these forces can be expressed in terms of a scalar potential field $\phi$ as follows

$$\boldsymbol{\rho} = \frac{\partial \phi}{\partial \mathbf{x}} \quad (9)$$

Thus, it is possible to solve for the scalar potential field, rather than the vector force field.

3. Non-local, i.e. weakly enforced rotation-free formulation

Here the generalisation of the local model to a weakly enforced rotation-free cell force field is considered. This generalisation is a consequence of the observation that cell has some small but finite size. Moreover, a cell has a complex pre-stressed structure which can transfer shear forces.

This problem is defined similarly to the local version. However, this time we add the additional non-local term,

$$\begin{align*}
\{ & \min J(\mathbf{u}, \rho) = \frac{1}{2}(\mathbf{u} - \mathbf{u}_d, S(\mathbf{u} - \mathbf{u}_d))_{S_u} + \frac{\epsilon_u}{2}(\rho, \rho - l^2\text{div}^2[\mathbf{\rho}])_{S_\rho}, \\
& \text{div}[\mathbf{\sigma}(\mathbf{u})] = 0 \quad \text{in } V \\
& \mathbf{n} \cdot \mathbf{\sigma} = \mathbf{\rho}
\} \quad (10)
\end{align*}$$

Reformulating this we have

$$\begin{align*}
\{ & \min J(\mathbf{u}, \rho) = \frac{1}{2}(\mathbf{u} - \mathbf{u}_d, S(\mathbf{u} - \mathbf{u}_d))_{S_u} + \frac{\epsilon_\rho}{2}(\rho, \rho)_{S_\rho} + \frac{\epsilon_l^1}{2}(\text{curl}^2[\mathbf{\rho}], \text{curl}^2[\mathbf{\rho}])_{S_\rho}, \\
& \text{div}[\mathbf{\sigma}(\mathbf{u})] = 0 \quad \text{in } V \\
& \mathbf{n} \cdot \mathbf{\sigma} = \mathbf{\rho}
\} \quad (11)
\end{align*}$$

where parameter $\epsilon_l$ controls the rotation-free term. As this parameter approaches zero, this formulation converges to the local variant presented above. Applying the same procedure as before, the set of Euler equations is derived

$$\begin{align*}
(\delta \mathbf{u}, \mathbf{u})_{S_u} + (\mathbf{\Sigma}, \text{grad}(\delta \mathbf{u}))_V = 0 \\
(\mathbf{\sigma}, \text{grad}(\delta \mathbf{Y}))_V - (\mathbf{\rho}, \delta \mathbf{Y})_{S_\rho} = 0 \\
(\epsilon_\rho \mathbf{\rho}, \delta \mathbf{\rho})_{S_\rho} + \epsilon_l^{-1}(\text{curl}^2[\mathbf{\rho}], \text{curl}^2[\delta \mathbf{\rho}])_{S_\rho} - (\mathbf{Y}, \delta \mathbf{\rho})_{S_\rho} = 0
\end{align*} \quad (12)$$

4. Finite element approximation

For the local version, standard piecewise continuous polynomials can be applied as an approximation basis. In general, functions approximating displacements $\mathbf{u}^h$, Lagrange multipliers $\mathbf{Y}^h$ and potential field $\phi^h$ have to belong to the standard finite dimensions Hilbert space, $H^1(V)$ for displacements and $H^1(S_\rho)$ for the potential field. Note that $\mathbold{\rho}^h$ is obtained by taking the gradient of the potential field $\phi^h$.

For the non-local version, it is required that the approximation of tractions $\mathbold{\rho}^h$ belongs to a finite vectorial space such that the tangential component of tractions is piecewise continuous, i.e. tractions belong to $H(\text{curl}, S_\rho)$ space.

In this work, complexities related to the construction of approximation spaces, integration of element matrices, problem assembly and pre- and post-processing are implemented in general purpose finite element code MoFEM [3]. Hierarchical approximation bases with an arbitrary polynomial order on the tetrahedron, prism or triangle element is used. Prism elements are used to model the very thin gel layer, see Figure 1.
5. Iterative solver and block preconditioner

In this implementation, the block structure of the matrix is utilised and solved using the PETSc block preconditioner with GEMREs solver [4]. The functionality of PETSc is enabled by the generic and multi-purpose MoFEM implementation of Discrete Manager Interface.

The problem discussed here has three unique matrices, i.e. $S$, $K$ and $B$. Such a problem can be solved efficiently applying Jacobi or Gauss-Seidel on matrix blocks or by applying Schur complement when convenient, see [5].

Utilising the capabilities of MoFEM and PETSc, the problem is decomposed on two nested sub-problems, which conveniently can be expressed by matrices $\bar{\bar{A}}$ and $\bar{\bar{X}}$, as follows,

$$\bar{\bar{A}} = \begin{bmatrix} \bar{\bar{X}} & \bar{\bar{V}} \\ \bar{\bar{H}} & \bar{\bar{D}} \end{bmatrix}, \quad \text{where} \quad \bar{\bar{X}} = \begin{bmatrix} K & 0 \\ S & K \end{bmatrix}, \quad \bar{\bar{V}} = \begin{bmatrix} -B^T & 0 \\ 0 & -B^T \end{bmatrix}, \quad \bar{\bar{H}} = \begin{bmatrix} 0 & -B^T \end{bmatrix}. \quad (13)$$

The problem associated with matrix $\bar{\bar{A}}$ is used applying Shur complement pre-conditioner, whereas the nested sub-problem associated with matrix $\bar{\bar{X}}$ is solved using block Gauss-Seidel solver. With this approach, only matrices $K$, $S$ and $B$ are stored physically in memory and matrix $K$ is only factored once. This enables efficient and robust solution for large systems, see example in Figure 2.

![Figure 2: Example of cell force identification using the non-local variant of the formulation.](image)

6. Summary

This paper has briefly introduced a methodology for identifying tractions exerted by cell forces. The unknown fields are approximated using the finite element method and solved with an iterative block solver. Three novelties are introduced in this paper. First, the method is generalised to be applied for heterogeneous (two layered) material. Second, a non-local variant is derived, and finally, an efficient and robust solution technique is proposed. Moreover, hierarchical and heterogeneous approximation bases of arbitrary order are used.

References


Contact and Error Estimation
HYPERDIMENSIONAL OFFSETS AND POLYNOMIAL REFINEMENT AND INTEGRATION SCHEME FOR HARMONIC BASIS FUNCTION FINITE ELEMENTS

*Pascal A. H. Gadoury*\(^1\) and Inna M. Gitman \(^2\)

\(^1\)Advanced Manufacturing Research Centre, University of Sheffield, Catcliffe, Sheffield, S60 5TZ
\(^2\)Dept. of Mechanical Engineering, University of Sheffield, Maplin Street, Sheffield, S1 3JD

* p.gadoury@sheffield.ac.uk

**ABSTRACT**

**Key Words:** Finite Elements; Boundary Elements; Meshing Techniques; Error Analysis & Adaptivity; Material Modelling

1. Introduction

A finite element method (FEM) formulation capable of defining arbitrary convex elements has been improved from previous work. The solution in question uses harmonic basis functions (HBFs) comprised of a weighted sum of radially symmetric fundamental solutions to the Laplace equation, or kernels, as described by Martin et al. [3]. HBFs form a suitable linear interpolation basis over the function domain, which can then be used to generate finite element shape functions within arbitrary concave elements. This flexibility makes these elements well suited to unstructured mesh problems where discontinuities may be isolated via an appropriate conformal domain partition and polynomial refinement can then be used to speed up convergence. To isolate singularities present at the centre of each kernel, it is necessary to offset the kernels away from the element domain. A new method to achieve this purpose is described in this paper which both simplifies the offset method and optimizes the condition of the HBF fitting problem. Integration schemes are examined to complete the element formulation.

2. Review of Harmonic Basis Function Elements

Harmonic basis functions are attractive as the basis for interpolation over elements because they are continuous, smooth, differentiable. With the proper Dirichlet boundary conditions, they also form a partition of unity and reproduce linear functions within the fitted solution domain [3]. As PDE’s solutions to the Laplace equations can be formulated using the method of fundamental solutions. In short, the harmonic basis functions can be expressed as follows:

\[
\zeta_i(x) = \sum_j w_{ij} \psi(\|x - k_j\|)
\]

where \(\zeta_i(x)\) is the harmonic coordinate associated with node \(i\) at position \(x\), \(w_{i,j}\) corresponds to the weights associated with node \(i\) and the radial calculation kernel function \(\psi\) centred at \(k_j\). This sum converges to the exact solution as the number of kernels along the boundary approaches infinity, but in practice, 5 kernels per edge (and a similar areal density in higher dimensions) suffice to reduce the L2 approximation error to 2-3% [3]. The kernel functions for any dimension vary solely with \(r\).

\[
\psi_{1D}(r) = r
\]
\[
\psi_{2D}(r) = \ln(r)
\]
\[
\psi_{3D}(r) = \frac{1}{r}
\]
\[
\psi_{nD}(r) = \frac{1}{r^{n-2}} \quad | \quad n > 2
\]
The weights can be solved from boundary collocation values $b_j(c_i)$ satisfying the lower-order linear HBFSs via the (possibly over-defined) following matrix equation using the SVD pseudo-inverse:

$$
\begin{pmatrix}
\psi(||c_1 - k_1||) & \cdots & \psi(||c_1 - k_n||) \\
\vdots & \ddots & \vdots \\
\psi(||c_n - k_1||) & \cdots & \psi(||c_n - k_n||)
\end{pmatrix}
\begin{pmatrix}
w_{1j} \\
\vdots \\
w_{nj}
\end{pmatrix} =
\begin{pmatrix}
b_j(c_1) \\
\vdots \\
b_j(c_n)
\end{pmatrix}
$$

In turn, weights corresponding to higher order shape functions may be subsequently calculated by inverting the Vandermonde matrix evaluating nth order monomials of these linear shape functions at each node and arbitrary midpoint. This formulation is especially useful because it makes it possible to generate an element that still conforms to domain boundaries or discontinuities all the while avoiding the mesh densities required to maintain low aspect ratio elements as a consequence of a dense surface mesh in the traditional tetrahedral meshes.

The original solution proposed by Martin et al requires kernels be offset away from the element boundary along the boundary normal by some empirical distance to isolate singularities at the kernel centres. The radius from a kernel near the boundary to a given point within the domain is given by:

$$\tilde{r}_M = ||x - \tilde{k}_M|| = \sqrt{\sum_{i=1}^{d}(x_i - k_i + \rho_M \hat{n}_i)^2}, \quad (x, k) \in \mathbb{R}^d$$

The offset $\rho_M \hat{n}$ guarantees points within the domain are some distance away from any kernel.

The replication of Martin’s results for the shape function of the corner node of a concave element is shown in Figure 1, with a variety of offset functions. It is evident within this figure that the interpolation is sensitive to the magnitude of the kernel offsets away from the element boundary. For sharp re-entrant corners, special care is also required to avoid offsetting kernels back into the element domain. Schemes to implement mitred offsets have been examined, for instance, and variable offset distances relative to edge lengths, but a more systematic approach to kernel offsetting was desired.

![Figure 1: Replication of Martin’s harmonic coordinate solution with varying coplanar kernel offsets factors](image)

**Legend:** 0 | 0.050 coplanar offset factor | 0.100 coplanar offset factor | 0.150 coplanar offset factor
---|---|---|---

Figure 1: Replication of Martin’s harmonic coordinate solution with varying coplanar kernel offsets factors

### 3. Improved Kernel Offsets

A simpler and more robust kernel placement scheme was developed which avoids these singularities and also inherently sidesteps degenerate cases caused by re-entrant corners. Specifically, the approach consists of offsetting the kernels in a hyperdimension normal to the interpolation...
domain. In this way, the kernels can be seeded directly on the domain boundary or indeed anywhere within the element’s native space without the need to calculate normals or mitre angles. An artificial offset coordinate is simply added to the radius vector:

\[ \tilde{r}_H = \| \mathbf{x} - \mathbf{k}_H \| = \sqrt{\sum_{i=1}^{d} (x_i - k_i)^2 + \rho_H^2}, \quad (\mathbf{x}, \mathbf{k}) \in \mathbb{R}^d \] (8)

Figure 2 shows the effect of a hyper-dimensional offset on an inverse radius kernel ($\phi_{3D}$ along a 4th dimension, in fact). The larger the offset (yellower lines further away from the origin), the more the sharp discontinuity at $r = 0$ is blunted, and the more the entire function is smoothed overall, its falloff is reduced. Away from discontinuities, this is advantageous, as the smoother function can describe a larger area, and fewer kernels are required nearby because of this. Near discontinuities (which coincide with the node positions, in our case), sharper falloffs are needed to match the larger function gradients present there.

\[ \phi_{3D} = 1/r \]

Figure 2: Effect of kernel offset for inverse radius kernel

Though this analysis makes intuitive sense, a more thorough treatment of the kernel spacings and their hyperdimensional offsets is required, especially since kernels may be placed anywhere in or around the element, and with any amount of offset. Optimizing the kernel positions with regard to the condition number of the alternate matrix $A_{ij} = \psi(\| \mathbf{c}_i - \mathbf{k}_j \|)$ yields the most numerically stable kernel placements suitable for the solution of the underlying Laplace equations of the HBFs. Indeed, it can be shown that kernel placements which minimize the condition number of the HBF fit must satisfy:

\[ \sum_{i=1}^{n} A_{ij}^2 = \text{const} \] (9)

Transforming the domain and fitting the constant on the RHS to satisfy the node boundaries yields a unique solution to the kernel placement for a given element geometry. Figure 3 shows optimal kernel placements and the consequent harmonic basis function for the same benchmark element examined by Martin. It should be noted that this method is not reliant heuristic constants, nor is it affected by concave corners.

4. Improved Integration Quadrature

To solve element integrals, a suitable quadrature method must be specified. Martin suggested Monte Carlo methods but a more deterministic, efficient and adaptive method was desired. In their work on mean value coordinates for 3D convex polyhedra [4], Wicke et al’s
suggest using a numerical quadrature whose samples positions are defined by a heuristic mix between the polyhedral nodal centroid and each point of a fixed quadrature set on the polyhedral triangulated surface. Wicke’s quadrature weights are based on the volume of the tetrahedra formed by this construction. Although the quadrature is effectively fixed this method proves to be an adequate substitute for the Monte Carlo method, at least for the first-order convex geometries examined in their work. To suit higher order polynomial shape functions, and to account for surface crossings which may occur along a line integrals going from some central point to a concave polyhedral surface, an adaptive quadrature was required. Based on the divergence theorem, this method consists of summing the products of line integrals between the nodal centroid and quadrature points on the element boundary by the corresponding surface quadrature weight and by the local cosine between the surface normal and path unit vector. This method is applicable in any dimension for airtight concave hulls. Both the surface and path quadratures in this method may be automatically refined to a user-determined tolerance using line and triangle adaptive quadratures. The triangle quadrature is that provided by Zhang et al. [5]. An optimisation to the line integration scheme can be applied whereby critical points along the path integrals can be identified a priori by evaluating the points nearest each kernel along a given integration path. These critical points were then fed as piecewise breaks in Chebyshev quadratures.

Of course, further work remains to be done in generating yet more efficient deterministic quadrature methods over arbitrary convex domains. Specifically, a Fekete node quadrature is currently being developed in following with work done by Briani [2], but requires further work towards validation of the current approach.

5. Polynomial convergence study

To make full use of the conformal meshing capabilities of HBF elements a polynomial refinement method was implemented, thereby laying down the groundwork for hp-adaptive elements, following Babuska [1]. An evaluation of the convergence speed of polynomial refinements on HBF elements versus the convergence speed for mesh refinements with the quintessential linear tetrahedra was carried out for a cantilevered slender beam, showing the promise of the approach. The results could therefore be benchmarked against the known Timoshenko symbolic beam bending solution. Figure 4 shows the resulting convergence rates relative to the beam bending solutions for these numerical experiments. As expected, because the beam deflection problem is exactly solved by a fourth order polynomial, the solution converged to within the specified integration tolerance on the element by its fourth polynomial refinement, and much faster than via mesh refinement.
Figure 4: Convergence testing of HBF element with polynomial refinement

References


Accuray control and non-intrusive implementation of Model Order Reduction based on Greedy Sampling for elasto-dynamics

*X Du\(^1\), A Kundu\(^2\) and P Kerfriden\(^3\)

\(^1,2,3\)Institute of Mechanics and Advanced Materials, Cardiff University, CF24 3AA

*dux8@cardiff.ac.uk

ABSTRACT

In this paper, we present a new adaptive error estimation technique for reduced basis methods applied to linear transient dynamics. The idea is to measure the numerical distance between finite element solution and reduced order approximation such that the adaptivity of Greedy sampling algorithm is under control. In order to do so, we will approximate the inverse of the dynamics operator over the parameter domain by using interpolations with Lagrange polynomials for the adjacent grid parameter points. This is achieved by interpolating a set of small-scale responses in order to circumvent the high cost of direct interpolation of dynamic operator inverse. Multiple spectral reductions are performed to further reduce the cost of the "Offline/online" approach. The comparison of low and high-order interpolation schemes will give us a measure of the "error in the error estimate", which will be used to drive the adaptivity of the error estimate, together with the adaptivity of the reduced basis itself.

Key Words: Greedy sampling algorithm; Finite element method; Model order reduction; H-refinement

1. Introduction

Model order reduction is widely applied to reduce the computational cost of predicting the time dependent behaviour of structures subjected to parameter variations [3]. The reduction is divided into an "Offline" and "Online" stage. The "Offline" stage consists a sequence of expensive pre-computations during which the solutions to the parameterised problem are learned and stored. The "Online" stage makes use of this accumulated data to predict the solution related to any particular parameter of interest at extremely cheap costs.

We rely on a reduced basis approach to construct "Offline/online" decompositions for affinely parametrised linear dynamics problems. It is of vital importance to select a representative projection basis from a set of exactly computed "snapshots". Moreover, a good "Offline" method for snapshot sample selection keeps the "Offline" cost under control. Greedy sampling algorithm has been proved to be an efficient solution [2]. However, the success of this family of techniques rely on the availability of a sharp error estimate, which are not readily available for hyperbolic problems [1, 4].

In this paper, we develop an implemented Greedy sampling algorithm which aims on searching for the best reduced basis over a parameter domain in order to minimise the Frobenius norm of the displacement error, which is defined as \( e = Q E = Q(A^{-1}R) \). This error estimate is robust as it enables the evaluation of error in the entire time domain rather than individual time steps. Original Greedy approach requires the solutions over entire parameter domain, thus an approximation \( A^{-1} \) is needed. Furthermore, a decomposition (in contrast to assembly) is performed to obtain a set of small scale responses for feasibility purposes. The adaptivity of Greedy algorithm is driven by the "error in the error estimate" with local parameter domain h-refinement.
2. Assembly of Newmark method

We aim to solve a finite discretised transient dynamic problem with parameter dependency, that is

\[ M(\mu)\ddot{u}^h(t_\tau; \mu) + C(\mu)\dot{u}^h(t_\tau; \mu) + K(\mu)u^h(t_\tau; \mu) = F(t_\tau), \forall t \in [0, T], \mu \in \mathcal{P} \]  

where \( \ddot{u}^h \), \( \dot{u}^h \) and \( u^h \) denote FE acceleration, velocity and displacement at time step \( t_\tau \). The conventional step-by-step Newmark method is

\[ \ddot{u}^h(t_\tau) = \frac{\gamma}{\beta \Delta t} \ddot{u}^h(t_{\tau-1}) - \frac{\gamma}{2 \beta} u^h(t_{\tau-1}) - \frac{\Delta t}{2} \left( \frac{\gamma}{\beta} - 1 \right) \dot{u}^h(t_{\tau-1}), \quad \tau \in [1, n_\tau] \]

\[ \dot{u}^h(t_\tau) = \frac{1}{\beta \Delta t^2} \ddot{u}^h(t_{\tau-1}) - \frac{1}{\beta \Delta t} \dot{u}^h(t_{\tau-1}) - \frac{1}{2 \beta} u^h(t_{\tau-1}) - \frac{1}{2 \beta} \dot{u}^h(t_{\tau-1}), \quad \tau \in [1, n_\tau] \]  

Equation (3) can be written as:

\[ \begin{pmatrix} M & C & K \\ 0 & I & -a_1 \mathbf{I} \\ I & 0 & -a_0 \mathbf{I} \end{pmatrix} \begin{pmatrix} \ddot{u}^h(t_\tau) \\ \dot{u}^h(t_\tau) \\ u^h(t_\tau) \end{pmatrix} + \mathbf{a}_5 \mathbf{I} \begin{pmatrix} \ddot{u}^h(t_{\tau-1}) \\ \dot{u}^h(t_{\tau-1}) \\ u^h(t_{\tau-1}) \end{pmatrix} = \begin{pmatrix} F^h(t_\tau) \\ 0 \\ 0 \end{pmatrix} \]  

Equation (4) can be written as: \( H^s x^h(t_\tau) + H^f x^h(t_{\tau-1}) = g^h(t_\tau) \), the matrix form for the entire time domain reads

\[ \begin{pmatrix} \tilde{H}^s & 0 & \cdots & 0 \\ H^f & H^s & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & H^s \end{pmatrix} \begin{pmatrix} x^h(t_1) \\ x^h(t_2) \\ \vdots \\ x^h(t_\tau) \end{pmatrix} = \begin{pmatrix} \tilde{g}^h(t_1) \\ g^h(t_2) \\ \vdots \\ g^h(t_\tau) \end{pmatrix} \]  

thus the equation of assembled Newmark method is

\[ A X^h(t) = G^h(t) \]  

Here name \( A \) as the dynamic operator. Equation (5) implies that (i) instead of step-by-step integration, a dynamic problem can be solved in one step, (ii) the intrinsic nature of a dynamic problem is static. However, the solution in eq. (5) is of no practical use as \( A \in \mathbb{R}^{3n_\tau \times n_\tau} \). The following equivalence between step-by-step Newmark method and assembly is established

\[ A^{-1}(\mu)G^h \overset{\text{assembly}}{\longrightarrow} X^h(\mu) \overset{\text{def}}{=} [F^h, M(\mu), C(\mu), K(\mu)] \overset{\text{step-by-step}}{\longrightarrow} [\ddot{u}^h(\mu), \dot{u}^h(\mu), u^h(\mu)] \]  

3. Assembly of Newmark method with reduced model

Reduced order model is particularly suitable to solve parameterised problem repeatedly with a cheap cost. After solving a set of high-fidelity problems (snapshots) and obtaining solutions, a truncated singular value decomposition (t-SVD) is performed and results in a set of orthogonal reduced basis \( \phi \in \mathbb{R}^{n_\tau \times n_\tau} \). The discretised problem is projected on the \( n_\tau \)-dimensional reduced space to compute the reduced state variables for desired parameter values. The reconstruction of responses is a linear combination of reduced basis and reduced state variables, which is efficient due to the preferably small \( n_\tau \).

The above linear combination of space and time response reads (omit acceleration and velocity)
\[ U^h(t; \mu) \approx U'(t; \mu) = \Phi \alpha(t; \mu) = \sum_{i} \phi_i \alpha_i(t; \mu) \] (7)

Vectorise in time and substitute in eq. (5)

\[ A \Psi \Pi(t) = AX'(t) = G'(t) \] (8)

where \( \Psi \) is square matrix contains \( \Phi \) in the diagonal line, \( \Pi(t) \) is the reduce state variable vector. The general residual vector is the difference between FE external force and reduced external force: \( R = G^h - G' = AE \), where \( E \) is the general error vector which contains acceleration, velocity, displacement error vector, respectively. \( E = A^{-1} R = A^{-1}(G^h - G') = \dot{X}^h - \dot{X}' \). As we are particularly interested in displacement error only, a general extractor \( Q \) is applied to extract displacement error: \( e = QE = U^h - U' \). Frobenius norm of displacement error is used to evaluate the numerical distance.

4. Lagrange interpolation of the dynamic operator inverse

The aim is to obtain the general error vector, thus requires to solve \( E = A^{-1} R, \forall \mu \in P \). However, this is not practical as it is equivalent to solve the exact problem for every \( \mu \). In order to circumvent this problem yet maintain the robust error estimate \( E \), an approximation of dynamic operator inverse \( A^{-1} \) is obtained by Lagrange interpolation, correspondingly the general error vector becomes an approximation

\[
\begin{align*}
\hat{E}(\mu) &= A^{-1}(\mu) R(\mu) = \sum_i L_i A^{-1}(\mu_i) R(\mu) = \sum_i L_i A^{-1}(\mu_i) \left( G^h - \sum_j A_j \Psi \Pi(\mu) \right) \\
&= \sum_i L_i \left( A^{-1}(\mu_i) G^h - \sum_j A^{-1}(\mu_i) A_j \Psi \Pi(\mu) \right) \forall \mu_i \in \mathcal{W}, \mu \in \mathcal{P}
\end{align*}
\] (9)

notice that \( \sum_j A_j \) denotes an affine decomposition, which is a crucial assumption in this paper. Direct interpolation of \( A^{-1} \) is too expensive due to its large size, therefore apply the equivalence in eq. (8), we obtain the displacement error vector

\[
\hat{e}(\mu) = Q \hat{E}(\mu) = \sum_i L_i \left( U^h(\mu_i) - \int_{\tau} \sum_j \sum_{\mu} U^{\hat{e}}_{ij}(\tau; \mu, \mu_i) d\tau \right)
\] (10)

Equation (10) describes an integration in time, summation in affine terms, system matrices and reduced basis, respectively. However, the integration in time is a convolution but also different from Duhamel’s integral due to the fact that \( U^{\hat{e}}_{ij} \) is an affine term. An impulse force needs to be generated and applied on the affine system in order to obtain \( U^{\hat{e}}_{ij} \). The Lagrange interpolation sample domain \( \mathcal{W} \) needs to be refined to improve accuracy. Therefore a local h-refinement is naturally applied to \( \mathcal{W} \). In order to control the adaptivity of h-refinement, we introduce the new "error in the error estimate" (in a relative form)

\[
e_{up} = \frac{\| \hat{e} \| - \| \hat{e} \|}{\| \hat{e} \|}
\] (11)

where \( \hat{e} \) denotes displacement error vector in a refined sample domain. The condition is: if \( e_{up} >= e^* \), perform local h-refinement; else if \( e_{up} < e^* \), cease h-refinement and continue the Greedy iteration.

5. Numerical Example and Results

5.1. The cantilever beam model
A linear elastodynamics problem is modelled to test the proposed method along with the new error estimate. The model is a 2D cantilever beam finitely discretised with 3-node triangular elements, results in 154 nodes and 250 elements. The model composes 2 inclusions each with a varied Young’s modulus $\mu_1 \in [10^1, 10^2]$ and $\mu_2 \in [10^1, 10^2]$. The parameter domain $\mathcal{P}$ is formed by $\mu_1$ and $\mu_2$. A dynamic load is applied at the right upper corner node, pointing to -y direction. Total time is 3 seconds with time step length $\delta t = 0.1s$, results in 30 time steps. The dynamic load lasts for 0.4 seconds. Homogeneous Dirichlet boundary condition is applied on the left edge. The model is generated and meshed in Abaqus, and corresponding affined system matrices are imported into MATLAB.

5.2. Preliminary results

Conventional and implemented Greedy algorithm have been tested in this paper. The implemented Greedy algorithm gives different samples, results in an improved reduced basis (contains 12 basis vectors) and gives a maximum error decay curve which converges a lot faster than the conventional one (‘truth’). Moreover, the decay is stable in the implemented Greedy while the conventional Greedy shows instability.

6. Conclusion

This paper describes an implementation of model order reduction based on Greedy sampling algorithm. The inverse of dynamic operator is interpolated in order to estimate error of dynamic problems in a global sense. In order to achieve this, further decompositions are implemented to reduce computational cost. A local $h$-refinement is applied to the interpolation with an “error in the error estimate” to control the adaptivity. The implemented algorithm shows a faster, more stable convergence of maximum error compare with the conventional one.

References


GENERALIZED FINITE ELEMENTS FOR BLOW UP SOLUTIONS TO REACTION-DIFFUSION EQUATIONS

*Gissell Estrada-Rodriguez*¹, Heiko Gimperlein¹

¹Maxwell Institute for Mathematical Sciences and Heriot-Watt University, Edinburgh, EH14 4AS, U.K.

*ge5@hw.ac.uk

**ABSTRACT**

We consider a Dirichlet problem for transient nonlinear heat diffusion problems, \( u_t = \Delta u + f(u) \), in a bounded domain. A Generalized Finite Element Method (GFEM) is studied with a particular emphasis towards blow up solutions. In this case, controlling the numerical errors is crucial. We discuss a residual error estimate to estimate a norm of the error in the whole domain. Using a GFEM, based on test and ansatz spaces enriched with Gaussian functions, we obtain rigorous error estimates and efficient approximations in the presence of blow up. To estimate the error in relevant quantities of interest, such as the error of the maximum temperature, we then present a goal-oriented two-level estimate. Mathematically, the residual a posteriori estimates are shown to provide reliable and practically useful upper bounds for the numerical errors, independent of the heuristically chosen enrichment functions. Numerical experiments underline the practical relevance of our theoretical results. First, the error estimates are shown to capture the decrease in the error as the number of enrichment functions is increased. Second, the estimate is used to predict the behaviour of the error where no exact solution is available.

**Key Words:** generalized finite element method; goal-oriented error estimates; non-linear heat equation

1. **Introduction**

Generalised finite element methods based on non-polynomial basis functions provide an efficient approximation of solutions with singularities or steep gradients. Using physical or analytical information about the problem, they enrich the approximation space of the finite element method with appropriate approximations of the singularities in the actual solution.

In this paper we present computable *a posteriori* error estimates for a GFEM in the case of nonlinear reaction diffusion equations, possibly in the presence of blow up. The estimates we present provide reliable upper bounds for the total error, respectively the error in quantities of interest. The distinctive characteristic of the approach that we present here is that they are independent of the choice of enrichment functions. See also [1] for a first work in the case of linear heat diffusion problems.

More precisely, we consider the initial-boundary value problem

\[
 u_t = \Delta u + f(u), \text{ in } (0, T) \times \Omega, \quad u(x, 0) = U_0(x), \text{ for } x \in \Omega, \quad \text{ and } \quad \partial_n u = 0, \text{ on } (0, T) \times \Gamma, \tag{1}
\]

where \( \Omega \in \mathbb{R}^2 \) is a polygonal bounded domain with boundary \( \Gamma \). We are interested in nonlinearities \( f(u) = u^p, \text{ for } p > 1 \).

In the presence of blow up solutions, quantities of particular interest include the maximum temperature and its error in a subregion, rather than global errors, or also blow up times. Hence the importance of using goal-oriented error estimates.
Our goal is to compute the quantity $L$ associated to the numerical approximation $\tilde{u}$. The primal problem (1) has a strong dual formulation, equivalent to the weak form (2), given by

$$
\int_T \int_{\Omega} v u_r \, d\Omega + \int_T \int_{\Omega} \nabla v \nabla u \, d\Omega = \int_T \int_{\Omega} f(v) v \, d\Omega.
$$

We look for a solution $u^{i+1}(x)$ that comprises the piecewise polynomial bases $N_j(x)$ and enrichment functions $G_q(x)$, which are going to be specified in Section 4. Therefore,

$$
u^{i+1}(x) = \sum_{j=1}^{M} \sum_{q=1}^{Q} A_q^{j} N_j(x) G_q(x),
$$

where $A_q^{j} \in \mathbb{R}$ are the new unknowns, $M$ is the total number of nodal points and $Q$ is the total number of enrichment functions. Using an implicit Euler method with step size $\Delta t$ such that $t^{i+1} = t^i + \Delta t$ and letting $v = N_j G_q$ in (2), the GFEM is, for $k = i/\Delta t$ and $F^{j+1} = (f^{j+1} + k u^j)$: Find $u^{i+1} \in H^1(\Omega)$ such that $u^0 = u_0$ and

$$
\int_T \int_{\Omega} \left( k N_j G_q u^{i+1} + \nabla N_j G_q \nabla u^{i+1} \right) \, d\Omega = \int_T \int_{\Omega} F^{j+1} N_j G_q d\Omega.
$$

3. A posteriori error estimates

The residual a posteriori error estimators are given as follows. See [1] for a Robin-type boundary condition.

**Theorem 1.** Assume that $U$ is the solution of the weak formulation (2) and $u$ is the solution of (4). Then there exists a constant $\delta > 0$ such that

$$
\int_{\Omega} |U(x, T) - u(x, T)|^2 \, d\Omega + \int_0^T \int_{\Omega} |\nabla(U - \tilde{u})|^2 \, dt \, d\Omega \leq \delta (\eta_1^2 + \eta_2^2 + \eta_3^2 + \eta_4^2 + \eta_5^2)
$$

where $\tilde{u}(x, t) = u(x, t_{j+1})$ and

$$
\eta_1^2 = \|U_0 - u_0\|^2_{L^2(\Omega)}, \quad \eta_2^2 = \sum_{j=0}^{T} \int_0^T \|f - u_t + \Delta \tilde{u}\|^2_{L^2(\Omega)} \, dt,
$$

$$
\eta_3^2 = \int_0^T \|f - \tilde{f}\|_{H^{-1}(\Omega)} \, dt, \quad \eta_4^2 = \int_0^T \|\tilde{\nabla}(u - \tilde{u})\|^2_{L^2(\Omega)} \, dt, \quad \eta_5^2 = \sum_{E} \int_0^T \|\frac{\partial \tilde{u}}{\partial n}\|^2_{L^2(E)} \, dt.
$$

In the numerical experiments below $\eta_2^2$, $\eta_4^2$ and $\eta_5^2$ will be dominant. They represent the residual of the equation, the approximation error from the time discretisation and the jump of $\partial u/\partial n$ across the edges $E$ of the elements $\square$.

Our goal is to compute the quantity $L(u)$, where $L$ is a linear functional of the solution $u$. The error associated to the numerical approximation $L(u_h)$ is given by $L(u - u_h) = L(e)$.

The primal problem (1) has a strong dual formulation, equivalent to the weak form (2), given by

$$
w_r + \Delta w = \Delta v, \text{ in } (0, T] \times \Omega, \quad w(x, T) = J(x), \text{ for } x \in \Omega, \text{ and } \partial_n w = 0, \text{ on } (0, T] \times \Gamma.
$$
where \( w \) is the influence function. It relates the error in the quantity of interest \( L(e) \), with the residual, which is the source of error.

Consider the numerical approximation \( u_Q \) of the primal solution \( u \) in a coarse mesh using \( Q \) enrichment functions, and define \( u_q \) but using \( q > Q \) enrichment functions. The error in the primal approximation now is \( \delta \approx u_q - u_Q \), provided \( u \approx u_q \). From \( u_q \), we obtain the dual problem for \( \hat{w} \) in a weak form. With \( \hat{w}_q \) an approximation of \( \hat{w} \), we obtain an error estimate for \( L(e) \) in terms of

\[
L(e) = \|u - u_Q\|^2 \approx \eta := \int_0^T \mathcal{R}_Q^u(\hat{w}_q)dt + \mathcal{R}_0^u(\hat{w}_q), \quad \|v\|^2 := \int_0^T B(v, v)dt + \|v(T)\|^2_{L^2(\Omega)} . \tag{7}
\]

Here, \( \mathcal{R}_Q^u \) is the residual of the primal problem given by \( \mathcal{R}_Q^u(\cdot) = F(\cdot) - (u_Q, \cdot) - B(u_Q, \cdot) \) and \( \mathcal{R}_0^u(\hat{w}_q) = (e(0), \hat{w}_q(0)) \) where \( e(0) = U_0 - u_Q(0) \).

For \( L(u) = \int_\omega u \) the integral of the temperature in a subdomain \( \omega \subset \Omega \), \( \hat{w} \) solves a heat equation with a constant heat source in \( \omega \). In this case, we may use the enrichment from \( [1] \) to resolve the gradient at the boundary of \( \omega \) in the dual problem.

**Theorem 2.** For \( \eta \) as in (7) and for \( r_1 \) and \( r_2 \) small, \( e = u - u_Q, e_q = u - u_q \) and \( \hat{w} \) the dual solution for \( u \approx u_q \), we obtain

\[
L(e) = \|e\|^2 = \eta + r_1 + r_2, \quad r_1 = 2(((e_q, e))_E - \|e_q\|^2, \quad r_2 = \int_0^T \mathcal{R}_Q^u(\hat{w} - \hat{w}_q)dt + \mathcal{R}_0^u(\hat{w} - \hat{w}_q) .
\]

As shown in \( [2] \), terms of the form \( r_1, r_2 \) are negligible even on coarse meshes.

### 4. Numerical examples

We compare the error estimates from Theorem 1 with the actual error in the model problem (1), with \( \Omega = (0, 1), f(u) = u^2 \) and \( U_0 = 1 \). In Figure 1 we compare the error indicators \( \eta_2 + \eta_4 + \eta_5 \) with the actual error for a standard \( h \)-FEM (no enrichment) with 90 respectively 3000 equidistant nodes and \( \Delta t/\Delta x \) constant. In this case the solution blows up for \( T \approx 0.08 \).

In both cases the error estimates capture the behaviour of the actual error in time. We also note that the constant \( \delta \) in Theorem 1 scales with the number of nodes. However, it will be constant for a GFEM on a fixed mesh and could easily be taken into account also here.

![Figure 1: Blow up profile of the solution (left) and comparison of actual error vs. error estimates for 90 nodes (middle) and 3000 nodes (right).](image)

First computational results for a GFEM in 2d use Gaussian enrichment functions together with piecewise polynomial shape functions. So \( G_\varphi \) in (3) is given by

\[
G_\varphi(x) = 1, \quad e^{-\left(\frac{x - x_c}{\varepsilon}\right)^2}, \quad e^{-\left(\frac{x - x_c}{\varepsilon}\right)^3} \quad \text{or} \quad e^{-\left(\frac{x - x_c}{\varepsilon}\right)^3 - \left(\frac{x - x_c}{\varepsilon}\right)^2} . \tag{8}
\]
The model problem (1), with $\Omega = (0, 1)^2$, $f(u) = u^2$ and $U_0 = 30$, is solved on a fixed mesh with 25 square elements, and we vary the number of enrichment functions in each square. The parameter $C$ in (8) is equal to $\frac{200}{239}$ and $(x_C, y_C) = (0.5, 0.5)$. We compute the profile of the solution and the corresponding error estimates varying the number of enrichment functions per element in Figure 2. Here, we evaluate $\eta_2^2 + \eta_4^2 + \eta_5^2$ for different numbers of enrichment functions in each element. From [1] the estimators capture the actual error. We see that the solution profile becomes smoother with increasing number of enrichments, as the total error decreases.

5. Conclusions

The residual a posteriori error estimate presented in this paper is shown to capture the behaviour of the actual error in a nonlinear reaction-diffusion problem with blow-up: The estimate is proven to be reliable even close to the blow up time, and numerically it tracks the behaviour of the actual error. In two dimensions we obtain accurate and efficient numerical approximations of the solution as we increase the number of enrichment functions per mesh element. A detailed analysis in this case as well as a numerical exploration of the goal-oriented estimate are work in progress.

References


THREE-DIMENSIONAL MORTAR CONTACT FORMULATION: AN EFFICIENT AND ACCURATE NUMERICAL IMPLEMENTATION

*Zahur Ullah¹, Łukasz Kaczmarczyk¹ and Chris J. Pearce¹

¹School of Engineering, Rankine Building, The University of Glasgow, Glasgow, UK, G12 8LT

*Zahur.Ullah@glasgow.ac.uk

ABSTRACT

The mortar contact formulation is a well-established technique to tie non-conforming finite element meshes in domain decomposition and is also the basis of many well-known contact algorithms. Mortar contact formulation allows for a variationally consistent treatment of contact conditions including mesh tying, non-penetration, frictionless and frictional sliding leading to satisfaction of contact patch test. Efficient, accurate and robust numerical implementation of the interface coupling terms associated with the mortar contact formulation remains challenging, especially in three-dimensional case. The computational contact algorithm presented in this paper is carefully designed for accuracy, efficiency and robustness and making use of the cutting-edge third-party computational tools including Mesh-Oriented datABase (MOAB), Portable, Extensible Toolkit for Scientific Computation (PETSc), Boost and clipper libraries. The computational framework is designed to take advantage of distributed memory high-performance computing and hierarchic basis functions. The numerical implementation is validated with two non-conforming mesh tying examples, which, on the one hand, remove some of the complexities associated with actual unilateral contact formulation but, on the other hand, clarify many of the conceptual and implementational aspects of the contact mechanics.

Key Words: finite element analysis; mortar contact formulation; mesh tying; numerical integration; hierarchical basis functions

1. Introduction

Mechanical interaction between different bodies often referred as "contact or impact", is of great importance in many engineering applications including prosthetics in biomedical engineering, pneumatic tires in automotive engineering and adhesion or slip between concrete and reinforcing steel in civil engineering. In mechanical engineering applications, contact can be found in gears, bearings, metal forming and car crash test [1, 2]. At the minimum, contact mechanics involves searching for the contact area between interacting bodies and subsequent prevention of inter-penetration. Relative movement or slip including both frictionless and frictional, intermittent interaction and wear also comes under the umbrella of contact mechanics. Due to the associated nonlinearities and complicated nature of problems involving contact, special assumptions were used in the past for their solution. Advances in Computational modelling allows solving these problems to be solved numerically with sufficient accuracy for engineering analysis/design. On the other hand, as compared to the current state of the art nonlinear finite element technology including finite deformation kinematics, inelastic material behavior and linear and nonlinear equations solvers, contact mechanics is relatively immature. Therefore, the design of efficient, accurate and robust contact algorithms is still a challenge for practical engineering problems.

In this paper, one of the most commonly used contact discretisation technique for the solution of contact problem, i.e. the mortar contact formulation is adopted, which is also referred to as a special type of segment-to-segment approach in the literature [3]. Alternative methods, including node-to-segment and enforcing contact condition at specific finite element node, cannot guarantee the satisfaction of contact patch test and suffers from non-physical oscillation in the contact forces. As compared to the strong or point-wise satisfaction of the interface continuity condition in the aforementioned contact mechanics approaches, a weak or integral form is used in the mortar contact formulation. The computational
contact algorithm presented in this paper is carefully designed for accuracy, efficiency and robustness and makes use of the cutting-edge third party computational tools including Mesh-Oriented datABase (MOAB), Portable, Extensible Toolkit for Scientific Computation (PETSc), Boost and clipper [4] libraries. The developed algorithm is implemented within our group’s finite element code, MOFEM [5]. Relatively simple, linear-elastic two body problems with non-conforming meshes are used to validate the numerical implementation. Tetrahedral elements are used to discretise the two contacting bodies leading to triangular elements on the common interfaces. The clipper library is used to create an intersecting polygon between every pair of triangles belongs to the two contacting surfaces. These polygons are then triangulated, with their integration points projected back on to the parent triangles, which are used subsequently for the numerical integration of the mortar contact integral. For the convenient and efficient handling of the mesh data associated with the contacting surfaces, prisms are inserted between every pair of contacting triangles and are stored in the multi-index containers. Furthermore, the computational framework is designed to take advantage of distributed memory high-performance computing and hierarchic basis functions [6].

2. Problem formulation

In this paper, we limit ourselves to the application of mortar contact formulation for tying non-conforming meshes in linear-elasticity by removing some of the complexities associated with unilateral contact mechanics. Nonetheless, this will clarify many of the conceptual and implementational aspects of the computational contact mechanics [7]. Consider two subdomains \( \Omega^{(i)} \subset \mathbb{R}^3, i = 1, 2 \) bounded by boundaries \( \partial \Omega^{(i)} \). The subdomain boundary \( \partial \Omega^{(i)} \) is divided into disjoint sets of Dirichlet boundary \( \Gamma_{u}^{(i)} \), Neumann boundary \( \Gamma_{\nu}^{(i)} \) and mesh tying interface \( \Gamma_{c} \). The body force acting over the individual subdomain is \( b^{(i)} \). The strong form of governing equations in the case of linear-elasticity for each subdomain is written as:

\[
\text{Div}\sigma^{(i)} + b^{(i)} = 0 \quad \text{in} \quad \Omega^{(i)},
\]

where \( \sigma^{(i)} \) is the Cauchy stress tensor. The associated boundary conditions are the Dirichlet, Neumann and mesh tying constraint and are written as:

\[
\begin{align*}
\mathbf{u}^{(i)} &= \bar{\mathbf{u}}^{(i)} & \text{on} & \Gamma_{u}^{(i)}, \\
\sigma^{(i)} \cdot \mathbf{n}^{(i)} &= \mathbf{t}^{(i)} & \text{on} & \Gamma_{\sigma}^{(i)}, \\
\mathbf{u}^{(1)} &= \mathbf{u}^{(2)} & \text{on} & \Gamma_{c}.
\end{align*}
\]

The weak formulation is subsequently derived together with Lagrange multipliers \( \lambda \) to enforce the mesh tying constraint. In Figure 1(a), \( \Omega^{(2)} \) is considered as the slave side and \( \Omega^{(1)} \) is considered as the master side. The final discretised set of equations is written as:

\[
\begin{bmatrix}
K_{NN} & K_{NM} & K_{NS} & 0 \\
K_{MN} & K_{MM} & 0 & -M^{T} \\
0 & K_{SN} & D^{T} \\
0 & 0 & D & 0
\end{bmatrix}
\begin{bmatrix}
d_{N} \\
d_{M} \\
d_{S} \\
\lambda
\end{bmatrix}
= \begin{bmatrix}
F_{N} \\
F_{M} \\
F_{S} \\
0
\end{bmatrix},
\]

where \( d_{S} \) and \( d_{M} \) are the degrees of freedom associated with slave and master contact surfaces and \( d_{N} \) consists of all the remaining degrees of freedom, \( K \) and \( F \) are the standard stiffness matrices and force vectors respectively. Both slave and master surfaces are not connected directly and are tied using the mortar contact formulation leading to blocks of zeros for both \( K_{MS} \) and \( K_{SM} \). Constraint matrices \( D \) and \( M \) are written as:

\[
D = \int_{\Gamma_{c}} N_{A} N_{S} d\Gamma_{c} = \sum_{p_{r}=1}^{n_{pr}} \left( \sum_{g=1}^{n_{gp}} w_{g}^{S} N_{A} \left( \xi^{S}(\xi_{g}), \eta^{S}(\eta_{g}) \right) N_{S} \left( \xi^{S}(\xi_{g}), \eta^{S}(\eta_{g}) \right) J^{S} \right),
\]

\[
M = \int_{\Gamma_{c}} N_{A} N_{M} d\Gamma_{c} = \sum_{p_{r}=1}^{n_{pr}} \left( \sum_{g=1}^{n_{gp}} w_{g}^{M} N_{A} \left( \xi^{M}(\xi_{g}), \eta^{M}(\eta_{g}) \right) N_{M} \left( \xi^{M}(\xi_{g}), \eta^{M}(\eta_{g}) \right) J^{M} \right),
\]
where $N_S$ and $N_M$ are matrices of shape functions for slave and master sides respectively. $N_A$ is a matrix of shape functions used for the discretisation of Lagrange multipliers, only exists on the slave side and is assumed the same as $N_S$, $w$ and $J$ are the weight and Jacobian associated with Gauss points. $(\xi_S(\xi_g), \eta_S(\eta_g))$ and $(\xi_M(\xi_g), \eta_M(\eta_g))$ represents the projection of Gauss points on the original slave and master triangles in local coordinates, explained below in detail.

A step-by-step procedure used for the 3D mortar contact formulation for one pair of slave and master triangles is shown in Figures 1(b-e). After projection of both triangles in $xy$-plane Figure 1(b), the clipper library is used to determine the clip polygon (Figure 1(c)), which is subsequently triangulated (Figure 1(d)) with their integration points projected back on both the original master and slave triangles (Figure 1(e)). For the easy and efficient data handling, prisms are inserted between each intersecting slave and master triangles. In Equation (4), $n_{pr}$ and $n_{gP}$ are the number of prisms and Gauss points respectively.

3. Numerical Example

The two pairs of both non-conforming and conforming meshes, as shown in Figure 2, are used to validate the numerical implementation of the mortar contact formulation. The dimensions, loading, boundary conditions and coordinate system are also shown in Figure 2. Young’s modulus and Poisson’s ratio used in this case are $E = 10$ and $\nu = 0.5$ respectively. For both pairs, the conforming meshes, i.e. cases shown in Figures 2(b, d), are used for validation and is solved without mortar contact formulation. In Figure 2(a) and Figure 2(c) non-conforming meshes exists at their curved interfaces. The contours of $z$-component of displacement, i.e. $u_z$ is also shown for all of the four cases. It can be seen that for each pair, the contours plots of $u_z$ is exactly the same, demonstrating the correct implementation of the computational framework.

4. Conclusions

In this study, an efficient, accurate and robust numerical framework is presented for three-dimensional mortar contact formulation, which allows consistent treatment of the contact conditions. The computational framework is implemented in our group’s finite element code, MOFEM, which uses state of
the art MOAB, PETSc and Boost libraries. The implementation is validated with two non-conforming mesh tying examples. Although, not demonstrated in this paper, the developed computational framework is designed to take advantages of the hierarchic basis functions and high-performance computing. This paper is restricted to linear-elastic problems but will be extended subsequently to include both material and geometric nonlinearities. The actual contact formulation including efficient contact search, non-penetration, frictionless and frictional sliding will be implemented next.

Acknowledgements
This work was supported by EDF Energy Nuclear Generation Ltd and the Royal Academy of Engineering (RAEng). The views expressed in this paper are those of the authors and not necessarily those of EDF Energy Nuclear Generation Ltd or RAEng.

References
Efficiency analysis of patch size and type for Error Estimates based on implicit residual and local Dirichlet patch problems.

Pedro Bonilla\(^1\), Abhishek Kundu\(^1\) and *Pierre Kerfriden\(^1\)

\(^1\) Institute of Mechanics Materials and Advanced Manufacturing, Cardiff University, CF24 3AA - United Kingdom

*KerfridenP@cardiff.ac.uk

ABSTRACT

The present work aims for a unified framework for different reduction of the residual to local patch approaches through Dirichlet boundary conditions, allowing its comparison, hybridisation and better understanding. The paper introduces the ideas of treating the residual as an element-wise pre-stress for the error problem rather than averaging patch contributions. This allows the use on any element and patch and some of this range of choice is analysed. A two steps estimation estimating first the error fluctuation across element edges and then projecting to the interior is also introduced. Computational results in terms of accuracy, computational time and cost-efficiency for the different approaches and some new estimates based on the combination of the known and new concepts are included. Poisson problems are used to compare the methods.

Key Words: error estimation ; patch residual approach ; comparison

1. Introduction

The Finite Element Method is a powerful tool to approximate boundary value problems for partial differential equations. A posteriori error estimation is recognized as a major tool not only to assess the accuracy of the computations, but to reduce the computational cost of the estimations through adaptive schemes.

The estimates based on reducing the Residual to local Dirichlet Problems retain most of the good properties of the Residual family, specifically those concerning the robustness for local non-linear phenomena. On the other hand, it lacks the property of a guaranteed upper bound provided by the Equilibrated Residual approaches. The method uses as main assumption that contributions to the error of neighbour elements is of higher order than the distant ones, enhancing prediction of local phenomena.

Several methods have been developed within this classification, for instance the ones based partition of unity, sub-space projection or space enhancement concepts. Each of them was presented independently. One of the present work’s aims is to fit these methods in a common framework that allows compare its performance. Then it is also possible to combine concepts already used in the tested methods, in an attempt to improve them.

2. Framework for error estimation from the residual.

Let us consider a weak form of an elliptic problem over a bounded domain \( \Omega \subset \mathbb{R}^d \), defined in a Sobolev Space \( V = \{ v \in H^1(\Omega) \mid v = 0 \text{ on } \Gamma_d \} \) which is also solution of the strong form of the problem provided suitable Boundary Conditions in the boundary \( \partial \Omega \). Usually \((C\nabla u) \cdot \vec{n} = g_n \text{ on } \Gamma_n \) and \( u = u_d \text{ on } \Gamma_d \), Neumann and Dirichlet complementary subsets of \( \partial \Omega \).

\[
a(u, v) := \int_{\Omega} (\nabla v \cdot (C\nabla u) + v \cdot b \cdot u) \, d\Omega = \int_{\Gamma_n} v \cdot g_n \, d\Gamma_n =: l(v), \; \forall v \in V. \quad (2.1)
\]
The term $f(x,y)$ is known, $u(x,y)$ is the solution, $\vec{n}$ is the unit outward normal vector to $\Gamma_n \subset \partial \Omega$ and $C$ and $b$ are parameters defining the problem, in our case the diffusion coefficient and advective velocity respectively.

Numerical methods are employed to approximate this solution in the continuum making use of a finite element space $V^h \subset V$ leading to a discrete coarse approximation $u^h$.

The discretisation error $e = u - u^h$ belongs to the space $V$ of continuous functions, and it is defined by $a(e,v) = l(v) - a(u^h,v), \forall v \in V$, where the energy of the discrete solution is subtracted from both sides of the global problem. We can therefore define the residual as $R(v) := l(v) - a(u^h,v)$.

We know from Galerkin orthogonality that the solution $u^h$ is the best one in space $V^h$, so in order to compute any error we need a discrete space richer than $V^h$.

In our work, the initial coarse space is defined by the size $'h'$ of its elements, while the reference space is defined by $h$ and the number of refinements $'R'$ in each direction for every element. For instance, figure 1.d) shows a particular case of a $1 \times 1.25$ squared, regularly meshed, coarse domain of $1/h \times 1.25/h = 4 \times 5$ quadrilateral elements where a refinement of $R \times R = 4 \times 4$ is applied creating a reference space of $(1/h)^*R \times (1.25/h)^*R = 16 \times 20$ sub-elements.

![Diagram](image)

**Figure 1:** Types of patch definition, used in this paper.

### 3. Elemental contribution and Vanishing assumption.

By splitting all the integral in the residual using each element as a local domain of additivity integration ($R(v) = \sum_{k=1}^{ne} R_k$), but keeping the whole domain as local patch problem and original B.C. for each one of the patches we are making no approximation, but computing a set of global contributions $\varepsilon_k$ such that $e = \sum_{k=1}^{ne} \varepsilon_k$, with extra computational cost.

$$R(v) = \sum_{k=1}^{ne} R_k = \sum_{k=1}^{ne} \left( \int_{\Omega_k} v \cdot f \, d\Omega + \int_{\Gamma_k} v \cdot g_n \, d\Gamma_n - \int_{\Omega_k} (\nabla v \cdot (C \nabla u^h) + v \cdot b \cdot u^h) \, d\Omega \right) \quad (3.1)$$

Despite the cost, this allows us to plot the elemental contribution to the error as an analogy with distributed loads (figure 2), and more importantly, its gradient, which is the magnitude that we will approximate to apply the vanishing assumption to reduce the local patch.

$$a(\varepsilon_k, v) = R_i(v) \approx a_p(\varepsilon_p, v) = R_k(v), \quad \forall v \in V \quad (3.2)$$

where $k$ stands for the number of element and $a_p(\cdot, \cdot)$ is obtained by neglecting all contributions of the elements outside the reduced local patch $p$. 

90
Elements outside star patch

Elements loaded

Elements in star patch unloaded

Elements loaded

Elements in star patch unloaded

Elements loaded

Initial mesh: structured quad 20x20 elements, R=4x4. Element loaded k=319 => row 15, col. 19. Full domain as patch. Coloured what would be approximated in a star patch type (fig. 1.b)

Figure 2: Elemental Contribution to the error and its gradient.

4. Formulations of the methods compared.

The most common estimate in the family uses first-order Lagrange basis function $\lambda_p$ to define the patches around the vertexes $n$ of our discretization. $\lambda_p(x_m) = \delta_{nm}$.

$$a(e, \tilde{\partial}u) = \sum_{p=1}^{p=nn} \lambda_p \cdot R(\tilde{\partial}u) = \sum_{p=1}^{p=nn} R_p(\lambda_p \cdot \tilde{\partial}u), \quad \forall \tilde{\partial}u \in \tilde{V} \quad (4.1)$$

Note that $\lambda_p \cdot \tilde{\partial}u$ fulfils all the criteria to be a test function in any subspace limited to the patch, but it is a different function than $\partial u$, so if the vanishing assumption is used instead of the original methods, the test function is different in left and right hand sides. Details of the method and how to compute bounds can be found in I. Babuska and A. Miller [1].

Space enhancement method was presented by K. Runesson and co-workers [3]. It is based on an enhancement of the subspace $V^h$ increasing the order of the elements by adding nodes only in its boundary.

We can decompose any solution $\tilde{u} \in \tilde{V}$ into $\tilde{u} = \tilde{u}_1 \in V^h + \tilde{u}_2 \in |\Delta \tilde{V}|$ being $\Delta \tilde{V} = \{v \in \tilde{V}, v = 0 \}$ at each node in $V^h$. Then the approximation $\tilde{u}_1 = u^h$ is introduced in the subspace $\tilde{V}$.

This method was modified with the vanishing assumption, to allow full neighbourhoud patches.

Subspace projection method was Presented by A. Huerta and co-workers [2]. The method defines a set of subspaces $\tilde{V}_k$ for each element on the domain that vanish on all the domain but the interior of the element. $V_k \subset \tilde{V} = \{v \in \tilde{V}_k | v = 0 in \Omega \setminus \Omega_k\}$.

The error $e$ can be split into the projection $\tilde{e}$ and the part omitted by the projection $e^{\perp \tilde{V}}$ which is orthogonal to the projection subspaces $\tilde{V}_k$ and hence to $\tilde{e}$ and any $\tilde{e}_k$. By the Pythagoras theorem $||e||^2 = ||\tilde{e}||^2 + ||e^{\perp \tilde{V}}||^2$ being $|| \cdot ||^2$ the energy norm $a(\cdot, \cdot)$. $e^{\perp \tilde{V}}$ is approximated by computing a solution in an alternative subset of bubble patches (figure 1.d) and enforcing its orthogonality to $\tilde{e}$ through Lagrange multipliers.

Another variation introduced in this work is to use the values computed at the boundary of each element as Dirichlet B.C. for a bubble problem taking advantage of the orthogonality shown in the sub-projection method. This allows to use p refinement and larger patches as a 1st step to save computational effort and still project to an h refined space.
Left, h refinement methods, Right p refined. initial 1/h=80, R varies from 2 to 16. Truth 1/h=640

5. Results.

The Poisson problem in the domain of the unit square \((0,1)\times(0,1)\) used to assess the different methods is 
\[- \Delta u = f \text{ in } \Omega \]
\[B.C. u = 0 \text{ on } \Gamma_d = \{y = 0, x \in (0,1)\}, \quad \frac{\partial u}{\partial n} = 0 \text{ on } \Gamma_n = \{\Omega \setminus \Gamma_d\}.
\]

The source term \(f(x,y)\) was set to the analytical solution of 
\[- \Delta u(x, y) \text{ being } u(x, y) = 5x^2(1-x)^2(e^{10x^2} - 1)y^2(1-y)^2(e^{10y^2} - 1)\]

After trying different patches and methods in the test case, results showed that the star patch works only for space enhancement if the enriched p test function is close to the original one (quad4 and quad8 elements). However, using the full immediate neighbourhood, made the vanishing assumption stable in all the methods.

Figure 3, shows that for h refinement and the test case, subspace projection is less accurate and the vertex patches are faster than full neighbourhood ones for similar accuracy. By using p refinement we reduce the computational cost significantly for better accuracy. Also, the improved accuracy of the introduced hybrid 2 steps methods, does not justify the increase of computational cost respect just the projection of the p enhanced solution.

Acknowledgements.

This project has been supported by the Engineering Research Network Wales Grant (Rhwydwaith Ymchwil Peirianneg Cymru) corresponding to project NRN071.

References


A-Priori Error Estimator based Hierarchical $p$ Adaptivity Scheme for Acoustic Problems

*X. Meng$^1$, J. Reboud$^2$ and Ł. Kaczmarczyk$^3$

$^1$School of Engineering, Rankine Building, The University of Glasgow, Glasgow, G12 8LT, UK

*E-mail: m.xuan.l@research.gla.ac.uk

ABSTRACT

In this paper the development of efficient computational method for Helmholtz equation is presented. Here we solve the Helmholtz equation in the frequency domain, applying hierarchical finite element approximation with generalized Duffy transformation based on unstructured meshes [3], where both pressure field and geometry are independently approximated with arbitrary and heterogeneous polynomial order. We demonstrate the implementation and performance of the numerical approach by benchmark problems, especially under pollution effects, which also validate the accuracy and efficiency of an object oriented a priori error estimator through numerical assessments.

Key Words: $p$ adaptivity scheme; Hierarchical basis; Lobatto shape functions; Duffy transformation; A priori error estimator

1. Introduction

It is widely accepted that acoustic problems have vast range of uses in different physical applications, in the context of microfluidic object subject to high frequency SAW (surface acoustic waves), the applications encompass disease diagnostics, biochemical analysis, drug delivery, aid to build the lab-on-chip system. However, the modelling of high frequency application is difficult in practical situations due to capacity of numerical methods.

The main idea of error analysis is to find the optimised numerical scheme allowed fast frequency sweep acoustic applications. There are mainly two subjects under the category of error estimator: a priori and a posteriori. The a priori error estimator is the estimation of the exact error before we reach the approximation solution which based on known information about the exact solutions in object specific norms. The major drawback of a posterior error estimator is that it requires the finite element solution calculated before the estimated error.

Proposed finite element technology is implemented in open-source finite element University of Glasgow in-house parallel computational code, MoFEM (Mesh Oriented Finite Element Method).

2. Mathematical formulation

Let $\Omega$ be a domain in $\mathbb{R}^3$ with smooth boundary and outward unit normal $n$. In the assumption of time harmonic wave, the steady part of the wave equation for the propagation of acoustic waves in an isotropic, ideal medium is described as

$$\nabla \cdot \nabla \Phi(\mathbf{r}) + k^2 \Phi(\mathbf{r}) = f(\mathbf{r}) \text{ in } \Omega \quad (1a)$$

$$\left( \frac{\partial \Phi(\mathbf{r})}{\partial n} + i \sigma \Phi \right) = g \text{ on } \Gamma \quad (1b)$$

where the variation of $f(\mathbf{r})$ in (1a) can be regarded as a point source of acoustic wave. Eq (1b) exhibits the mixed boundary condition (MBC) with material constant $\sigma$ and acoustic energy $g$, which can be used to describe any BCs by modifying the parameters. The example of benchmark problem with plane wave impinging on a sound hard sphere are shown in Figure 1 where diffraction of energy can be observed.
3. Generalized Duffy transformation for simplex

The accurate higher order Gauss points and weights lying within the element domain are extremely difficult to derive for simplex geometry. The difficulty of searching quadrature rules generally leads to well known problem of finding the zeros or minima of high-order multi-variate polynomials, as well as general limitation of $p$ order below 7.

In 1982, Duffy introduced an integration techniques which can increasing the accuracy of integration while eliminates the integrand with a $\frac{1}{r}$ singularity on vertex. In this paper, we present a special case of generalised Duffy transformation which collapse the hexahedron to tetrahedron directly by changes the transformation to:

$$Q^3 □ (u, v, w) \rightarrow T^3 △ (x, y, z) : x = u^2v^2w, y = xv(1-z) = u^2v(1-w), z = x(1-y) = u^2(1-v)$$ [2]. In this paper, we employ generalized Duffy transformation to integrate simplex element for volume and surfaces, it guarantees the exactness of integrand with arbitrary polynomial orders.

4. Hierarchical Lobatto basis for tetrahedron

The difficulty arisen in acoustic problem is the increasing of frequency causes the grows of condition number of system matrix, which is $\kappa = ||A|| \cdot ||A^{-1}||$ for system of linear equations $Ax = b$. Where $||A||$ can represents any specific norms (typically $L_2$). The quantity of memory required to store and factorize the system matrix also related to the conditioning of matrix. The reason of keeping condition number relative low is to maintain a stable and rigorous solution particular for large problems with huge size of system matrix using iterative solvers. The Legendre basis functions are:

$$L_n(\tilde{\zeta}) = \frac{2n+1}{n} \tilde{\zeta} L_{n-1}(\tilde{\zeta}) - \frac{n-1}{n} L_{n-2}(\tilde{\zeta}), \text{ for } n = 1, 2, \ldots, N$$ (2)

where $-1 \leq \tilde{\zeta} \leq 1$ for the first order functions, $L_0(\tilde{\zeta}) = 1$ and $L_1(\tilde{\zeta}) = \tilde{\zeta}$. Legendre basis has orthogonality property in $L_2$. The Lobatto basis functions are derived from modified integrated Legendre basis, thus inherited the hierarchical orthogonal property. The $p_{ih}$ order Lobatto basis for edges are computed based on $p - 1_{th}$ Legendre basis:
\[ l_i(\zeta) = \sqrt{i - \frac{1}{2} \int_{-1}^{\zeta} L_{i-1}(\xi) d\xi}, \text{ for } i = 2, 3, \ldots, p \]  

(3)

for \( L_i(\zeta) \) is the Legendre basis of order \( i \). Its orthogonality property up to first order derivative in \( H_1 \) can delivery coarser stiffness matrix together with the Duffy transformation of Gauss quadrature. Intuitively, they together lead to better conditioning for sparse system matrix with high wavenumbers [3]. Figure 3 reveals the fact that hierarchical Lobatto basis is better conditioned than the Legendre basis especially for high frequencies.

![Figure 3: Lobatto basis versus Legendre basis coupled with Duffy transformation, condition number against number of polynomial orders. Impinging sound hard sphere in 3D with \( r = 4, a = 0.5 \)](image)

5. A simple object oriented error estimator

In the basic assumption of relation between 1D element and higher dimensional element, error incurs from higher order element can be estimated from error in 1D element. In essence, the error indicator estimates the average of errors occurred in each element from a given mesh. The detailed implementation procedures are depicted in Chart 4.

The efficiency of adaptivity scheme can be improved by calculate the criterion of \( \chi_{kh} = kh' \) value corresponding to the best polynomial order \( p \), and put into a table in the premise of pre-defined error level \( \eta \). Consequently, the value of \( kh \) in each element is compared with the criterion value \( \chi_{kh} \), if actual \( kh < \chi_{kh} \), the best \( p \) corresponding to \( \chi_{kh} \) is employed.

The piecewise \( H^1 \) actual error is calculated on the computational domain for benchmark problem in Figure 4. The dispersion error caused by phase lag is a global effect that builds up itself over the whole computational domain. Figure 4b identifies the fact that there are large parts of errors occurred around the boundary of scatterer, the infinite domain, and along the propagation direction. The former can be sufficiently eliminated through \( p \) adaptivity algorithm as shown in 4b (p order: blue = 3, cyan = 4, green = 5, red = 6.), where the latter contributed by the dispersion errors can only be alleviated. Nevertheless, these dispersion errors can be minimised by hierarchical shape functions of Lobatto basis through \( p \) adaptivity, in such a way that the phase accuracy of higher order element is greater than lower order element with approximately same total no. of DOFs. The total relative \( H^1 \) error is approximately
0.2496% when the predefined error level is 0.5%. In addition, the \( p \) adaptivity scheme has successfully spotted the errors around 34%, which are indicated by red colour region in plot 4b.

### 5.0.1. Adaptivity schemes efficiency analysis

In the following numerical tests, we assessed plain \( h \) refinement \((p = 2)\), uniform \( p \) enrichment and automatic \( p \) adaptivity, whilst fixed the mesh resolutions in descending order: \( \tau_i = \frac{\tau_0^p}{h_{\text{max}}} = [8.6820, 5.7880, 5.2092, 4.3410, 3.4728, 3.0387, 2.7782] \) by varying \( h_{\text{max}} \) and \( f \) for \( h&p \) adaptivities respectively. \( h_{\text{max}} \) denotes maximum element size in mesh. As for the automatic \( p \) adaptivity, we replace \( p \) in \( \tau_i \) by the average of \( p \) over whole computational domain. From both Figures, automatic \( p \) adaptivity delivers lowest error with decreasing resolution, and its efficiency has been guaranteed by less memories occupied compared to \( h \) adaptivity technique, but it requires more memories than uniform \( p \) adaptivity since it allocates more higher order elements based on error indicator. Overall, automatic \( p \) adaptivity with partly refined mesh is more stable than other adaptivity schemes since its natural of predefined error level, this fact can be observed from the plateau area of error (red solid line) in Figure 5a.

![Graph](image)

**Figure 5:** Automatic \( p \) adaptivity versus uniform \( h&p \) adaptivity based on mesh resolution \( \tau_i \), Impinging sound hard sphere problem, \( a = 0.5 \) and \( r = 4 \)

### 6. Conclusions

Pertaining to the demand of efficient adaptivity method for solving high frequency acoustic problems, an object oriented a priori error estimator proposed by Prinn.A[1] has been implemented with both hierarchical Lobatto basis and generalized Duffy transformation. We omitted the plots of pollution error analysis (increasing domain length gradually), efficiency analysis (time, memory, no.DOFs), and effectivity indices in order to be concise in contexts. Although the a priori error estimator does not account for pollution effect, it enables to control the pollution effect within the frequency limit. Results shown the \( p \) adaptivity scheme based on a priori error estimator outperforms \( h&p \) adaptivity scheme in every aspects, while maintains the predefined error level within certain frequency band. This found of acoustic solver with \( p \) adaptivity have practical importance since in industrial applications, problems with high frequency sweeps are considered, it will be extremely expensive to refine the mesh within each frequencies and created a large number of meshes. On contrast, we can solve our problem with initial coarse mesh, and enrich our approximation basis in each frequencies.

### References


Failure, Fracture and Damage
COUPLING ENRICHED RBF AND MFS FOR ANTI-PLANE SHEAR CRACKS

*Faisal M. Mukhtar¹ and Husain J. Al-Gahtani²

¹, ²Department of Civil & Environmental Engineering, King Fahd University of Petroleum & Minerals, 31261, Dhahran, Saudi Arabia

*faisalmu@kfupm.edu.sa

ABSTRACT

The paper presents enriched RBF (e-RBF), enriched MFS (e-MFS) and coupled enriched RBF-MFS for anti-plane shear (mode III) crack analysis. The enrichments help in capturing the singularity behaviour at the crack-tip while the coupling strategy helps in minimizing the discretization density which in turn reduces computational cost with better accuracy.

Keywords: anti-plane crack; singularity; RBF; MFS; enrichment; coupling

1. Introduction

The stress field in the vicinity of a crack tip governs the crack growth and, hence, behaviour of the crack-tip-field stresses is very essential in fracture mechanics. As shown in Figure 1, mode III is a consequence of loading a cracked body with an anti-plane shear \( \tau \). In order to have an idea about the extent of stress singularity at a crack tip, the stress intensity factor (SIF) is defined. This parameter provides a useful information that helps in characterizing the state of stress near the crack tip due to remote loading.

![Figure 1: Anti-plane shear loaded arbitrary shaped cracked body](image)

The non-availability of exact solution to crack problems with complex shapes and/or loading conditions necessitates the adoption of numerical tools. RBF and MFS are famous meshless methods that are handy in solving different engineering problems including anti-plane crack analysis [1 – 3].

2. Governing equation and singular analytical solution for a crack under anti-plane shear

General elasticity, in the absence of body forces, yields Eq. (1) as the governing equation for anti-plane shear cracks in terms of the transverse displacement \( w \). The shear stress components given by Eq. (2) are functions of the shear modulus \( \mu \). The general boundary condition \( \Gamma \) acted upon by the boundary operator \( \delta \) is subdivided into the far boundary 1 and the crack faces/boundary 2 as described in Eq. (3). Where, \( f \) and \( g \) are continuous functions of space variables.

\[
\nabla^2 w = 0
\]  

(1)
\[ \tau_{xx} = \mu \frac{\partial w}{\partial x}; \quad \tau_{yy} = \mu \frac{\partial w}{\partial y} \quad (2) \]

\[ \mathbb{B}_{\Gamma_1} w = f \quad \text{on} \quad \Gamma_1; \quad \mathbb{B}_{\Gamma_2} w = g \quad \text{on} \quad \Gamma_2; \quad (3) \]

There exists an analytical solution, \( K_0 = \tau_0 \sqrt{\pi a} \), for the stress intensity factor of symmetrically cracked infinite body under anti-plane shear of magnitude \( \tau_0 \) and crack size \( a \). This solution does not apply to unsymmetrical cases and/or finite elastic bodies and, therefore, more robust approaches are needed. Fortunately, meshless numerical methods such as RBF and MFS are handy in solving such cases. However, still, such methods cannot capture the singularity behaviour at the crack-tip as does the analytical methods. Consequently, enriched formulations (e-RBF and e-MFS) are used in resolving the issue.

3. RBF and MFS: Enrichments and coupled formulations

Both RBF and MFS do not require the geometry to be meshed using elements. Instead, as shown in Figure 2 (a and b), some distributed nodes are used in their discretizations. The source points in MFS are placed at an off-set distance from the actual boundary.

![Figure 2: Cracked body](image)

In both the two methods, the solution is approximated in the form given by Eq. (4). In RBF method, \( \phi \) is chosen as a suitable RBF centered at \( x_j \) points, while in the MFS it is chosen to be the fundamental solution \( w^* \) which satisfies the domain of the problem. Hence, in case of RBF, the coefficients \( \alpha \) are determined by forcing Eq. (4) to satisfy Eqs. (1) and (3). On the other hand, these coefficients are determined, in the case of MFS, by collocating over only the boundary nodes to satisfy Eq. (3).

\[ w(x) = \sum_{j=1}^{N} \alpha_j \phi(\|x - x_j\|) \quad (4) \]

Unfortunately, in crack analysis, Eq. (4) cannot capture the crack tip singularity. Hence, the present study proposes the coupled RBF-MFS given by Eq. (5) as a modified form of Eq. (4), which involves the sum of three series as the overall solution. Choice is made of the multiquadric RBF \( \phi = \sqrt{r^2 + c^2} \), the fundamental solution \( w^* = (1/2\pi) \ln(r) \) and \( N_i \) singular terms as functions of the analytical solution \( \psi_k = r^{k-1} \sin \left( \frac{k - 1}{2} \right) \theta \) in the vicinity of the crack tip. \( r = \|x - x_j\| \) is a radial distance between two points and \( c \) is a constant called shape function. Since the singular stresses manifest only in the first term of \( \psi_k \), \( N_2 = 1 \) is used in this study and \( \psi = \sqrt{r} \sin \left( \frac{\theta}{2} \right) \) is chosen to be entered at the crack tip \( x_c \). The system of algebraic equations given by Eq. (6) is ultimately generated via collocation procedure. This makes it possible to solve for the unknowns \( \alpha, \beta \) and \( \gamma \). It would be interesting to note that when \( w^* = \sqrt{r^2 + c^2} \) is used in Eq. (5), the problem becomes e-RBF. On the other hand, when \( \phi = 0 \) is used, the problem becomes e-MFS. When, in either of the cases, \( \psi = 0 \) is used, the problem becomes unenriched formulation.
\[
W(x) = \sum_{j=1}^{N_d} \alpha_j \phi(||x - x'_d||) + \sum_{j=1}^{N_F} \beta_j w^r(||x - x'_r||) + \sum_{k=1}^{N_S} \gamma_k \psi_k(||x - x'_k||)
\]

(5)

Some crack configurations require the use of domain-decomposition approach for more convenience and/or accuracy. This could be achieved by subdividing the original domain $\Omega$ into a number of sub-domains. As shown in Figure 2(c), the far boundary and the crack face/boundary for the $i$th sub-domain $\Omega_i$ are denoted by $\Gamma_{1,i}$ and $\Gamma_{2,i}$, respectively. The interface boundary is denoted as $\Gamma_i$. The coupled RBF-MFS formulation based on this domain-decomposition can be written in the form given by Eq. (7).

\[
\begin{bmatrix}
\nabla^2 \phi(x'_d) - \nabla^2 w^r(x'_r) - \nabla^2 \psi(x'_k)
\end{bmatrix}
\begin{bmatrix}
\phi\{x'_d\}
\psi\{x'_r\}
\phi\{x'_k\}
\end{bmatrix}^T =
\begin{bmatrix}
0
0
0
\end{bmatrix}
\]

(6)

\[
\begin{bmatrix}
\phi\{x'_d\}
\psi\{x'_r\}
\phi\{x'_k\}
\end{bmatrix}^T =
\begin{bmatrix}
\alpha
\beta
\gamma
\end{bmatrix}^T
\]

(7)

4. Numerical results

The rectangular plate shown in Figure 3(a) is analysed using the formulations presented above. This problem may represent an internal central crack in a plate of dimensions $2W \times 2H$ or an edge crack in a plate with dimensions $W \times 2H$. Due to symmetry, the single-domain formulation (Eq. (6)) works well when half of the problem is modeled. The domain-decomposition approach (Eq. (7)) becomes useful when the full domain is considered. The ratio $H/W = 1$ is used.

Figure 3(b) shows a typical case where the conventional RBF and MFS fail to model the crack-tip field satisfactorily. This issue is resolved in e-RBF, e-MFS and their coupled form as seen in Figure 3(c).

![Figure 3: Plate of the example problem](image)

SIF results achieved for different crack sizes are reported in Table 1 along with other literature results for comparison. Relative performance of the methods formulated in this study can be assessed based on the foregoing discussion and the summary given in Table 2, where capability of the suggested
formulations to capture the singularity is emphasized. In addition, the coupled RBF-MFS entails less number of discretization points.

Table 1: SIF results for the plate of the example problem

<table>
<thead>
<tr>
<th>$\tilde{K}_{III}$</th>
<th>$a/W$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.1</td>
</tr>
<tr>
<td>Present</td>
<td>e-RBF</td>
</tr>
<tr>
<td></td>
<td>e-MFS</td>
</tr>
<tr>
<td></td>
<td>RBF-MFS</td>
</tr>
</tbody>
</table>

Table 2: Summary of performance of the enriched formulations in the example problem

<table>
<thead>
<tr>
<th>Method</th>
<th>Captures singularity</th>
<th>Enriched Crack-tip field solution</th>
<th>Far-field solution</th>
<th>Discretization</th>
<th>Shape function/off-set</th>
</tr>
</thead>
<tbody>
<tr>
<td>RBF</td>
<td>No</td>
<td>No</td>
<td>×</td>
<td>✓</td>
<td>60 by 60</td>
</tr>
<tr>
<td>MFS</td>
<td>No</td>
<td>Yes (e-RBF)</td>
<td>✓</td>
<td>×</td>
<td>60 by 60</td>
</tr>
<tr>
<td>RBF-MFS</td>
<td>Yes</td>
<td>Yes (e-MFS)</td>
<td>✓</td>
<td>✓</td>
<td>60 by 60</td>
</tr>
</tbody>
</table>

✓ Provides accurate solution × Fails to provide accurate solution - Not applicable

5. Conclusions

Enriched formulations of RBF, MFS and their coupling for anti-plane shear cracks have been presented in this study. The same have been implemented to find the stress intensity factor for mode III cracked plates. The results show that while the enrichments helps in capturing the singularity behaviour at the crack-tip, the coupling strategy helps in minimizing the discretization density which in turn reduces computational cost with better accuracy.

Acknowledgements

The authors would like to acknowledge the support provided by the Deanship of Scientific Research at King Fahd University of Petroleum & Minerals (KFUPM) under Research Grant JF-151003.

References


Simulating evolution of fluid lag during hydraulic fracture propagation using finite element method

Bin Chen, *Chenfeng Li and Beatriz Ramos Barboza

Zienkiewicz Centre for Computational Engineering, Swansea University, Swansea, SA1 8EN

*c.f.li@swansea.ac.uk

ABSTRACT

A plane 2D model is developed to simulate the evolution of fluid lag during propagation of mixed mode hydraulic fracture. Rock deformation and fluid flow are both modelled by standard finite element methods and are solved in fully coupled manner while linear elastic fracture mechanics theory is utilized to dictate the propagation of fracture. An elaborate adaptive remeshing strategy is adopted to update the unstructured mesh when new fracture surface is presented. The model is verified by existing semi-analytical and numerical results.

Keywords: hydraulic fracture; fluid lag; finite element, remeshing

1. Introduction

Since the first field test in Kansas in 1947 on a gas well in the Hugoton field [1], hydraulic fracturing has become a vital step to get a commercial or higher production from oil, unconventional gas, especially for low-permeability and tight reservoirs. Diverse simulators have been developed to optimize the design or understand some specific mechanisms. However, there are still some situations which have not been treated properly, for example, the evolution of lag in complex conditions.

Existence of lag, the gap between the fluid front and crack tip during propagation of hydraulic fracture, has been recognized since the beginning of the development of hydraulic fracturing models [2]. By combining Poiseuille’s law, mass conservation and an integral equation derived from elasticity theory, a more rigorous KGD model is constructed and is adopted to simulate a hydraulic fracture with an always existing lag systematically [3,4]. The self-similar solutions for early-time and late-time stages are derived in a semi-analytical way [3] while the evolution of lag in transient stage is simulated numerically in this scheme [4]. This process is also simulated in FEM and XFEM manner [5]. All above semi-analytical or numerical analysis only focus on the straight propagation of hydraulic fractures.

In this paper, we develop a plane 2D model using finite element method to simulate the evolution of lag during mixed mode propagation of hydraulic fracture. Application of standard finite element in hydraulic fracturing simulation is highlighted here and more complicated constitutive model or heterogeneities of rocks is allowed to be inserted.

2. Problem formulation and coupled solution system

In this paper, a plane strain assumption is applied on the plane orthogonal to the vertical wellbore (see Figure 1). The rock media is assumed to be impermeable linear elastic block and the fluid is assumed to be incompressible, Newtonian and fluid flow is assumed to be laminar. An initial fracture with length of \( L_0 \) and orientation angle \( \alpha \) with respect to maximum horizontal stress is assumed. A domain 50\( L_0 \) by 50\( L_0 \) is used in the finite element analysis to approximate the infinite rock media. The effect of gravity is not considered since it is orthogonal to the plane. In the following part, the theory and (or) numerical methods adopted for simulating the three basic physical processes are discussed with the coupled solution system followed.
2.1 Rock deformation

The rock is assumed to be linear elastic media suffering small deformation in this paper. The constitutive model for the rock is expressed as

\[ \sigma_{ij} = c_{ijrs} \varepsilon_{rs} \quad i, j, r, s = 1, 2 \]  \hspace{0.5cm} (1)

\[ c_{ijkl} = \frac{vE}{(1 + v)(1 - 2v)} \delta_{ij} \delta_{kl} + \frac{E}{2(1 + v)} (\delta_{ik} \delta_{j} + \delta_{ij} \delta_{kl}) \]  \hspace{0.5cm} (2)

Where \( \sigma \) is the stress tensor, \( \varepsilon \) is the strain tensor, \( v \) is the Poisson’s ratio, \( E \) is the young’s modulus. A quasi-static analysis is conducted and the gravity acts in the direction orthogonal to the plane, so the equilibrium equations can be simplified as

\[ \nabla \cdot \sigma = 0 \]  \hspace{0.5cm} (3)

Standard FEM is adopted to solve the rock deformation due to its feasibility to more advanced constitutive models. Weak form of the equivalent equation is expressed as:

\[ \int_{\Omega} \delta \varepsilon_{ij} c_{ijrs} \varepsilon_{rs} d\Omega - \int_{\Gamma_e} \delta u_i t_j d\Gamma_e - \int_{\Gamma_f} \delta u_i p_i d\Gamma_f = 0 \]  \hspace{0.5cm} (4)

Where \( \Omega \) is domain of rock, \( \Gamma_e \) is the external boundary, \( p_i \) and \( \Gamma_f \) are the fluid pressure and the fracture boundary respectively. \( \delta \varepsilon_{ij} \) is the strain corresponding to virtual displacement \( \delta u_i \).

2.2 Fluid flow

The application of lubrication theory is assumed to be valid and is very common in great amount of literatures. Without the gravity term, Poiseuille law (or cubic law) reads as:

\[ q = \frac{w^3}{12 \mu} \frac{dp}{dx'} \]  \hspace{0.5cm} (5)

Where \( q \) is the flow rate, \( w \) the fracture width, \( \mu \) the viscosity of the fracturing fluid, \( p \) the fluid pressure and \( x' \) is the coordinates aligned with the tangential direction to the fracture path.

The continuity equation is expressed as:

\[ \frac{dw}{dt} - \frac{dq}{dx'} = 0 \]  \hspace{0.5cm} (6)

Plugging the cubic law into the weak form of the continuity equation results in:

\[ \int_{\Gamma_p} \delta p \frac{\partial w}{\partial t} d\Gamma_p + \int_{\Gamma_p} (\delta p) \frac{w^3}{12 \mu} p_i d\Gamma_p - \delta p(0) Q_{\text{outlet}} + \delta p(L_f) \bar{Q} = 0 \]  \hspace{0.5cm} (7)
Here, $\Gamma_p$ is the fracture path occupied by fluid. $Q_{\text{inlet}}$ being imposed injection flow rate and $\bar{Q}$ is the flow rate at fluid front $L_f$.

2.3 Fracture propagation

For maximum tensile stress criterion [6], the fracture propagates once the following expression is satisfied:

$$\cos \frac{\theta}{2} \left( K_I \cos^2 \frac{\theta}{2} - \frac{3}{2} K_{II} \sin \theta \right) \geq K_c$$

(8)

Where $K_I$, $K_{II}$, $K_{IC}$ are the stress intensity factors for mode I, mode II and fracture toughness respectively. The stress intensity factors $K_I$ and $K_{II}$ are computed by using interaction energy integral method. $\theta$ dictates the direction of propagation and is expressed as

$$\tan \left( \frac{\theta}{2} \right) = \frac{1}{4} \left( \frac{K_I}{K_{II}} - \text{sgn}(K_{II}) \sqrt{\left( \frac{K_I}{K_{II}} \right)^2 + 8} \right), \quad -\pi < \theta < \pi$$

(9)

2.4 Discretization and coupled solution system

As for the solid part, an unstructured triangular mesh is utilized to discretize the solid phase domain. An elaborate remeshing strategy with mesh generator GMSH [7] combined is put forward to update the global mesh when a new fracture surface emerges. The 1D mesh used for fluid computation is from the 2D mesh. After the discretization of space, Newton-Raphson method is used to solve the two finite element problems together.

3. Advancement of crack tip and fluid front

Both the crack tip and fluid front are tracked in our model. At the beginning of the simulation, a minimum mesh size ($L_{\text{min}}$) is set to control the simulation accuracy and computation cost. We define the minimum mesh size as one advancement step for both the crack tip and fluid front. The fluid front is advanced firstly, and then the crack tip is advanced until the fracture criterion is not satisfied.

4. Numerical case

This model has been verified with the early-time and late-time semi-analytical results firstly and the comparison is omit here. The following case is for the evolution of lag during mixed-mode propagation of hydraulic fracture. The two far-field stresses are set to be 19.4MPa and 9.7MPa. The direction of the initial crack is 89° with respect to the maximum horizontal stress and half-length is $L_0/2=0.1m$. Viscosity of the fluid used here is 100cP (0.1Pa·s) and injection flow rate is 0.002m²/s. The rock properties are: Young’s modulus $E=25$GPa, Poisson’s ratio $v=0.3$, and crack toughness 1.2MPam¹/². The initial relative position of fluid front is determined to be 0.8. The minimum mesh size is $L_0/60$. Fracture trajectory and evolution of lag size and relative position of fluid front are shown in Figure 2.

As shown in Figure 2, the tangential direction at crack tip changes from the direction of minimum horizontal stress to the direction of maximum horizontal principle stress. The lag size shows a wavelike increase while the lag ratio varies in a more complex mode. At the beginning, the fracture propagates almost along the direction perpendicular to the maximum horizontal stress. The relative position of fluid front increases dramatically until a significant curve occurs at around 31th step. After that, the relative position of fluid front decreases in a wavelike mode due to the change of stress condition until 76th step where the intersection degree between tangential direction of the crack at crack tip and maximum horizontal stress is around 20°. Then the relative position of fluid front tends to one gradually in a wavelike mode as time elapsed.
Figure 2. Fracture trajectory (left), evolution of lag size (middle) and relative position of fluid front (right) for poropagation of mixed mode hydraulic fracture in anisotropic stress field. The whole process is divided into three stages by the cross symbol or the dashed line.

5. Conclusions

A plane 2D model is developed to simulate the evolution of lag during mixed mode propagation of hydraulic fracture using finite element method. The accuracy and capacity of our model in dealing with the lag evolution is verified by the self-similar solutions. In addition, by using an elaborate remeshing strategy, the effect of anisotropic stress on evolution of lag is presented. Application of standard finite element in hydraulic fracturing simulation is highlighted here and more complicated constitutive model or heterogeneities of rocks is allowed to be inserted in this model, which is one of the future works.

Acknowledgements

The author Bin Chen gratefully acknowledges the financial support from China Scholarship Council/Swansea University Joint Scholarships Program.

References

A NON-ORDINARY STATE BASED PERIDYNAMICS IMPLEMENTATION FOR ANISOTROPIC MATERIALS

*G. Hattori*¹ and J. Trevelyan*¹

¹School of Engineering and Computing Sciences, Durham University, South Road, DH1 3LE, Durham, UK

*gabriel.hattori@durham.ac.uk

ABSTRACT

In this work we present a peridynamics (PD) formulation for generally anisotropic materials. PD has been shown as a new approach for modelling fracture mechanics, and can easily model different dynamic effects, such as crack branching. The non-ordinary state-based framework allow us to model the material properties in the same way as in the classical continuum mechanics. The crack propagation path follows the same behaviour as seen in experimental results for unidirectional fibre composites. Damage is modelled through a deformation criterion.

Key Words: peridynamics; non-ordinary state-based formulation; anisotropic materials; crack propagation

1. Introduction

Fracture mechanics is a difficult problem to deal with since there are discontinuities arising from cracks. The continuum mechanics equilibrium equation presents a partial derivative, which becomes infinite at the discontinuities. Numerical models have different approaches in order to deal with this particular case, such as the quarter-point for the finite element method (FEM) and the dual formulation for the boundary element method (BEM).

Peridynamics (PD) is a novel numerical method developed by Silling [1] to treat fracture mechanics problems. The equilibrium equation is defined in an integral form, which eliminates the rising of discontinuities in fracture mechanics problems. For this reason, the same formulation of PD is used whether there is a discontinuity or not, being ideal for modelling crack initiation, branching and coalescence for example. These crack propagation behaviour are very difficult to model with conventional numerical methods.

PD is receiving increased attention over recent years, due to its potential for fracture mechanics. So far, most of the works considered only isotropic materials, but some works for PD in composite materials have been investigated (see [2] for instance). Nevertheless, a full anisotropic model for PD has not been developed to date, and it is shown in this work for the first time. A non-ordinary state-based formulation is used [3, 4], where elements of continuum mechanics such as the deformation gradient are employed in the PD framework. This formulation is a generalisation of the first PD proposed in [1].

2. Non-ordinary state-based peridynamics

In the classical continuum mechanics, the equation of motion is defined as

\[ \nabla \cdot \sigma + b(x,t) = \rho \ddot{u} \] (1)

where \( \sigma \) represents the Cauchy stresses, \( b(x,t) \) stands for the body forces, \( \rho \) is the mass density and \( \ddot{u} \) is the acceleration.

The equation of motion in state-based peridynamics (PD) is defined as

\[ \int_{\mathbb{R}^n} [T(x,t)(x' - x) - T(x',t)(x - x')] dV_{x'} + b(x,t) = \rho \ddot{u}(x,t) \] (2)
with $\mathbf{T}$ as the force vector state field, and square brackets denote that the variables are taken in the state vector framework.

In order to Eq. (2) to be valid, it must satisfy both balance of linear and angular momentum. The proofs can be found in [5] for instance.

Figure 1 illustrates the reference (or initial) configuration, and the deformed configuration after a displacement $\mathbf{u}$ and $\mathbf{u}'$ has been imposed on particles $\mathbf{x}$ and $\mathbf{x}'$, respectively. In the original bond-based formulation, the particles inside the horizon of $\mathbf{x}$ make a contribution for the displacement solution. However, the fact that these other particles $\mathbf{x}'$ also possess their own horizon is not taken into account. This leads to a restriction of the material properties [1]. The state-based theory [3] removes this limitation, allowing to model any material properties.

![Reference and deformed configuration in state-based PD.](image)

There are 2 types of state-based formulation: ordinary and non-ordinary. In the ordinary theory, the forces in the bonds are defined in the direction of the bonds, in the same way as in the bond-based formulation. The main issue is how to obtain the equivalent material properties from the classical continuum mechanics. An energy equivalent approach can be used, as detailed in Madenci and Oterkus [6].

In the non-ordinary framework, the forces between particles are not constrained to the bond direction, which provides a more general formulation. In this case, some of the main parameters in continuum mechanics, such as the deformation gradient, are expressed in terms of the PD formulation. Additionally, the material constitutive matrix can be used, overcoming this limitation in the ordinary state-based PD theory.

The peridynamics state-based formulation consists in the use of the so called state fields. They are fully detailed in [3]. The deformation vector state field is stated as

$$\mathbf{y}(\mathbf{x}, t)[\xi] = \mathbf{y}(\mathbf{x} + \xi, t) - \mathbf{y}(\mathbf{x}, t)$$  \hspace{1cm} (3)

The non-local deformation gradient $\mathbf{F}(\mathbf{x})$ for each particle is given by

$$\mathbf{F}(\mathbf{x}) = \left[ \int_{\mathcal{H}} \omega(|\xi|)(\xi \otimes \xi) dV_{\xi} \right]^{-1}$$ \hspace{1cm} (4)

$$\mathbf{B}(\mathbf{x}) = \left[ \int_{\mathcal{H}} \omega(|\xi|)(\mathbf{Y}(\xi) \otimes \xi) dV_{\xi} \right] \mathbf{F}(\mathbf{x})$$ \hspace{1cm} (5)

where $\mathbf{B}(\mathbf{x})$ is the shape tensor, $\otimes$ denotes the dyadic product of two vectors, and $\omega(|\xi|)$ is a dimensionless weight function, used to increase the influence of the nodes closes to $\mathbf{x}$. In this work, we assumed that $\omega(|\xi|) = 1$. 

107
To incorporate the kinematic stress into the PD model, the transpose of the first Piola-Kirchhoff stress is equivalent to [7]

\[ \mathbf{P}(x)^T = \frac{\partial W}{\partial \mathbf{F}} \] (6)

with \( W \) being the strain energy density function.

The force vector at time \( t \) is finally stated as [7]

\[ \mathbf{T}[x,t](x' - x) = \omega(|x' - x|)\mathbf{P}(x)^T \cdot \mathbf{B}(x) \cdot (x' - x) \] (7)

The processing of mapping a stress tensor as a peridynamic force state is the inverse of the process of approximating the deformation state by a deformation gradient tensor. A peridynamic constitutive model that uses stress as an intermediate quantity results in general in bond forces which are not parallel to the deformed bonds.

3. Numerical discretisation

In order to obtain the values for the acceleration, velocity and displacements, we need to integrate the PD solution using an explicit approach. The values of acceleration are calculated directly from Eq. (1). In order to obtain the values for the acceleration, velocity and displacements, we need to integrate the equation of motion,

\[ m \ddot{u}(x,t) = \mathbf{T}[x,t] \] (11)

where \( \Delta t \) is the time step, \( \mathbf{u}(x,t) \) are the velocities and \( \mathbf{u}(x,t) \) are the displacements. Since we are using an explicit approach, the time step must be smaller than a certain threshold in order to the analysis to be valid. In this work we considered that the \( \Delta t \propto \delta/c_p \), where \( c_p = \sqrt{C_{22}/\rho} \) and \( c_p \) is the dilatational wave speed and \( C_{22} \) comes from the material properties. The time step was obtained by \( \Delta t = 0.01 \frac{\delta}{c_p} \).

4. Results

We investigate the dynamic effects in an anisotropic square plate containing an edge crack. The plate has dimensions 100 mm x 100 mm, the crack tip is located at the centre of the plate, and the length of the crack is 50 mm. The dimensions of the plate were chosen just to assess the formulation. The plate is a graphite-epoxy where the fibre forms an angle of 45° with respect to the horizontal axis. The material properties in global coordinates system are given by (in Voigt notation): \( C_{11} = 5.01 \) GPa, \( C_{12} = 3.08 \) GPa, \( C_{16} = 3.34 \) GPa, \( C_{22} = 5.01 \) GPa, \( C_{26} = 3.34 \) GPa, \( C_{66} = 3.80 \) GPa. The plate is subjected to an initial velocity gradient \( \mathbf{L} \) given by

\[ \mathbf{L} = \begin{bmatrix} 0 & 0 & \frac{1}{s} \\ 0 & 350 \end{bmatrix} \] (11)

Figure 2 depicts some stages of the crack propagation with respect to a damage parameter. If damage is 0, all the bonds are active, while if damage is 1, all the bonds are broken. In Figure 2(a), the crack is about to start propagating, while in Figure 2(c) the crack has propagated through the entire plate. One can note that the angle of crack propagation is 45°, which is consistent with experimental results for a unidirectional composite fibre [8].

The time step of the analysis is \( \Delta t = 6.0 \times 10^{-9} s \), and the total time until complete failure is \( t = 1.50 \) \( \mu s \), resulting in 5000 steps of the integration. The bond breaking criterion is defined in the same way as in [4], and it consists in using a deviatoric deformation component. If the deformation between two particles exceeds a critical deformation, the bond breaks. In this work we assumed \( \epsilon_{cr,tt} = 0.0042 \).
5. Conclusions

A peridynamics model for fully anisotropic materials has been presented for the first time in the literature. The non-ordinary state-based framework has been used to model a general anisotropic material. The crack propagation path is consistent to the one find in experiments in the literature for an unidirectional fibre composite. Future work include using different horizon sizes and other problems such as anisotropic bimaterials or inclusions.

Acknowledgements

The first author acknowledges the Faculty of Science, Durham University, for his Postdoctoral Research Associate funding.

References


A constitutive model for elastic-plastic behaviour and delamination damage in fibre metal laminates

Ahmad S.M. Al-Azzawi¹,²,³*, L.F. Kawashita² and C.A. Featherston¹

¹School of Engineering, Cardiff University, The Parade, Cardiff, CF24 3AA, UK
²Advanced Composites Centre for Innovation and Science, University of Bristol, Bristol, BS8 1TR, UK
³College of Engineering, University of Babylon, Babylon, Iraq

*Corresponding author: Email address. Al-AzzawiAS@cardiff.ac.uk

ABSTRACT

This study focusses on the development of a constitutive material subroutine to simulate damage at the interfaces of elastic-plastic materials under quasi-static loading. The code, based on a novel cohesive zone model using a trapezoidal traction-separation law enables the definition of cohesive interfacial properties representative of those observed for Glare® fibre-metal laminates. By considering elastic-plastic damage behaviour, this model provides more accurate results for the simulation of ductile adhesives than the commonly used bilinear cohesive zone model. It is also computationally more robust when compared with implicit techniques since it is coded for dynamic explicit solution schemes which can simulate highly nonlinear material behaviour easily. It is implemented through a user-defined VUMAT subroutine in the Abaqus/Explicit software. Elastic results correlate well with the bilinear cohesive zone model for cohesive elements available in the Abaqus library after which behaviour consistent with the trapezoidal traction law is observed.

Keywords: Fibre Metal Laminates, Cohesive Zone Model, VUMAT subroutine, elastic-plastic behaviour, traction-separation law.

1. Introduction

Cohesive zone models have been widely used for predicting delamination in adhesively bonded composite structures under static loading. Models used in these analyses which are mostly based on a bilinear traction-separation law have been found to be a particularly efficient approach for elastic materials. This approach however has not been found to be accurate for elastic-plastic materials where a trapezoidal traction-separation law proved to be more efficient in predicting the plastic flow of ductile adhesives [1]. The trapezoidal traction-separation law has been adopted by researchers such as [2, 3] to model the interface damage behaviour in elastic or elastic-plastic materials in either mode I or mode II independently under static loading. In this work a mixed mode trapezoidal traction-separation law has been developed to model static damage in fibre metal laminate (FML) structures including adhesively bonded joints. Ongoing work will extend this static damage model to high cycle fatigue.

2. Theory

A mixed mode cohesive zone model with both pure mode I and mode II VUMAT code was implemented in Abaqus/Explicit for static analysis. This model included calculation of damage variables for both initiation and evolution stages based on the trapezoidal traction-separation law (Figure 1). The damage initiation variable was predicted using a quadratic nominal stress criterion (Equation 1) [4]. Strain energy release rates $G_I$ and $G_{II}$
were then calculated from the area under the trapezoidal traction-separation curve. The damage evolution variable was then calculated using a power law failure criterion (Equation 2) based on strain energy and the power law parameter $\phi$ determined from best fit to mixed-mode delamination data from the literature [5].

Figure 1: Mixed mode trapezoidal traction-separation law

$$\left(\frac{\sigma_I}{\sigma_{IC}}\right)^2 + \left(\frac{\sigma_{II}}{\sigma_{IIc}}\right)^2 = 1$$  \hspace{1cm} (1)

$$\left(\frac{G_I}{G_{IC}}\right)^\phi + \left(\frac{G_{II}}{G_{IIc}}\right)^\phi = 1$$  \hspace{1cm} (2)

3. FE Model

A simplified three element model was generated as shown in Figure 2, in order to validate the developed model for both pure mode I and mode II under static loading. The simplified model incorporated three two dimensional cohesive elements COH2D4 of length 0.25mm and thickness 0.01 mm with both pure mode I and mode II VUMAT code implemented. The properties of cohesive materials used are illustrated in Table 1. Element 1 is subjected to vertical and horizontal loads representing mode I and mode II respectively. The other two elements are fixed in x-axis and y-axis.

Table 1: Cohesive zone properties for GFRP-metal interfaces

<table>
<thead>
<tr>
<th>$G_{IC}$</th>
<th>$G_{IIc}$</th>
<th>$\sigma_{I\text{max}}$</th>
<th>$\sigma_{II\text{max}}$</th>
<th>$K_I$</th>
<th>$K_{II}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(kJ·m$^{-2}$)</td>
<td>(kJ·m$^{-2}$)</td>
<td>(MPa)</td>
<td>(MPa)</td>
<td>(N·mm$^{-3}$)</td>
<td>(N·mm$^{-3}$)</td>
</tr>
<tr>
<td>0.45</td>
<td>1.0</td>
<td>40</td>
<td>40</td>
<td>$2.189 \times 10^3$</td>
<td>$0.823 \times 10^3$</td>
</tr>
</tbody>
</table>
4. Results

The results for the developed trapezoidal traction-separation curve are validated against the bilinear traction-separation relation available in the Abaqus software as shown in Figure 3. Mode I VUMAT results (Figure 3 (a)) show that a yield stress 40 MPa is reached in the damage initiation region at a displacement of 1.827 $\times 10^{-4}$ mm for a normal stiffness of 218900 N/mm$^3$ and that this is identical to the Abaqus results in elastic region. The VUMAT results then show damage evolution starting, with stress remaining constant whilst displacement increases to 0.0068598 mm (the constant-stress region), before degrading to zero in the softening region at a failure displacement of 0.016 mm. This is in contrast to the Abaqus results which follow a bilinear traction-separation law with no constant stress region and linear degradation following damage initiation phase to failure at zero normal stress with a deflection of 0.0456674 mm.

The pure mode II VUMAT results in Figure 3 (b) show similar behaviour in the elastic region with linear behaviour up to damage initiation at the same shear yield stress (40 MPa) but as shear stiffness is lower than in the normal direction (83200 N/mm$^3$) corresponding to a displacement of 4.86 $\times 10^{-4}$ mm. This is again identical to pure mode II Abaqus results in the elastic region. Stress then remains constant up to a displacement of 0.01518 mm when softening region with degradation in stress up to failure displacement of 0.0353 mm. As for mode I, mode II Abaqus results follow a bilinear law with damage evolution starting once the shear yield stress has been achieved with displacement increasing to 0.1 mm accompanied by linear stress softening to failure at zero shear stress. Thus good correlation is found between the developed VUMAT code and Abaqus results in the elastic region for both mode I and mode II validating this part of the code with subsequent behaviour being representative of the trapezoidal traction law reported via Hutchinson[5] again for both mode I and mode II.

Contour plots of the Abaqus static damage variable SDEG and the VUMAT code static damage variable SDV for the simplified model are compared in Figure 4 (a). Both mode I and mode II results show very similar behaviour for the two codes, with both damage variables reaching one (red) for element one and indicating no damage (blue) in the other two elements due to their fixed boundary conditions. Figure 4 (b) shows the relationship between these two damage variables and the simulation time in element 1 for mode I with mode II results being very similar. The damage variables for both Abaqus and VUMAT can be seen to increase steadily with simulation time up to the maximum value of one,

![Figure 3: Comparison between VUMAT code and Abaqus software results for simplified model a) Pure mode I, b) Pure mode II](image)

Contour plots of the Abaqus static damage variable SDEG and the VUMAT code static damage variable SDV for the simplified model
and then remain constant up to the final failure. Again therefore, the results predicted by the VUMAT code are verified.

5. Conclusion

A trapezoidal traction-separation law model was proposed to simulate the elastic plastic behaviour at the interfaces of a Glare fibre metal laminate specimen. Results showed good correlation in the elastic region with those predicted using elements based on the bilinear law available in Abaqus/Explicit with overall behaviour replicating the trapezoidal law proposed by others. Thus, the model was shown to be able to simulate delamination propagation in FMLs interfaces and adhesive joints effectively.

References


DYNAMIC BRITTLE FRACTURE VIA MATERIAL POINT METHOD - A PHASE-FIELD IMPLEMENTATION

Emmanouil G. Kakouris,*Savvas P. Triantafyllou

Centre for Structural Engineering and Informatics, Faculty of Engineering, The University of Nottingham, NG7 2RD, Nottingham, UK

*savvas.triantafyllou@nottingham.ac.uk

ABSTRACT

Over the past twenty years, a number of numerical methods has been introduced to simulate dynamic brittle fracture problems. However, dynamic crack propagation is still an open problem mainly due to the fact that crack paths are highly influenced by the stress waves propagating within the material. In dynamic crack propagation, cracks can both result in or being produced by stress waves. Therefore, accurate models should be formulated to account for these phenomena. Currently, three classes of models are mainly used to simulate dynamic crack propagation. These are atomistic, lattice and continuum-based models. Atomistic models demand large computational resources, making simulation of an entire structure an arduous task. Lattice models have been reported to result in unrealistic velocities that are not observed in the experiments. Continuum-based models modify the local continuum mechanics equations and introduce cracks by considering either time-consuming remeshing strategies or discrete discontinuities in the displacement field (e.g. XFEM). In the first approach, the crack path is forced to coincide with the mesh geometry whereas in the second approach the computational complexity is increased due to the enrichment techniques within each element as the crack progresses.

Very recently, Phase field method has been introduced [1] within a fracture mechanics setting. Phase field fracture models represent cracks by means of an additional continuous field, i.e., the Phase Field that smoothly varies from zero (inside the crack) to one (away from crack). As a result, Phase-Field models overcome the need for algorithmic tracking of discontinuities. Therefore, Phase-Field method is able to handle complex crack paths, including crack branching and crack merging that are commonly observed in dynamic brittle fracture problems.

Phase Field models have already been implemented within a Finite Element setting to account for dynamic brittle fracture. However, grid based methods depend on the quality the underlying mesh. As a result, mesh distortion errors, e.g., when large deformation significantly degenerate the accuracy of the simulated response. In the case of dynamic crack propagation in particular, even minor mesh distortion results in spurious stress waves that reduce the accuracy of the numerical solution and the resulting crack path. Taking these into account, a new continuum-based method, namely Material Point Method (MPM), was developed [4]. MPM is a particle in cell method that has the potential to inherit the advantages of both Eulerian and Lagrangian approach, resulting no distortion errors. In this work, a novel, Phase-Field formulation for dynamic crack propagation of structures with Material Point Method is presented.

Key Words: Material Point Method, Phase-Field Model, Dynamic Brittle Fracture.

1. Introduction

In this work, the case of a deformable domain $\Omega$ is considered with an internal crack $\Gamma$ (see. Fig. 1(a)). According to Griffith theory [2] the potential energy of this solid body is expressed as

$$\Psi_{pot} = \Psi_{el} + \Psi_f = \int_{\Omega} \psi_{el} (\varepsilon) d\Omega + \int_{\Gamma} G_c d\Gamma$$  \hspace{1cm} (1)

where $\Psi_{el}$ and $\Psi_f$ correspond to the total elastic strain and fracture energy respectively. The term $\psi_{el} (\varepsilon)$ corresponds to the elastic strain energy density, whereas $\varepsilon$ is the strain tensor expressed as

$$\varepsilon (u) = \frac{1}{2} \left( \nabla u + \nabla u^T \right)$$  \hspace{1cm} (2)
according to infinitesimal strain theory. Furthermore, $G_c$ is the critical fracture energy density which is the energy that is required to produce a unit of fracture surface $\int d\Gamma$. According to fracture phase field theory, the fracture energy $\Psi_f$ can be approximated by introducing a crack density $Z_c$ in the whole domain $\Omega$ as

$$\Psi_f = \int_{\Gamma} G_c d\Gamma \approx \int_{\Omega} G_c Z_c(c) d\Omega$$  (3)

In this work, the crack density functional introduced in [1] is considered, which is expressed in the following form

$$Z_c(c) = \left[ \frac{(c - 1)^2}{4l_0} + l_0|\nabla c|^2 \right]$$  (4)

where $c(x, t)$ is a scalar variable called phase field and $l_0$ is the length scale parameter that controls the diffusion of damage around the crack path. In view of the potential energy introduced in Eq. (1), any increase in the fracture energy must be accompanied by a corresponding decrease in the elastic energy stored within the medium. In phase field fracture theory, this is introduced through the degradation of the elastic properties as

$$\psi_{el}(\epsilon) = g(c)\psi_{el}^+(\epsilon) + \psi_{el}^-(\epsilon)$$  (5)

where $\psi_{el}^+$ and $\psi_{el}^-$ are the strain energy density due to tension and compression respectively, while $g(c)$ is a degradation function. A widely used degradation function is [3]

$$g(c) = (1 - k)c^2 + k$$  (6)

Conversely, the energy balance equation is defined by

$$\dot{\mathcal{K}}(\dot{u}) + \dot{W}^{int}(\dot{u}, \dot{c}) - \dot{W}^{ext}(\dot{u}) = 0$$  (7)

where $\dot{\mathcal{K}}(\dot{u})$, $\dot{W}^{int}(\dot{u}, \dot{c})$ and $\dot{W}^{ext}(\dot{u})$ are the rate of kinetic, internal and external energy work functional expressed as

$$\dot{\mathcal{K}}(\dot{u}) = \frac{d}{dt} \int_{\Omega} \frac{1}{2} \rho |\dot{u}|^2 d\Omega$$
$$\dot{W}^{int}(\dot{u}, \dot{c}) = \frac{d}{dt} \int_{\Omega} (\psi_{el}(\epsilon) + G_c Z_c(c)) d\Omega$$
$$\dot{W}^{ext}(\dot{u}) = \int_{\partial \Omega} (\tilde{\tau} \cdot \dot{u}) d\Omega + \int_{\Omega} (b \cdot \dot{u}) d\Omega$$  (8)

respectively. After the necessary algebraic manipulation, the strong form is eventually derived from Eq. (7) as

$$\nabla \cdot \sigma + b = \rho \dot{u}$$  and  $$\left( \frac{4l_0 (1 - k) \mathcal{H}}{G_c} + 1 \right) c - 4l_0^2 \Delta c = 1, \text{on} [\Omega_t, \Omega_f]$$  (9)
where \( H \) is the history field defined as the maximum \( \psi^+ \) obtained in time space \([t_0, t]\). The coupled field equations (9) are subject to the following set of boundary and initial conditions

\[
\begin{align*}
\sigma n &= \bar{t} \text{ on } \partial \Omega_0, \partial \Omega_t, \\
\mathbf{u} &= \bar{u} \text{ on } \partial \Omega_0, \partial \Omega_t, \\
\mathbf{u} &= \mathbf{u}_0 \text{ on } \Omega_0, \\n\dot{\mathbf{u}} &= \ddot{\mathbf{u}}_0 \text{ on } \Omega_0, \\
\nabla c \cdot n &= 0 \text{ on } \partial \Omega_0, \partial \Omega_t,
\end{align*}
\]

where \( n \) is the outward unit normal vector of the boundary, \( \bar{u} \) is the prescribed displacement field on \( \partial \Omega_0 \) boundary, \( \bar{u} \) is the velocity field, \( \ddot{u} \) is the acceleration field and \( \rho \) is the mass density. The discrete form of phase field material point method is derived through a Galerkin approximation of the strong form defined in Eq. (9) as

\[
\begin{align*}
R^u_I(u_I) &= \sum_{p=1}^{N_p} \left[ \rho_p u_p N_I(x_p) \right] \Omega_p + \sum_{p=1}^{N_p} \left[ \sigma_p \cdot \nabla N_I(x_p) \right] \Omega_p \\
- \int_{\partial \Omega_t} \left[ \bar{t} N_I(x_p) \right] d\partial \Omega_t + \sum_{p=1}^{N_p} \left[ b_p N_I(x_p) \right] \Omega_p = 0 \\
R^c_I(c_I) &= \sum_{p=1}^{N_p} \left[ \left( \frac{4l_0^2}{G_c} \left( 1 - k_p \right) H_p \right) + 1 \right] c_p N_I(x_p) \right] \Omega_p \\
+ \sum_{p=1}^{N_p} 4l_0^2 c_p \nabla N_I(x_p) \right] \Omega_p - \sum_{p=1}^{N_p} N_I(x_p) \Omega_p = 0
\end{align*}
\]

(11)

where \( I = 1, \ldots, N_n \) and \( N_n \) corresponding to the number of grid nodes, whereas \( N_p \) is the number of material points. The acceleration, displacement and phase field values at the material points are interpolated from the corresponding grid node values with the following relations.

\[
\begin{align*}
w_{pi} &= \sum_{I=1}^{N_n} N_I(x_p) w_{li}, \\
\nabla w_{pi} &= \sum_{I=1}^{N_n} \nabla N_I(x_p) w_{li}
\end{align*}
\]

(12)

2. Test case

A benchmark test with the proposed scheme is illustrated in Figs. 4 for a plate under impact loading. The geometry, boundary conditions and material parameters are presented in Figs. 2. The pressure is considered to be \( \sigma = 1 \text{ [N/mm}^2] \). Both \( C^0 \) and \( C^1 \) B-splines are considered for this problem with cell spacing \( h = 0.125 \text{ [mm]} \). An explicit time integration is implemented with a timestep \( \Delta t = 0.025 \text{ [\mu s]} \). The resulting total elastic and fracture energy during the simulation are presented in Figs. 3(a) and 3(b) respectively.

![Figure 2: Plate under impact loading: Geometry (a) and (b) material parameters.](image)

<table>
<thead>
<tr>
<th>Material Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Elastic Material Properties</strong></td>
</tr>
<tr>
<td>Young's modulus</td>
</tr>
<tr>
<td>Poisson ratio</td>
</tr>
<tr>
<td>( \rho )</td>
</tr>
<tr>
<td><strong>Phase-Field Material Properties</strong></td>
</tr>
<tr>
<td>( l_0 )</td>
</tr>
<tr>
<td>( G_c )</td>
</tr>
<tr>
<td>( k )</td>
</tr>
</tbody>
</table>
Figure 3: Plate under impact loading: (a) Total elastic strain energy (b) Total fracture energy.

Figure 4: Plate under impact loading: Phase field for timestep (a) $t = 0 \, [\mu s]$ (b) $t = 50 \, [\mu s]$ (c) $t = 65 \, [\mu s]$ and (d) $t = 80 \, [\mu s]$.

References


Adaptive Hierarchical Refinement in Isogeometric Analysis for Cohesive Fracture

*L. Chen, R. de Borst

1Department of Civil and Structural Engineering, University of Sheffield, Sir Frederick Mappin Building, Mappin Street, Sheffield, S1 3JD

*lin.chen@sheffield.ac.uk

ABSTRACT
This paper is concerned with the use of adaptive hierarchical refinement in isogeometric analysis (IGA) for cohesive fracture modeling. In the analysis, the crack interface is introduced by knot insertion in the NURBS basis, which yields $C^{-1}$ continuous basis functions. To capture the stress state smoothly in the vicinity of crack tip, the hierarchical refinement in IGA is used with successive $h$-refinement of a coarse initial mesh. In this respect, a multi-level mesh is constructed. It is employed to describe the moving mesh around the crack tip. An element-wise viewpoint and Bézier extraction are adopted, which allows to implement the method in any finite element code. The accuracy of the approach is validated by a numerical example.

Key Words: fracture; cohesive zone model; NURBS; isogeometric analysis; hierarchical refinement

1. Introduction
Cohesive zone models are widely employed in fracture modeling [1]. In contrast to the brittle fracture model, the cohesive zone model considers the tractions between the crack faces to vanish gradually upon further crack opening. To describe this model mathematically, the traction in the fracture zone is related with the crack opening by a traction-opening law [1, 2]. Over the past decades, various finite element technologies have been presented to incorporate the cohesive zone model [1]. Recently, isogeometric analysis (IGA) has been introduced in crack propagation analysis [3, 4]. It has been suggested that IGA can predict the structural response accurately when the crack propagates along a pre-defined interface. However, standard refinement in IGA will lead to more degrees of freedom due to the tensor-product structure of splines. Hence, the local refinement is necessary for improving the efficiency. In this contribution, we will employ adaptive hierarchical refinement [5] for cohesive crack modelling. Knot insertion will be used to introduce the crack interface, while adaptive hierarchical refinement will be adopted in the mesh refinement around the crack tip. A smooth stress state will result that be captured accurately with less degrees of freedom.

2. Cohesive zone formulation
In the cohesive zone model the crack is represented as an adhesive interface $\Gamma_c$ in the physical domain $\Omega$, see Figure 1. The strong form of equilibrium equations is given as

$$\nabla \cdot \sigma = 0 \quad \text{on} \quad \Omega; \quad u = \hat{u} \quad \text{on} \quad \Gamma_u; \quad \sigma \cdot n = \hat{t} \quad \text{on} \quad \Gamma_t; \quad \sigma \cdot n = t(\|u\|) \quad \text{on} \quad \Gamma_c$$

in which $n$ denotes the normal vector at the boundaries, $\hat{u}$ and $\hat{t}$ represent the prescribed displacements and tractions, respectively. $\sigma$ is the Cauchy stress tensor, which relates to the infinitesimal strain tensor $\varepsilon$ as $\sigma = C\varepsilon$ with $C$ the elastic stiffness tensor. The crack opening $\|u\|$ is defined as $\|u\| = u^+ - u^-$ with $u^+$ and $u^-$ the displacement at $\Gamma_+^c$ and $\Gamma_-^c$, respectively, see Figure 1.

In a standard isoparametric sense, NURBS basis functions will be employed to describe the geometry of the solid [3], but also to interpolate the displacement field $u$:

$$x(\xi^1, \xi^2) = \sum_{I=1}^{n_f} N_I(\xi^1, \xi^2) X_I \quad u(\xi^1, \xi^2) = \sum_{I=1}^{n_f} N_I(\xi^1, \xi^2) U_I$$
in which $X_I$ represents the coordinates of so-called control points, $U_I$ denotes the degrees of freedom at the control points, and $n_c$ is the total number of control points. The NURBS basis function $N_I(\xi^1, \xi^2)$ could be obtained from [3], which is defined upon two univariate NURBS basis functions $N_{pi}^p$ and $N_{pq}^q$ ($p, q$ denote polynomial degrees). In general, $N_{pi}^p$ is $C^{p-m_i}$ continuous, which means $N_{pi}^p$ is $p-m_i$ times continuously differentiable over the knot $i$, and $m_i$ is the multiplicity of knot vector employed to define $N_{pi}^p$. This higher-order continuity is beneficial for solving higher-order differential equations. It is also favourable to produce interface $\Gamma_c$ in the solid [3], which requires $C^{-1}$ continuity. In this contribution, we will employ this approach for the crack description.

To solve Eq. (1), the weak form of the equilibrium equation is employed:

$$
\int_{\Omega} B^T \sigma d\Omega + \int_{\Gamma_c} H^T t (\|u\|) d\Gamma = \int_{\Gamma_t} N^T \hat{t} d\Gamma
$$

(3)

in which $\sigma$ is the Cauchy stress tensor. $N$, $B$ and $H$ are matrices that contain the shape functions, the derivatives of the shape functions, and the jump in the shape functions, respectively [3]. Linearisation of Eq. (3) yields the tangential stiffness matrix.

$$
K = \int_{\Omega} B^T C B d\Omega + \int_{\Gamma_c} H^T R^T T_d R H d\Gamma
$$

(4)

where $R$ denotes the rotation matrix [4]; $T_d$ represents the tangential stiffness matrix of the traction-opening law at the interface $\Gamma_c$ [4].

3. Hierarchical refinement for cohesive crack growth

In this contribution, the hierarchical basis functions are considered in an element-wise viewpoint, which conforms ideally to the Bézier extraction framework [5]. In the implementation, the hierarchical basis functions are defined over multiple hierarchy levels. We firstly construct a hierarchy of $P$ levels. The basis functions on each hierarchy level are defined over the knot vector $\Xi_i$ ($i = 0, 1, \ldots, P - 1$) with identical polynomial degree $p$. $\Xi_i$ is obtained by successive uniform knot insertion within $\Omega_d$ from the initial knot vector $\Xi_0$ and $\Omega_d$ denotes the parametric domain. Consequently, one obtains nested parametric domains $\Omega_d^i \subset \Omega_d^{i+1}$ and nested knot vectors $\Xi_i \subset \Xi_{i+1}$. Each knot vector $\Xi_i$ defines a set of NURBS basis functions $N^i = \{N_{ij}^i\}_{j=1}^{ni}$ which in turn forms a nested NURBS approximation space $N^i$. Due to the nested nature of $N^i$, the basis functions of hierarchy level $i$ can be described by the basis functions on hierarchy level $j$:

$$
N^i = S^{i,j} N^j = \sum_{l=i}^{j-1} S^{l,l+1} N^{l+1}
$$

(5)

where $S^{l,l+1}$ is the subdivision or refinement operator [5].

Figure 1: Domain $\Omega$ with crack interface $\Gamma_c$. Here, $\Gamma_c$ is represented by overlapping positive and negative sides $\Gamma_c^+$ and $\Gamma_c^−$, respectively.
To construct the hierarchical basis function space \( \mathcal{A} \), one needs to identify the active elements and basis functions in the multi-level hierarchy. The active element is chosen by a certain marking criterion, such as a posteriori error estimator \([5]\). It is defined across different hierarchy levels without any overlap or gap. Starting from the active elements, one needs to define a linearly independent hierarchical basis function space \( \mathcal{A} \), which will be employed to describe the geometry of the solid and to approximate the solution space. Here, we have taken an element-based selection approach to construct \( \mathcal{A} \) \([5]\).

Given the active elements and basis functions, one can subsequently insert the hierarchical basis functions to obtain the stiffness matrix in a multi-level adaptivity approach \([5]\). The final system of equations is

\[
K_h U_h = F_h \quad \text{with} \quad K_h = M_h K M_h^T \quad \text{and} \quad F_h = M_h F
\]

where \( K \) denotes the assembly of the stiffness matrix on each hierarchy level, with no consideration of interaction between multi-level basis functions, \( U \) includes the nodal degrees of freedom on each level such that \( U = M_h^T U_h \), \( F \) represents the force vector, \( M_h \) is the hierarchical subdivision operator.

With the multi-level implementation of hierarchical basis functions in place, we proceed to its application in the adaptive refinement during cohesive crack growth simulation. The steps for the adaptive hierarchical refinement are listed below:

1. Solve Eq. (6) to obtain the displacements \( U_h \) and \( U \).
2. Compute the crack opening \( \| a \| \) at the interface \( \Gamma_c \) by Eq. (1).
3. Check the crack opening \( \| a \| \) and mark elements for refinement and coarsening.
4. Refine or coarsen the marked elements. If no element is required to be refined or coarsened, stop the calculation here; otherwise return to S1.

Figure 2: Fibre with a circular cross section. (a) schematic representation of the full model; (b) one quarter of the fibre considering symmetric boundary conditions; (c) initial mesh for the fibre-epoxy model.

### 4. Numerical example

The example of a fibre-epoxy debonding experiment is chosen here, which has been studied before in, for example, \([3]\). The problem is analyzed using a two dimensional model and applying plane-strain conditions. The geometry of the specimen is shown in Fig. 2. By virtue of symmetry, only one quarter of the specimen has been considered. The material properties of the bulk material are: (a) fibre elastic modulus \( E = 225 \text{GPa} \) and Poisson’s ratio \( \nu = 0.2 \); (b) epoxy elastic modulus \( E = 4.3 \text{GPa} \) and Poisson’s ratio \( \nu = 0.34 \). The traction on the fibre-epoxy interface \( \Gamma_c \) is determined by Xu-Needleman law with a fracture strength \( t_u = 50 \text{MPa} \) and a fracture toughness \( G_c = 4 \times 10^3 \text{N/mm} \). A hierarchy of 3 levels has been constructed on the basis of the initial mesh of Figure 2c. The order of the NURBS basis functions is \( p, q = 2 \). The response of the model is presented in terms of the horizontal stress \( \sigma_1 \) as a function of the prescribed displacement \( \bar{u} \) in Figure 3a. As shown in the figure, the results agree well with the
reference solution [3]. Initially, the stress increases with the rise of the presented displacement. Then, a softening behavior is observed in the response curve due to the debonding of the fibre and epoxy. After the complete debonding, the stress increases again as the prescribed displacement is increased.

The debonding process of the fibre and epoxy is illustrated in Figures 3b and 3c. The crack propagates gradually with the increase of prescribed displacement. The element refinement is performed with the crack growth. The displacement and stress remain smooth in both the fibre and the epoxy. During debonding, the interface still carries tractions due to the traction-opening law.

Figure 3: Response curve, horizontal displacement and stress distribution for the fibre-epoxy. (a) response curve for the model; the stress component $\sigma_1$ at $x_A = (15, 0) \mu m$ is plotted versus $\bar{u}$; (b) $u_1$ contour plot under $\bar{u} = 0.1 \mu m$; (c) $\sigma_1$ contour plot under $\bar{u} = 0.2 \mu m$. The crack opening has been amplified by a factor 10.

5. Conclusion

Herein, a NURBS basis has been employed to represent the crack interface. It is achieved by knot insertion until $C^{-1}$ continuity attained. To capture the stress state accurately around the crack tip, hierarchical refinement has been used, in which a coarse mesh was refined by successive knot insertion in the domain of interest. The use of an element-wise point of view allows to dynamically change the mesh during the simulation. Moreover, the application of Bézier extraction enables to implement the method into any existing finite element code. A numerical example shows that the ability of hierarchical refinement is well suited for the analysis of crack propagation. An accurate solution has been obtained for a relatively coarse initial mesh.

Acknowledgements

The financial support of the European Research Council (ERC Advanced Grant 664734 PoroFrac) is gratefully acknowledged.

References


HIGHER ORDER GRADIENT CONTINUA: AN ISOGEOMETRIC APPROACH

*Isa Kolo¹, Harm Askes¹ and René de Borst¹

¹Department of Civil and Structural Engineering, University of Sheffield, Mappin Street, Sheffield, S1 3JD

*ikolo1@sheffield.ac.uk

ABSTRACT

Standard continuum mechanics theories are largely insufficient in capturing size effects observed in many engineering materials: metals, composites, rocks etc. This is attributed to the absence of a length scale that accounts for microstructural effects inherent in these materials. Enriching the classical theories with an internal length scale solves this problem. One way of doing this in a theoretically sound manner is introducing higher order gradient terms in the constitutive relations. In elasticity, introducing a length scale removes the singularity observed at crack tips using the classical theory. In plasticity, it eliminates the spurious mesh sensitivity observed in softening/localisation problems by defining the width of the localisation zone thereby maintaining a well-posed boundary value problem. However, this comes at the cost of more demanding solution techniques.

Higher order continuity is usually required for solving higher order gradient continuum theories. While this is not straightforward using traditional finite elements, isogeometric analysis, which exploits spline-based shape functions naturally, incorporates higher-order continuity. In this work, we take advantage of the higher order continuity provided by isogeometric analysis to solve problems in gradient elasticity and gradient plasticity. Specifically, cases with Laplacian (second-order) gradient terms are considered.

Key Words: higher-order gradient continuum; gradient elasticity; gradient plasticity; isogeometric analysis; NURBS

1. Introduction

In higher-order gradient continuum models, a length scale is incorporated by adding higher-order spatial derivatives. This regularises the model so that well-posedness of the boundary value problem is preserved upon the development of a localisation zone for a quasi-static elastoplastic material with a softening behaviour. In a purely elastic material, it is motivated by removal of singularities at crack tips. In both cases, the incorporated length scale enhances robustness so that size effects can be captured.

The gradient elasticity model where the stress depends on the Laplacian of the strain in addition to its usual dependence on the strain is considered here [1]. This gives rise to a single length scale and the equilibrium equation becomes a fourth-order partial differential equation:

\[ D_{ijkl} (u_{k,jl} - \ell^2 u_{k,jlmm}) = 0 \]  \hspace{1cm} (1)

where \( u_i \) are the displacements, \( \ell \) is the length scale, \( D_{ijkl} \) contains the elastic constants and the body forces have been ignored. To discretise the weak form of this equation, \( C^1 \)-continuous shape functions are required.

For elastoplastic materials, we consider the von Mises gradient plasticity model with linear softening in which the yield function depends on the effective plastic strain measure, \( \kappa \), as well as its Laplacian, \( \nabla^2 \kappa \) [3]. The yield function is given as:

\[ F = \sqrt{\frac{3}{2} \sigma^T \mathbf{P} \sigma} - (\sigma_y + H \kappa + \ell^2 H \nabla^2 \kappa) \]  \hspace{1cm} (2)
where $\mathbf{\sigma} = [\sigma_{xx}, \sigma_{yy}, \sigma_{xy}]^T$ is the stress vector (in plane strain configuration), $\sigma_y$ is the initial yield strength, $H$ is the constant softening modulus, $\ell$ is a length scale and the symmetric matrix $\mathbf{P}$ is expressed as:

$$
\mathbf{P} = \begin{bmatrix}
\frac{2}{3} & \frac{-1}{3} & 0 \\
\frac{-1}{3} & \frac{2}{3} & 0 \\
0 & 0 & 2
\end{bmatrix}.
$$

(3)

To employ the finite element method, the gradient-dependent yield function (2) has to be satisfied only in a weak sense like the classical equilibrium equation:

$$
D_{ijkl} u_{k,ji} = 0
$$

(4)

In addition to the displacement field, the plastic strain field has to be discretised. As a result, there is a need for $C^1$-continuous shape functions.

Isogeometric analysis [5] exploits Non-Uniform Rational B-Splines (NURBS) shape functions with which one straightforwardly obtains $C^{p-1}$-continuity for NURBS of order $p$. This makes the method well suited as a solution technique, in addition to its advantage of eliminating geometric discretisation errors.

2. NURBS Shape Functions

In isogeometric analysis, the spline-based (NURBS) shape functions used to describe the geometry in computer-aided design (CAD) are directly used for analysis. A univariate NURBS is expressed as:

$$
R_{a,p}(\xi) = \frac{w_a B_{a,p}(\xi)}{W(\xi)}
$$

(5)

where $B_{a,p}(\xi)$ is the B-spline shape function, $w_a$ is the NURBS weight and the weight function,

$$
W(\xi) = \sum_{b=1}^{n} w_b B_{b,p}(\xi)
$$

(6)

The B-Spline shape function for a polynomial of degree $p = 0$ is defined as:

$$
B_{a,0}(\xi) = \begin{cases}
1, & \xi_a \leq \xi \leq \xi_{a+1} \\
0, & \text{otherwise}
\end{cases}
$$

(7)

for any knot (parametric coordinate) $\xi$. For $p > 0$, it is defined by the Cox-de Boor recursion formula [5]. Multivariate NURBS shape functions are obtained as tensor products of the univariate shape functions. Unlike Lagrange shape functions, NURBS shape functions are not local to an element. In order to make NURBS shape functions suitable for analysis in the standard finite element format, Bézier extraction [2] is employed. This approach has been used herein to implement the formulations of gradient elasticity and gradient plasticity in the C++ open source code, Jive [4].

3. Gradient Elasticity

Figure 1 shows the simulation results for a quarter cylinder with inner and outer radii 0.05 m and 0.5 m respectively. Young’s modulus $E = 8000$ MPa and Poisson ratio, $\nu = 0.35$. A polynomial of order 3 is adopted. A convergence analysis carried out (results not shown) revealed a theoretical convergence rate of $-1.5$ which matches the theoretical value of $O(nDOF^{- \frac{p}{2}})$ based on the number of degrees of freedom ($nDOF$) [6].

4. Gradient Plasticity

To demonstrate the applicability of NURBS-based discretisation in gradient plasticity, we consider a 100 mm long elastoplastic bar subjected to tension as shown in Figure 2. The initial yield strength $\sigma_y$ is 2 N/mm$^2$, the softening modulus $H = -2000$ N/mm$^2$, and $E = 20000$ N/mm$^2$. To trigger localisation, an
imperfection is introduced at the centre 3.125 mm of the bar by a 10% reduction in the yield strength. Two uniform meshes, with 64 and 128 elements respectively, are considered. Cubic interpolation ($p = 3$) is used for the displacement and quadratic interpolation ($p = 2$) for the plastic strain. This is because the displacement is one order higher than the strain.

As demonstrated in Figure 3, the load-displacement curves for both discretisations perfectly match, indicating no mesh dependence. Moreover, they are in agreement with the analytical solution, cf. [3]. This is further examined by checking the evolution of the effective plastic strain shown in Figure 4. The width of the localisation zone for both meshes matches well with the theoretical value $w = 10\pi \approx 31.4$ mm.
5. Conclusion

Isogeometric finite elements have been shown to be capable of solving problems in gradient elasticity and gradient plasticity, where discretisation requires the shape functions to be $C^1$-continuous. This is possible because NURBS shape functions naturally offer higher-order continuity.

References


Self-similarity of a Brittle Fracture Phase Field Model

*Arne C. Hansen-Dörr¹, Markus Kästner¹ and René de Borst²

¹ Institute of Solid Mechanics, TU Dresden, 01062 Dresden, Germany
² Department of Civil and Structural Engineering, University of Sheffield, Sheffield, S1 3JD

*arne.hansen-doerr@tu-dresden.de

ABSTRACT

The brittle fracture phase field model introduced by Francfort et. al. [2] and adapted by Miehe et al. [1] offers an elegant way to simulate crack nucleation and propagation in bulk solids. No crack path has to be specified since it emerges as a part of the solution. Phase field models are capable of reproducing qualitatively good results when it comes to physical crack patterns. Besides the Young’s modulus and Poisson’s ratio, the fracture toughness and the characteristic length scale directly influence the cracking behaviour. We vary the fracture toughness in order to improve the quantitative understanding of the model. The fracture toughness determines how much energy is dissipated during the fracture process. Larger values lead to a proportionally higher energy dissipation during crack growth. We will show that this relation does not only hold globally, i.e. for the complete failure process, but for every single point during failure. In other words, one obtains the solution for any value of the fracture toughness knowing the result of a single simulation. This local scaling behaviour is referred to as self-similarity.

The theoretical reasoning is supported by two 2D computational examples dealing with mode-I and mixed-mode cracking.

Key Words: brittle fracture; phase field; self-similarity

1. Introduction

The phase field approach used to model brittle fracture in homogenous media makes use of a regularisation procedure. Following Miehe et al. [1], the total free Helmholtz energy of a brittle, linear elastic material reads

\[ \Psi = \Psi^\text{el} + \Psi^c = \int_\Omega \psi^\text{el} + \psi^c \, dv = \int_\Omega g(c) \cdot (\psi^\text{el}_+ + \psi^\text{el}_-) + \frac{G_c}{4l_c} \left\{ (1 - c)^2 + 4l_c^2 c_{,ij} c_{,ij} \right\} \, dv. \]  

(1)

For the specific elastic free Helmholtz energy \( \psi^\text{el} = \frac{1}{2} e_{ij} E_{ijkl} e_{kl} \) a tensile split according to Borden [3] into a tensile \( \psi^\text{el}_+ \) and a compressive \( \psi^\text{el}_- \) part is carried out to degrade the material’s tensile loading capacity. Often, the degradation function \( g(c) = c^2 \) is used. In addition to the linear and angular momentum equations a micro force balance [3] is used to derive the small strain local balance equations

\[ \sigma_{ij,i} = 0 \quad \text{with} \quad \sigma_{ij} = \sigma_{ji} \]  

(2)

and

\[ (1 - c) + 4l_c^2 c_{,ii} = \frac{2g'(c)c_l}{G_c} \mathcal{H} \]  

(3)

with the history variable \( \mathcal{H}(t) = \max_{\tau \leq t} \psi^\text{el}_+(\tau) \) and \( \tau \in [0, t] \) taking the value of the highest \( \psi^\text{el}_+ \) ever reached. This prevents crack healing. The right hand side of equation (3) is referred to as the phase field driving force \( \mathcal{F} \). The equations are complemented by the boundary conditions \( \sigma_{ij} n_i = \bar{t}_j \) on \( \partial \Omega_t \), \( u_i = \bar{u}_i \) on \( \partial \Omega_u \) with \( \partial \Omega = \partial \Omega_t \cup \partial \Omega_u \), \( \emptyset = \partial \Omega_t \cap \partial \Omega_u \) and \( c_{,ij} n_i = 0 \) on \( \partial \Omega \).
Figure 1: Total and incremental dissipation: (a) The specimen is loaded until complete failure (orange mark) occurs. The hatched area equals the energy dissipated during cracking. (b) Both specimen are loaded until points P and Q. Afterwards, the load is reduced to $u = 0$ mm. The hysteresis-like areas between the loading and unloading curves resemble the dissipated energy.

2. Dissipation of Energy

In the following the Young’s modulus $E$, the Poisson’s ratio $\nu$ and the length scale $l_c$ are set to a constant, non-zero value. The fracture toughness is set to a reference value $G_c = G_{c1}$. Figure 1a describes the force displacement curve of a fictional specimen loaded under previously mentioned conditions. The force $F$ is recorded at the same point as the displacement load $u$.

As the loading starts, the driving force $F$ takes non-zero values and the phase field and the crack starts to develop. At a certain point, the crack propagates and eventually, the specimen is fully cracked (orange marker). The elastic energy $\Psi_{el}$ has become zero and the crack energy takes a value $\Psi_c \neq 0$ which is characterized by the current phase field and the fracture toughness. The latter is equal to the hatched area under the force displacement curve resembling the dissipated energy.

This procedure is repeated with the same values except for the fracture toughness $G_{c2} = 2G_{c1}$. Since the fracture toughness is higher, the driving force $F$ is inversely proportional, and therefore lower than in the first case. Compared to the first case the phase field’s evolution is delayed. The slower development of the phase field in the second case affects the history variable and the degradation function used for a second load step since both are (in-)directly influenced by the phase field. Generally speaking the driving force is continuously scaled for the second case. However, this does not affect the crack topology obtained at the end of loading (orange marker) because a simple scaling of the driving force for each point within the domain does not influence the topology. As soon as the second specimen is fully broken, the phase field is identical to the fully broken first specimen’s phase field. As a consequence, the dissipated energy $\Psi_c$ is twice as high for the second case as for the first one because everything is identical except for the fracture toughness.

Both cases, $G_{c1}$ and $G_{c2}$, are reconsidered with a slight load modification. As Figure 1b depicts, both specimens are unloaded at points P and Q before complete failure in a way their elastic unloading curves match. The area below the unloading curve is equivalent to the remaining elastic energy after partial degradation. Note that in both cases the bulk must have degraded equally since they share the same elastic unloading path. We recall that the elastic degradation is implemented by the degradation function $g(\varepsilon)$ which acts on the tensile part of the elastic energy $\Psi_{el}$. As the crack topology evolves similarly
Figure 2: Geometry and boundary conditions for the square specimen under (a) tensile and (b) shear load. The reference values are $l_{\text{ref}} = 0.5 \text{ mm}$ and $h_{\text{ref}} = 1 \text{ mm}$. The pre-existing crack $\Gamma$ is incorporated discretely by introducing double nodes, one for the upper and one for the lower crack boundary.

(but at different ‘speeds’) for both cases, there is but one possibility to achieve the same global elastic degradation: the phase field is identical for the points $P$ and $Q$. Hence, the dissipated energy accumulated in $\Psi^c$ and visually described as the area between the loading and elastic unloading curves proportionally scales like the fracture toughness. Thus, the dissipated energy does not only scale globally but also incrementally for any time or load step. This behaviour is referred to as self-similarity.

3. Numerical Examples

The theoretical reasoning is illustrated by two simulations featuring a square specimen subjected to tensile and shear load. The geometry and boundary conditions are described in Figure 2. The Young’s modulus, the Poisson’s ratio and the characteristic length scale were set as $E = 2.1 \times 10^5 \text{ MPa}$, $\nu = 0.3$, $l_c = 15 \mu\text{m}$. Plane strain conditions were assumed. The specimens were loaded using displacement control. The force displacement curves were recorded at the loading points as indicated in Figure 2.

Figures 3 and 4 give the force displacement curves. For each case three simulations are presented with different fracture toughnesses. Since the area under the force displacement curves scales proportionally, similar to the fracture toughness, the force $F$ and the displacement $u$ have to be normalized by $\sqrt{G_c}$ to achieve a proper scaling.

4. Conclusion

The fracture toughness scales proportionally to the amount of energy which is dissipated during the fracture process for homogenous materials. It does not have an influence on the crack topology and reduces to a constant which may be adjusted to different values knowing the results of a single simulation. This local scaling behaviour is referred to as self-similarity.

References


Figure 3: *Square specimen* tensile load: (a) The curves do not exactly reach $F = 0$ N due to a residual stiffness preserved to avoid numerical instabilities. (b) Scaling reveals self-similarity.

Figure 4: *Square specimen* shear load: (a) The curves of the mixed-mode crack simulation are much less smooth than those of both mode-I simulations. (b) However, the tiny peaks scale perfectly.
Explicit 3D crack modelling by the Cracking Particle Method

*Weilong Ai\(^1\) and Charles E. Augarde\(^1\)

\(^1\)School of Engineering and Computing Sciences, Durham University
South Road, Durham, DH1 3LE, United Kingdom

*weilong.ai@durham.ac.uk

ABSTRACT

A robust approach for explicit description of 3D cracks by the Cracking Particle Method is presented. Crack surfaces are simulated by a set of cracking particles with discontinuous segments cutting through their supports. The discontinuities of cracks are achieved by the visibility criterion and particles located on crack surfaces are assumed cracked and split into two groups on opposite sides of cracks. Crack shapes are obtained directly by capturing the locations of cracking particles rather than by extra description functions like level sets. This method is tested by an example of penny-shaped crack in an infinite cube and good accuracy is obtained.

Key Words: 3D cracks; cracking particle method; meshless

1. Introduction

Computational fracture modelling is of great importance to study the failure of engineering structures. Currently, the majority focus on two dimensional (2D) crack problems and few are working on three dimensional (3D) situations due to their complexities. Moving from 2D to 3D not only leads to a heavier calculation burden for one more degree of freedom but also brings more complicated crack patterns. Crack fronts can be arbitrary curves rather than a point in 2D, giving more difficulties for the description of crack geometries.

Over the past decades, several numerical methods have been tried to solve 3D crack problems. The Finite Element Method (FEM), as the most common numerical method for solid mechanics, divides a problem domain with small meshes (usually tetrahedrons or hexahedrons in 3D). It makes use of mesh faces to represent crack surfaces [1] but suffers from the requirement of remeshing to match mesh faces with crack directions during the crack propagation process. The eXtended Finite Element Method (XFEM) [2] can make the crack representation independent with the mesh by introducing discontinuous enrichment functions and therefore is widely used for crack modelling. The Element Free Galerkin Method (EFGM) [4] discretizes a problem domain with only nodes so problems of mesh distortion and volumetric locking can be avoided. However, both methods needs other methods like level sets to capture crack geometries, and updating those functions is not cheap computationally. There is also a requirement of additional node arrangements for calculating level set functions as in [5] if those methods are used.

The Cracking Particle Method (CPM) is a promising alternative, in which cracks are approximated by a collection of cracking particles and no level set functions are required [6, 7]. Cracking particles possess discontinuous segments cutting through their supports. Crack propagation is treated by transforming normal particles into cracking particles. The original CPM mainly focused on dynamic fracture problems, and a modified CPM was presented in [8] and applied to static problems providing solutions with smoother crack path. This paper extends the modified CPM to 3D problems and demonstrates its advantages with a penny-shaped crack problem.
2. Fundamental equations

The CPM is a meshless method based on the EFGM where the approximated displacements $u^h(x)$ are given by a summation of shape functions $\Phi_I(x)$ and nodal values $u_I$ as

$$u^h(x) = \sum_{I}^{n} \Phi_I(x)u_I,$$  \hspace{0.5cm} (1)

where $I$ is the node index and $n$ is the number of nodes with support covering $x$. The shape functions are determined through a moving-least square process as in [3], which are evaluated as

$$\Phi_I(x) = p(x) \cdot A(x)^{-1} \cdot \sum_{I}^{n} w_I(x)p(x_I),$$ \hspace{0.5cm} (2)

$$A(x) = \sum_{I}^{n} w_I(x)p^T(x_I) \cdot p(x_I),$$ \hspace{0.5cm} (3)

where $p^T(x)$ are the basis functions. A linear basis in 2D is $p^T(x) = [1, x, y]$ and $p^T(x) = [1, x, y, z]$ in 3D. The weight functions used here are

$$w_I(x) = w(s) = \begin{cases} 1 - 6s^2 + 8s^3 - 3s^4 & \text{if } s \leq 1, \\ 0 & \text{if } s > 1. \end{cases}$$ \hspace{0.5cm} (4)

where $s$ is the ratio of distance between $x$ and $x_I$ and the support size $R_I$.

3. Crack modelling

The discontinuity at a crack surface can be achieved by modifying either basis functions or weight functions. The original CPM [6] uses the first way by introducing discontinuous enrichment functions, which leads to an increase of unknowns in the problem. Those extra unknowns can be removed by splitting the cracking particles as in [7]. The original CPM suffers from spurious cracks and this kind of problems is alleviated by introducing a strategy of bilinear segments as in Fig 1 (a) [8]. In this paper the strategy is extended to 3D crack problems. A sphere support of a cracking particle is split into two parts and each part has discontinuous segments with shapes according to cracks, e.g. half circles in Fig 1 (b).

The visibility criterion is used to distinguish these particles on both sides of cracks. The crack opening is evaluated by the following equation in which $[\cdot]$ stands for the relative displacements,

$$\|u(x)\| = \sum_{l \in S^+} \Phi_I(x^{S^+})u_I - \sum_{l \in S^-} \Phi_I(x^{S^-})u_I.$$ \hspace{0.5cm} (5)

Figure 1: Strategy of splitting the cracking particles: (a) 2D support; (b) 3D support
4. Numerical examples

A penny-shaped crack problem is shown in Fig 2 where the dimensions are $h = w = t = 200$ mm, $2a = 20$ mm. The material is linear elastic with Young’s modulus $E = 100$ GPa and Poisson’s ratio $\nu = 0.3$. Uniform loading is applied onto the top and bottom faces with $\sigma = 100$ N/mm$^2$. A regular arrangement of nodes $15 \times 15 \times 15$ is used initially and the volume integrations are performed on $14 \times 14 \times 14$ cells each with $4 \times 4 \times 4$ Gauss points. The surface integrations of external forces are calculated on $14 \times 14$ cells each with $8 \times 8$ Gauss points. The analytical solutions for crack opening and mode I stress intensity factor (SIF) $K_I$ from [9] are

$$u = \frac{4(1 - \nu^2)}{\pi E} \sigma \sqrt{a^2 - r^2}, \quad (6)$$

$$K_I = \frac{2}{\pi} \frac{\sigma}{\sqrt{\pi a}}, \quad (7)$$

An adaptive approach from [8] is used for error control. Cells are refined around crack fronts automatically and the number of nodes increases from 3696 to 13550 during adaptivity. Final displacements are shown in Fig 3 and some curvatures of displacements can be found in Fig 3 (b). From Fig 4 (a), it can be seen that the predicted crack opening shape agrees well with Eq (6) in four different directions, in which $\theta$ is the angle along the front measured anticlockwise from the $x$-axis. Good agreements can also be found in...
the comparison between calculated $K_I$ and analytical results, where $K_I$ is normalized by $F_I = \frac{K_I}{\sigma \sqrt{\pi/a}}$ and calculated by an interaction integration used in [8].

5. Conclusions

A new methodology for 3D crack modelling has been proposed, which is based on the cracking particle method. Cracks are modelled explicitly by a set of cracking particles and no level set functions are required. Crack opening shapes can be accurately obtained by capturing the displacements of cracking particles. An adaptive approach is introduced to control the errors around crack fronts and there is good accuracy for the calculation of SIFs.

Acknowledgements

Support from the China Scholarship Council and Faculty of Science, Durham University is acknowledged.

References


AN IMPLICIT IMPLEMENTATION OF NON-ORDINARY STATE-BASED PERIDYNAMICS

*Nur A. Hashim¹, ², W. M. Coombs¹, G. Hattori¹ and C. E. Augarde¹

¹School of Engineering and Computing Sciences, Durham University, South Road, DH1 3LE, Durham, UK
²Department of Civil Engineering, School of Environmental Engineering, Universiti Malaysia Perlis, 02600 Arau, Perlis, Malaysia

*nur.a.hashim@durham.ac.uk

ABSTRACT

Peridynamics is a non-local continuum theory that was introduced by Silling. Its key advantage is its use of integral equation forms of the underlying physics, as compared to the partial differential equations in, say the finite element method and therefore does not need any extra assumptions to treat singularities. In this paper we present an implicit implementation of the non-ordinary state-based peridynamics formulation. Fracture is introduced into the peridynamic model by allowing bonds to break irreversibly. Bond breakage occurs when a damage criterion is satisfied, for instance, if the bond exceeds a critical stretch. This paper presents for the first time an implicit formulation of non-ordinary state-based peridynamic theory for finite deformation mechanics. An iterative procedure based on the Newton-Raphson method is used to solve the discretised problem.

Key Words: peridynamics; non-local models; non-ordinary state-based formulation; fracture; implicit model

1. Peridynamic Theory

An implicit time integration scheme allows us to perform a dynamic simulation with a larger time step for convergence and thus reduce the computational time than what would be permitted with an explicit integration scheme. However, an implicit time integration scheme can be much harder to implement. There are only a few existing examples of implicit implementations of peridynamics in the literature. A small-strain linearly elastic static implementation of the non-ordinary state-based peridynamics formulation is developed in [5, 6] and it is used to solve non-linear deformation problems for crystal plasticity simulations in [7].

In preparation for the derivation of the implicit non-ordinary state-based peridynamic scheme, a brief review of the underlying peridynamic theory is needed. In peridynamics, the problem domain is discretised by particles through bonds. The interaction between particles \( x \) and \( x' \) occurs over a finite distance defined by a given ‘horizon’, \( R \). The kinematics of peridynamics theory in 2D is shown in Figure 1.

![Figure 1: Particle x interacts with particle x' within a spherical neighborhood, R.](image)

The relative position of two particles is denoted by \( \xi = x' - x \) and relative displacement by \( \eta = u' - u \) where \( u \) and \( u' \) are the displacement of particle \( x \) and \( x' \). The relationship among the variables is illustrated in Figure 2.
In classical continuum mechanics, the equation of motion derived from the conservation of linear momentum and can be expressed as

$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \nabla \cdot \mathbf{\sigma} + \mathbf{b}(\mathbf{x}, t),$$

(1)

where $\rho$ is the mass density in the reference configuration, $\ddot{\mathbf{u}}$ denotes the acceleration, $\mathbf{\sigma}$ is the Cauchy stress and $\mathbf{b}$ is the prescribed body force density field [3]. However, in (1), the spatial derivative is undefined along discontinuities.

In contrast, peridynamics uses an integral function of a force on particle at $\mathbf{x}$ to replace the divergence of the stress term, that is

$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \int_R \mathbf{f}(\eta, \xi) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t),$$

(2)

where $\mathbf{f}$ is the pairwise peridynamic force function that the particle $\mathbf{x}'$ exerts on $\mathbf{x}$, $dV_{\mathbf{x}'}$ is volume associated with particle $\mathbf{x}'$. These basic equations can be applied anywhere in the body, so no additional theories are needed for studying fracture using the peridynamic method.

However, the original “bond-based” theory proposed in [1] and defined in Equation (2) places limitations on the choice of the material properties. For this reason, a “state-based” formulation was developed in [2] to allow arbitrary constitutive relations to be implemented within the peridynamics framework. The equation of motion in the state-based Peridynamics can be expressed as

$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \int_R \mathbf{T}[\mathbf{x}, t](\mathbf{x}' - \mathbf{x}) - \mathbf{T}[\mathbf{x}', t](\mathbf{x} - \mathbf{x}') dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t), \quad \forall \mathbf{x}' \in R$$

(3)

where $\mathbf{T}[\mathbf{x}, t](\mathbf{x}' - \mathbf{x})$ and $\mathbf{T}[\mathbf{x}', t](\mathbf{x} - \mathbf{x}')$ are the force-vector states [2]. $\mathbf{T}$ depends on the deformations of all bonds connected from particle $\mathbf{x}$ and $\mathbf{x}'$. The model is called ordinary when the force exerted by a bond between particles is in the same direction as the deformed bond. However, there is no requirement that force states be in the same direction as their deformation states, and models in which they are not in the same direction are called non-ordinary.

2. Non-ordinary peridynamic numerical implementation

Dividing the body $R$ into a number of cells, each represented by a particle, the integral expressions in (3) can be approximated with a finite sum as in [4], i.e.

$$\rho \ddot{\mathbf{u}}(\mathbf{x}_i, t) = \sum_{j=1}^{m} \mathbf{T}[\mathbf{x}_i, t](\mathbf{x}_j - \mathbf{x}_i) - \mathbf{T}[\mathbf{x}_j, t](\mathbf{x}_i - \mathbf{x}_j) V_j + \mathbf{b}(\mathbf{x}_i, t).$$

(4)

Some specific states that are used in the peridynamic concept are:

- reference position vector state : $\mathbf{X}(\xi) = \xi = \mathbf{x}' - \mathbf{x}$
- displacement vector state : $\mathbf{U}(\xi) = \eta = \mathbf{u}' - \mathbf{u}$
- deformation vector state : $\mathbf{Y}(\xi) = \eta + \xi = (\mathbf{u}' + \mathbf{x}') - (\mathbf{u} - \mathbf{x})$
with respect to the displacements can be written using (16) as:

\[ F(x) = \left[ \int_R \omega(\xi) (\dot{Y}(\xi) \otimes \xi) dV_\xi \right] \cdot B(x) \]  

(8)

and the shape tensor \( B(x) \) as

\[ B(x) = \left[ \int_R \omega(\xi) (\xi \otimes \xi) dV_\xi \right]^{-1}. \]  

(9)

where \( \otimes \) denotes the tensor product of two vectors and \( \omega(\xi) \) is a constant non-negative weighting function that defines the horizon in which the force relationship between particles is nonzero and all particles \( x' \) have equal influence on \( x \) [5]. The ideal value of constant weighing function is still under investigation and is currently taken to be unity [4]. For a discrete system, the non-local deformation gradient (8) at a particle \( i \) can be expressed as [4]

\[ F(x_i) = \left[ \sum_{j=1}^m \omega(\xi_j) (\dot{Y}(\xi_j) \cdot \xi_j) V_j \right] \sum_{j=1}^m \omega(\xi_j) (\dot{Y}(\xi_j) \cdot \xi_j) V_j \cdot B(x_i), \]

(10)

and shape tensor (9) as

\[ B(x_i) = \left[ \sum_{j=1}^m \omega(\xi_j) (\xi_j \cdot \xi_j) V_j \right] \sum_{j=1}^m \omega(\xi_j) (\xi_j \cdot \xi_j) V_j \cdot \left[ \sum_{j=1}^m \omega(\xi_j) (\xi_j \cdot \xi_j) V_j \right]^{-1}. \]

(11)

Using the deformation gradient (8), the left Cauchy-Green strain matrix \( C(x) \) and logarithmic strain \( \epsilon \) can be calculated as

\[ C(x) = F(x)F(x)^T \]  

(12)

\[ \epsilon = \frac{1}{2} \ln C(x). \]  

(13)

For 2D plane strain deformation, the Cauchy stress, \( \sigma(x) \) can be written as

\[ \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ 2\epsilon_{12} \end{bmatrix} \]  

(14)

and the first Piola-Kirchoff stress tensor is expressed as

\[ P = J \sigma(x) F(x)^{-T} \]  

(15)

where \( J = \det F(x) \). The force state of a bond with the bond vector \( \xi \) in terms of stress tensor \( \sigma \), takes the form [4]

\[ T(\xi) = \omega(|\xi|) [P(F)]^T \cdot B(x) \cdot \xi \]  

(16)

and the derivative of \( T \) with respect to the displacements can be written using (16) as:

\[ \frac{\partial T(\xi)}{\partial u} = \frac{\partial T(\xi)}{\partial F} \frac{\partial F}{\partial u} = \omega(|\xi|) \frac{\partial P}{\partial F} \frac{\partial F}{\partial u} \cdot B(x) \cdot \xi. \]  

(17)

The stiffness matrix can be written as:

\[ K(x) = \frac{m}{\omega} \left( \frac{\partial T}{\partial u} [x(x')] - \frac{\partial T}{\partial u} [x(x')] \right) V_{x'}. \]  

(18)

where \( m \) is the number of neighbour particles of \( x \) and \( V_{x'} \) is the volume occupied by each neighbour particles. For a 2D problem, the global matrix is \( 2N \times 2N \) where \( N \) is the total number of particles in the simulation.
3. Future work

The capability of the explicit implementation of non-ordinary state-based peridynamic problems has been successfully illustrated in numerous studies [4]. Therefore, it is planned to extend the implicit implementation to a comparison of fracture predictions using different damage criteria and compare the results with reference solutions found in the literature [2,4].

4. Conclusions

This paper offers for the first time an implicit implementation of non-ordinary state-based peridynamic theory for finite deformation mechanics. Newton-Raphson implementation of the peridynamic method developed here to allow the solution procedure extended towards solving non-linear deformation problems and therefore, to a range of damage criteria.

References


A discontinuous Galerkin hp-adaptive finite element method for brittle crack propagation

*R. Bird, W.M. Coombs and S. Giani

†School of Engineering and Computing Sciences, Durham University, South Road, Durham, DH1 3LE

*robert.e.bird@durham.ac.uk

ABSTRACT

In this paper the discontinuous Galerkin symmetric interior penalty (SIPG) method is used to model brittle fracture propagation. The criterion for fracture propagation and its direction are determined using configurational forces (CF).

Currently in literature, existing mesh refinement strategies are naïve and are only able to achieve accuracies in the region of 0.01% for the value of the CF at the crack tip, [1]. This lack of accuracy has prompted the derivation of an a posteriori error estimator, combined with a hp-adaptive scheme, for linear elastic problems. Discontinuous Galerkin methods are highly suited to hp-adaptive techniques due to their ability to easily incorporate hanging nodes and varying polynomial orders in a mesh.

In this paper the efficacy of the error estimator for improving the accuracy of the CF is verified against the analytical double crack problem, presented by Westergaard [2], for mode 1, 2 and mixed mode problems. The error estimator combined with the hp-adaptation strategy produced accuracies for the CF at the crack tip, using the tip method [3], which up to now have been unobtainable in literature. An exponential convergence rate in the CF value is achieved, verifying the proposed posteriori error estimator for fracture problems. Finally, this paper describes a method to consistently incorporate CF values that exist at hanging nodes attached to the crack tip.

Key Words: fracture mechanics; configurational force; a posteriori; hp-adaptivity; discontinuous Galerkin

1. Introduction

Crack propagation is the generation of new surfaces in a domain through crack growth. Here, the criterion for propagation and crack growth direction is determined using the configurational force (CF) at the crack tip [4]. The CF is determined from the stress field which is inherently singular at the crack tip [5]. Achieving an accurate representation of the stress field, and thus the CF, at the crack tip remains one of the most challenging aspect when modelling cracks with finite element methods.

In this paper a rigorous a posteriori error estimator is combined with a hp-adaptive scheme, [6], to achieve accuracies in the CF not yet achieved in literature for linear elastic problems modelled using SIPG, [7]. Due to the simple communication at element interfaces discontinuous Galerkin finite elements methods (FEM) are highly suited for hp-adaptive schemes, it is simple to incorporate hanging nodes (for h-refinement) and elements varying in polynomial order (for p-refinement).

After this introduction the CF within a FEM context is presented, then in Section 3 a description of the SIPG method is given. In Section 4 the error estimator is outlined along with the hp-adaptive method in Section 5. Lastly in Section 6 a numerical example is presented to show the effectiveness of the error estimator on improving the error in CF, conclusions are drawn in Section 7.

2. Configuration force

Miehe et al., [3] provide a robust derivation, based on the work of Eshelby [4], to determine the CF at the crack tip for small strain hyperelasticity. The CF at the crack tip node is defined as

\[ g_{el} = - \sum_{n=1}^{n_{h}} \sum_{K \in A} \nabla_{K} B_{f}^{T} \Sigma dV, \]
where \( n_b \) is a list of nodes at the crack tip, \( A \) is the set of elements \( K \) which share a node with the crack tip \( \partial \Gamma \) and \( B_1 \) is matrix of shape function derivatives with respect to the underformed state. Last \( \Sigma = \psi(\varepsilon)\dot{\varepsilon} - \frac{\partial u}{\partial x}^T \sigma \) is the Eshelby stress where \( \dot{\psi} \) is the free energy function for hyperelasticity, \( \sigma \) is Cauchy stress, \( \varepsilon \) is small strain, \( u \) is the small strain displacement, and \( x \) is the coordinate system of the undeformed reference state.

A slight variation of (1) is the domain approach, dicussed by [3, 1], which was shown to achieve higher accuracy solutions of the CF. It is obtained by redefining \( A \) as a set of elements which have a node within a radial distance \( r \) away from the crack tip and \( n_b \) as the set of nodes within \( r \).

3. SIPG method for linear elasticity

Here we consider the following model problem on a bounded Lipschitz polygonal domain \( \mathcal{B}_\Gamma \) in \( \mathbb{R}^2 \), with the boundary \( \partial \mathcal{B}_N \cup \partial \mathcal{B}_D = \partial \mathcal{B}_\Gamma \), where \( \partial \mathcal{B}_D \) and \( \partial \mathcal{B}_N \) are the Dirichlet and Neumann boundary conditions respectively. The strong form of the problem, for small strain hyperelasticity, is defined as

\[
\nabla \cdot \sigma(u) = 0 \text{ in } \mathcal{B}_\Gamma, \quad \sigma(u) \cdot n = g_N \text{ on } \partial \mathcal{B}_N \text{ and } u = g_D \text{ on } \partial \mathcal{B}_D,
\]

where \( g_D \) and \( g_N \) are the prescribed values for the Dirichlet and Neumann boundary condition respectively and both are data in \( L^2(\mathcal{B}_\Gamma)^2 \). \( n \) is the normal unit vector to the boundary and \( u \) is a displacement vector. The finite element mesh \( \mathcal{T} \) is comprised of elements \( K \), where \( \mathcal{T} \) is in general irregular. \( K \) is the image of the reference triangle under an affine elemental mapping \( F_K : \hat{K} \rightarrow K \). We denote by \( \mathcal{T}(K) \) the set of the three elemental faces of an element \( K \). If the intersection \( F = \partial K \cap \partial K' \) of two elements \( K, K' \in \mathcal{T} \) is a segment, we call \( F \) an interior face of \( \mathcal{T} \). The set of all interior faces is denoted by \( \mathcal{T}_I(\mathcal{T}) \). Analogously, if the intersection \( F = \partial K \cap \partial \mathcal{B}_\Gamma \) of an element \( K \in \mathcal{T} \) and \( \partial \mathcal{B}_\Gamma \) is a segment, we call \( F \) a boundary face of \( \mathcal{T} \). The set of all boundary faces of \( \mathcal{T} \) is \( \mathcal{T}_B(\mathcal{T}) = \mathcal{T}_N(\mathcal{T}) \cup \mathcal{T}_D(\mathcal{T}) \) for the boundaries \( \partial \mathcal{B}_N \) and \( \partial \mathcal{B}_D \) respectively.

For any mesh \( \mathcal{T} \) of \( \mathcal{B}_\Gamma \) with the degree vector \( p \), we then define the \( hp \)-version discontinuous Galerkin finite element space by

\[
W_p(\mathcal{T}) = \{ w \in L^2(\mathcal{B}_\Gamma)^2 : w|_K \in [P_{pK}(K)]^2, K \in \mathcal{T} \},
\]

with \( P_{pK}(K) \) denoting the set of all polynomials on the triangle \( K \) of degree no more than \( p_K \). The SIPG method, in the bilinear form, for the approximation of the model problem (2) is now introduced. Find the displacement \( u_h \in W_p(\mathcal{T}) \) such that \( a(u_h, w) = I(w) \) for all \( w \in W_p(\mathcal{T}) \), where

\[
a_K(u_h, w) = \sum_{K \in \mathcal{T}} (\sigma(u_h) \cdot \varepsilon(w))_F - \sum_{F \in \mathcal{T}_I(\mathcal{T}) \cup \mathcal{T}_D(\mathcal{T})} \langle (\sigma(u_h))_F, [w]_F \rangle - \sum_{F \in \mathcal{T}_I(\mathcal{T}) \cup \mathcal{T}_D(\mathcal{T})} \langle [\varepsilon(w)]_F, ([\sigma(u_h)]_F + \sum_{p \in K} \beta p_F^2 h_F^2 [u_h], [\sigma(u_h)]_F) \rangle + \sum_{p \in K} \beta p_F^2 h_F^2 [u_h], [\sigma(u_h)]_F) F, \tag{3}
\]

\[
I(w) = -\sum_{F \in \mathcal{T}_D} \langle g_D, n \cdot \sigma(w) \rangle_F + \sum_{F \in \mathcal{T}_D(\mathcal{T})} \beta p_F^2 h_F^{-1} \langle g_D, \sigma(w) \rangle_F + \sum_{F \in \mathcal{T}_N(\mathcal{T})} \langle g_N, w \rangle_F, \tag{4}
\]

\( \beta \) is a penalty term for linear elastic SIPG defined in [8], \( E_Y \) the material’s Young’s modulus and \( \nu \) as Poisson’s ratio. Further, \( h_F \) is the element face length and \( p_F = \max(p_{K'}, p_{K''}) \) if \( F \in \mathcal{T}_I(\mathcal{T}) \), or \( p_F = p_K \) if \( F \in \mathcal{T}_D \) where \( K', K'' \in \mathcal{T} \) are neighbours. The outer diameter of the triangular element \( K \) must also be defined as \( h_K \). Last \( \{ \cdot \}, \langle \cdot, \cdot \rangle, \langle \cdot, \cdot \rangle \) and \( \langle \cdot, \cdot \rangle \) are defined in [7].

4. Error Estimator

The derived error estimator for the mesh \( \mathcal{T} \) is calculated after \( u_h \) has been found. The estimated error is given by

\[
\eta_{en} = \sqrt{\sum_{K \in \mathcal{T}} \left( \eta_{R,K}^2 + \eta_{J,K}^2 + \eta_{F,K}^2 \right)}, \tag{5}
\]

where,

\[
\eta_{R,K}^2 = \frac{h_K^2}{p_K} \| \nabla \cdot \sigma(u_h) \|_{0,K}^2, \quad \eta_{J,K}^2 = \frac{1}{2} \sum_{F \in \mathcal{T}_I} \beta^2 p_F^2 \frac{h_F}{h_F} \| [\varepsilon(u_h)]_F \|_{0,F}^2 + \sum_{F \in \mathcal{T}_D} \beta^2 p_F^2 \frac{h_F}{h_F} \| u_h - g_D \|_{0,F}^2, \tag{6}
\]
The estimated error for an element $K \in T$ is given by $\eta^2_{T,K} = \eta^2_{R,K} + \eta^2_{J,K} + \eta^2_{T,K}$. 

5. hp-adaptive scheme

hp-adaptive schemes can be either driven by the error estimator alone [6] or by the error estimator and a smoothness indicator [9, 10]. Here the simple marking scheme defined in [6] is used as it was shown to give exponential convergence rates of the true norm for singular problems. It is noted that this hp-scheme is not as robust as others in [6] or those in [9, 10] as this scheme over-refines in $h$ for smooth problems.

Once $S_h$ and $S_p$ have been defined the mesh is refined accordingly. Elements are then h-refined further if along one of their faces there exists more than one hanging node or p-refined if an element has a polynomial order difference of at least 2 less compared to a neighbour.

6. Numerical example

The value of the error estimator and the true norm will decrease exponentially with the number of the degrees of freedom (ndof) in the problem, [11], when combined with a hp-adaptive scheme. However it is necessary to confirm that the error in CF also improves at an exponential rate. Although the CF is a function of stress, the error estimator is a not a function of the CF and so the hp-adaptive scheme will not be driven directly by the error in the CF.

A crack problem with an analytical stress solution will give a CF which can be used to test the accuracy, and error decrease rate, of the numerical CF. Westergaard in [2] provides an analytical stress solution to a centred crack in an infinite plate. The analytical solution of the CF [12] is given by the relation between the energy release rate and stress concentration factors $K_I$ and $K_{II}$, [5], for mode I and II respectively for plane strain

$$ g_{CT} = \begin{cases} \left(\frac{K_I^2 + K_{II}^2}{E'}\right), & \text{if } K_I = \sigma_0 \sqrt{\pi a}, \quad K_{II} = \tau_0 \sqrt{\pi a}, \quad \text{and } E' = \frac{E_Y}{(1 - \nu^2)}. \end{cases} $$

$\sigma_0$ and $\tau_0$ are the far field normal and shear stress applied at the far field of the Westergaard problem, $E_Y$ and $\nu$ are the Young’s modulus and Poisson’s ratio respectively, and $a$ is the half crack length shown in Figure 1b.

A truncated version of Westergaard’s problem where only half the crack for a finite plate is modelled is shown in Figure 1b. Here $L = 1 \text{ m}$, $a = 0.5 \text{ m}$, $E_Y = 5/2 \text{ Pa}$ and $\nu = 0.2$. The convergence rate of the CF using the error estimator combined with the hp-adaptive scheme was tested for three static crack problems, mode I ($\sigma_0 = 1, \tau_0 = 0$) Pa, mode II ($\tau_0 = 1, \sigma_0 = 0$) Pa and, mixed mode ($\sigma_0 = \tau_0 = 1$) Pa. The results of the CF, computed using the domain method [1], against the cube root of the ndof are shown in Figure 1b. The CF is plotted against ndof$^{1/3}$ as this is the best exponential convergence rate achieved using hp-adaptive schemes for singular problems [6]. For all three problems the CF consistently converged exponentially achieving accuracies in the CF not yet achieved in literature. The error estimate combined with the hp-adaptive scheme therefore works successfully in improving the accuracy of the CF with no sign of polynomial convergence.
Figure 1: (a): A plot of the relative error between the numerical CF, $g_{cI}$, and analytical CF, $g_{cIa}$. (b): A schematic of the problem modelling half of Westergaard’s crack [2] where $n_x$ and $n_y$ are the normals components of the vector perpendicular to the outer surface and, $\sigma_{xx}$, $\sigma_{yy}$ and $\sigma_{xy}$ are stress solutions in [2].

7. Conclusion

This paper presented an error estimator for linear elastic problems using the SIPG method. The error estimator was combined with a hp-adaptive method to improve the accuracy of finite element models. Through testing the error estimator combined with the hp-adaptive method was shown to decrease the error in the CF at an exponential rate consistently and displayed potential for the error to decrease further. Additionally the accuracy in CF obtained here has not yet been obtained in literature.

8. Acknowledgements

The first author acknowledges finical support during the completion of this work from the Engineering and Physical Science Research Council (EPSRC).

References

A FINITE ELEMENT MODEL FOR FAULT RUPTURE

*Sepideh Alizadeh Sabet1, René de Borst1

1Department of Civil and Structural Engineering, University of Sheffield, Sheffield, S1 3JD

*salizadehsabet1@sheffield.ac.uk

ABSTRACT

Herein we set up a finite element framework to investigate fault rupture. Damage/slip evolution in the fault is one of the main failure mechanisms. Zero-thickness interface elements are used to simulate crack propagation and are inserted in the mesh a priori, at the pre-existing fault locations. A cohesive-like traction slip law at the interface allows for progressive damage evolution and progressive slip at the fault. Conventionally, the initial nearly rigid behaviour at the fault is simulated by inserting a high dummy stiffness in order to suppress unphysical deformations in the pre-cracking phase, and post-peak exponential softening is used to capture the strength and stiffness degradation at the interface. The fracture energy controls the softening curve. Plane-strain conditions are assumed throughout. The behaviour of the interface model is investigated in a numerical example.

Key Words: fault rupture; interface element; cohesive zone models; traction slip laws

1. Introduction

Geologic faults are considered to be one of the main sources for earthquakes from where they originate and propagate. Several numerical methods, e.g. the boundary element method and the finite difference method have been used in the literature to model the fault rupture and propagation [1, 2]. An alternative to these methods are finite element models which incorporate a discrete, zero-thickness interface on which a cohesive-like slip weakening model is prescribed. These are inspired by the approach pioneered by Dugdale and by Barenblatt [3, 4]. In the latter approach, a fracture process zone is modeled by cohesive surfaces ahead of the crack tip. A traction-separation law prescribes how the cohesive tractions change as a function of the relative displacements between the cohesive surfaces. These laws can have different shapes, e.g. bilinear or exponential. In these laws, a tensile strength criterion regulates the damage initiation and when the fracture energy for the considered fracture mode is fully absorbed by the element, the cohesive tractions vanish and full debonding of the layers has occurred. Here the interface elements should be inserted in the finite element mesh a priori and therefore require the knowledge of the crack path in advance.

2. Governing equations

In this paper, we consider an initial linear elastic behaviour at the interface in the pre-cracking phase and an exponential softening behaviour post-peak, as can be seen in Fig. 1, such as follows:

\[
    t_s = \begin{cases} 
    K_s \cdot \lVert u \rVert_s, & \lVert u \rVert_s < \lVert u \rVert_{s,0} \\
    \text{sgn}(\lVert u \rVert_s) \left( t_{\text{s,ult}} - t_r \right) \exp \left( -\frac{t_{\text{s,ult}}}{\tau_f} \left( \lVert u \rVert_s - \lVert u \rVert_{s,0} \right) \right) + t_r & \lVert u \rVert_s \geq \lVert u \rVert_{s,0}
    \end{cases}
\]

where

\( t_s \) is the shear traction,  \\
\( K_s \) is the initial dummy shear stiffness,  \\
\( \lVert u \rVert_s \) is the relative shear displacement,  \\
\( \lVert u \rVert_{s,0} \) is the value of the relative shear displacement at which the damage starts,
Figure 1: Exponential traction-slip law for mode II loading

\( t_{s,ult} \) is the maximum shear strength,
\( t_r \) is the residual shear strength, which remains in the material after damage,
\( G_{IIc} \) is the critical mode II fracture energy.

In order to suppress unphysical deformations in the initial pre-cracking phase a high value is assigned to \( K_s \) to simulate a nearly rigid behaviour at the fault.

The element stiffness matrix and nodal internal force vector are then given as:

\[
K = \int_{S_d} R^T B^T K_{loc} B R \ dS
\]

\[
f^{int} = \int_{S_d} R^T B^T t \ dS
\]

where
\( S_d \) refers to the area of the interface element,
\( K \) is the element stiffness matrix,
\( R \) is the rotation matrix to transform the local quantities to global ones,
\( K_{loc} \) is the local material stiffness matrix
\( B \) is a matrix which when applied to the nodal displacements, gives the relative displacements in the integration points.
\( f^{int} \) is the nodal internal force vector
\( t \) is the local traction vector.

For a better insight into the concept and formulation of cohesive zone models, the reader is referred to [5].

3. Numerical example

A \( 10 \times 10 \text{ mm}^2 \) plate with an initial notch of length 4 mm in the middle is considered (see Fig. 2). Cohesive interface elements are inserted along the dashed line. The plate is sheared by a displacement load prescribed on top edge of the plate (\( \bar{u} \)). The bulk material is considered to behave elastically with \( E = 100 \text{ GPa} \) and \( \nu = 0.3 \), while interface elements obey a constitutive law as described in Eq. 1 with \( G_{IIc} = 0.2 \text{ KN/mm} \), \( t_{s,ult} = 1.0 \text{ GPa} \), \( t_r = 0.15 \text{ GPa} \) and \( K_s = 10000 \text{ GPa/mm} \). The plate was tested with three different mesh sizes and for different values of \( K_s \).

Fig. 3(a) shows the traction profile along the x-axis in the plate for a mesh of \( 50 \times 50 \) elements with Gauss integration and Fig. 3(b) shows the same using Newton-Cotes integration. As can be seen from the figures, when Gauss integration is used, tractions in the interface elements show strong spurious oscillations. The magnitude of these oscillations increases for higher values of \( K_s \). However, using Newton-Cotes integration scheme results in a smoother traction profile in the interface elements.
is a well-known problem in using cohesive interface elements [6]. Therefore, one should bear in mind that using Gauss integration scheme can lead to unrealistic early initiation of damage in the material due to these spurious oscillations as is shown in Fig. 4. Using Gauss integration in the $50 \times 50$ mesh with $K_s = 10000$ GPa/mm at $\bar{u} = 0.04$ mm, leads to some interface elements already reaching the ultimate shear strength and thereafter damage initiation, whereas the model is predicted to still be in the elastic regime using Newton-Cotes integration.

Fig. 5 illustrates the traction profile during the crack propagation for different values of displacement loads for the $50 \times 50$ mesh with $K_s = 10000$ GPa/mm. As the crack propagates, the shear traction in the interface elements reaches the value of residual shear strength.

Next the effect of mesh size has been studied. As can be seen from Fig. 6(a), the coarser meshes with $10 \times 10$ and $20 \times 20$ elements result in a lower predicted value for the maximum traction in the interface elements compared to the fine mesh with $50 \times 50$ elements. The spurious oscillations are seen here as well, for the Gauss integration, whereas in Fig. 6(b) the smoother traction profile obtained by Newton-Cotes integration for these meshes are shown.

4. Conclusions and future work

In this work, a cohesive interface element model was developed and implemented to capture the initiation and the progressive slip at faults. Gauss integration scheme was found to produce artificial oscillations in the traction profile at the interface. Newton-Cotes integration scheme on the contrary results in a
smoother approximation and hence more reliable to be used with cohesive interface elements. The next step involves investigating the energy dissipation in the bulk surrounding the fault and how this affects the total failure process.

Acknowledgements
The financial support by ERC Advanced Grant 664734 “PoroFrac” is gratefully acknowledged.

References


Numerical analysis of flow parameters in hydraulic fracturing

*D. Mahdavian¹, A.A Javadi²

¹Department of Engineering, University of Exeter, North Park Road, Exeter, EX4 4QF
²*dm464@exeter.ac.uk

ABSTRACT

Hydraulic fracturing is a process of fluid injection into the well. This process creates tensile stresses in formation in order to overcome the tensile strength of formation. This creates fractures in the formation that start from the wellbore wall and propagate until the fluid is injected continuously at a high rate. Fluid flow in a porous medium can have a major influence on the deformation and crack propagation. This paper presents a study on the effects of fluid velocity and viscosity on hydraulic fracturing process using the finite volume and computational fluid dynamics methods. The results show that the pressure around the crack increases with increasing the relative velocity and fluid viscosity. The fluid viscosity is also an important parameter, which can affect the crack propagation and the production rate in hydraulic fracturing. The pressure in the cracks also increases by increasing the fluid viscosity. The crack length increases with increasing the pressure in the cracks. The relationship between viscosity, velocity and pressure in crack is investigated.

Keywords: Hydraulic Fracturing; Viscosity; Velocity; Finite Volume; Crack Length

1-Introduction

Optimal design of hydraulic fracturing is a fundamental problem in Petroleum Engineering and plays a critical role in many applications within the oil and natural gas industry. The process of hydraulic fracturing can be generally defined as initiation and propagation of fractures due to the pressurization of fluid flow within existing fractures. Hydraulic fracturing involves the interaction between four different phenomena:

(1) porous medium deformation;
(2) pore fluid flow;
(3) fracturing fluid flow; and
(4) fracture propagation.

The equations and constitutive relations governing these coupled processes are Biot’s theory of poroelasticity for porous media, Darcy’s law for pore fluid flow, Reynold’s lubrication theory for fracturing fluid flow and the cohesive zone model to characterize fracturing. The focus of this study is the effect of velocity and viscosity of fluid flow on hydraulic fracturing process.

5-4.4. Fluid mechanics and fluid flow in the fracture

The major fluid flow parameters are the fluid viscosity \( \mu \) and injection rate \( q_i \). Consider a Newtonian fluid flowing laterally through a narrow slit (Fig. 1). In the case of laminar flow (the general case for flow inside hydraulic fractures), the pressure drop along some length \( \Delta x \) of the slit is:

\[
\frac{\Delta p_{net}}{\Delta x} = \frac{12\mu q}{h_f w^2} \tag{1}
\]

where \( h_f \) is fracture height, \( \Delta p_{net} \) is pressure drop and \( w \) is fracture width.
The fracture essentially is a channel of varying width over its length and height. The local pressure gradient within the fracture is determined by the fracturing fluid rheology, fluid velocity and fracture width. Equations governing fluid flow within the fracture can be derived using the principle of conservation of momentum and lubrication theory applied to a fluid travelling in a narrow conduit. The rheology of fracturing fluids is generally represented by a power law model that incorporates two parameters $K$ and $n$. In recognition that fluid flow within a fracture is laminar for most fracturing applications [2], the global pressure gradient along the length of a fracture can be expressed as:

$$\frac{dp}{dx} = \frac{Kv^n}{\bar{w}^{n+1}}$$  \hspace{1cm} (2)

where $v_x$ is the average fluid velocity along the length of the fracture and is defined in terms of the volumetric injection rate $q_i$, fracture height $h_f$ and height-averaged fracture width $\bar{w}$. Material balance or conservation of mass suggests that $v_x$ is proportional to $q_i/h_f$. Equation 2 then becomes

$$\frac{dp}{dx} = \frac{K}{\bar{w}^{n+1}} \left( \frac{q_i}{h_f} \right)^n$$  \hspace{1cm} (3)

In the special case of a Newtonian fluid ($n = 1$ and $K = \mu$, where $\mu$ is the fracturing fluid viscosity), Eq. 3 reduces to

$$\frac{dp}{dx} = \frac{\mu}{\bar{w}^3} \left( \frac{q_i}{\bar{w} h_f} \right)$$  \hspace{1cm} (4)

where the term $\bar{w} h_f$ is readily recognized as the average fracture cross-sectional area. Equation 4 is essentially Darcy’s law with the permeability proportional to $\bar{w}^2$. Equations 2 and 3 are formulated in terms of the average velocity and implicitly ignore change in the fracture width over its height. The varying width profile has an effect on the flow resistance relative to the case of a constant-width channel. The increase in the flow resistance is accentuated during periods of fracture height growth into barriers at higher stress. The varying width profile affects other physical phenomena that are highly sensitive to the velocity [1].

3-Numerical analysis

The Computational Fluid Dynamics (CFD) code, FLUENT, was used for numerical analysis. The code uses a finite volume based technique to convert the governing mathematical equations to algebraic equations that can be solved numerically. The code is supplemented by a proprietary ANSYS based geometry construction and meshing engine, which allows users to build and mesh complex flow models to be used by the solver [3].
Like most CFD programs, Fluent is based on the finite volume method (FVM). The finite volume method is a generalization of the finite difference method to unstructured meshes. Unlike the finite element method, FVM yields values across the entire volume contained within a cell. This has a particular advantage in preserving the flux of state variables across intercellular surfaces[4].

We are interested, in CFD, in solving the Navier–Stokes equations or some coherent simplified subset of these. These are the set of equations which, taken together, completely describe continuum hydrodynamics. The momentum conservation equations are:

\[
\begin{align*}
\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) &= -\frac{\partial P}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) \\
\rho \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) &= -\frac{\partial P}{\partial y} + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) \\
\rho \left( \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) &= -\frac{\partial P}{\partial z} + \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) 
\end{align*}
\]  

(5)

The associated continuity equation is

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0
\]  

(6)

where, \( u, v, w \) are \( x, y, z \) components of velocity respectively. The continuity equation (equation 6), and the Navier-Stokes equations (equation 5) completely describe the motion of an incompressible fluid in a continuum media in 3D [4].

Broadly, the strategy of CFD is to replace the continuous problem domain with a discrete domain using a grid. In the continuous domain, each flow variable is defined at every point in the domain. Appropriate initial conditions and boundary conditions need to be applied in order to solving the Navier-Stokes equation and continuity equations. The boundary conditions in a 2D crack on the wall of a production well, which are used in this study, are as follows:

- No-slip boundary condition is used to bound fluid and solid regions.
- Velocity inlet boundary conditions are used to define the velocity and scalar properties of the flow at inlet boundaries.
- Pressure inlet boundary conditions are used to define the total pressure and other scalar quantities at flow inlets.
- Pressure outlet boundary conditions are used to define the static pressure at flow outlets.

In addition, material properties including density and viscosity for each zone are specified. It is important to accurately represent a boundary layer or fully developed turbulent flow at the inlet but in this study laminar flow is used. Multiple upstream meshes can be used in Fluent, giving users the flexibility to select the most efficient mesh combinations for different applications but Quadrilateral mesh, is used in this study.

**Results:**

Figure 2 and 3 show the variation of pressure with fluid flow and fluid viscosity in hydraulic fracturing. The results cover a range of flow with low and high velocity and viscosity. Hydraulic fracture propagation could be easily affected by not only fluid velocity around the borehole but also viscosity of the injected fluid. Using high velocity fluid can increase the influence of the injection rate on hydraulic fracture propagation and, especially, using high viscosity fluid is effective in crack propagation.
Conclusion:

To study the effectiveness of using high viscosity fluid in hydraulic fracturing, numerical simulations using a 2D crack was performed. The results show that pressure around hydraulic fracture is decreased in the low velocity fluid injection, while it is increased in high velocity fluid injection. This is caused by the strong fluid injection rate on the borehole wall in the high velocity case. The results also show that the fractures could be easily propagated when the fluid viscosity is high. It can be concluded that higher fluid velocity and viscosity can be effective in the hydraulic fracturing process and can result in a higher production rate in the production well.

References

Fluid Mechanics
and
Fluid-Structure interaction
Simulation of Aerodynamic Behaviour of a Road Vehicle in Turbulent Flow

*Ahmed Al-Saadi, Ali Hassanpour, Yousef Ghaffari Motlagh, Tariq Mahmud

School of Chemical and Process Engineering, University of Leeds, Woodhouse Lane, Leeds, LS2 9JT

*pmaash@leeds.ac.uk

ABSTRACT

This study concentrates on different aerodynamic drag reduction techniques to reduce the aerodynamic drag coefficient and increase the stability of a three-dimensional full-size road vehicle. There are many modern aerodynamic add-on devices and modifications which are used in this research. All of these aerodynamic devices and modifications are used individually or in combination. Optimization of mesh parameters is carried out by analysis of the mesh data. Unstructured tetrahedral cells are used throughout the global domain to cope with the geometrical complexity of the car model. Inflation layers with prismatic cells are used to provide an accurate estimation of the velocity profiles near the surfaces of the car. Computational Fluid Dynamics (CFD) analysis based on steady state Reynolds-Averaged Navier-Stokes (RANS) turbulence modelling is used. Realizable k–ε, Standard k–ω, Shear Stress Transport k–ω (SST) and a Reynolds Stress Model (RSM) turbulence models are considered in this study. Good agreement has been achieved between the calculated drag coefficient for the baseline models and the experimental data for all types of turbulence models. It is found that the use of some types of aerodynamic modifications and devices can reduce the aerodynamic drag coefficient and increases the car stability.

Keywords: Simulation; Aerodynamics; Road Vehicle; Turbulent Flow.

1. Introduction

A rise in fuel prices has led to increasing concern about fuel consumption especially for vehicles. A large part of the engine power is used to overcome the air resistance force and improvement of aerodynamic behaviour can lead to a decrease in fuel consumption. Experimental tests and computational simulations have been performed to reduce the drag coefficient of road vehicles and to improve the aerodynamic behaviour. The simple geometry of wagon model was achieved with modifications of the front part by Guo et al. [2] using computational fluid dynamics analysis. The k-ε turbulence model was used to calculate the drag coefficient. The bottom part of the body was assumed as a flat surface. Some parts of car as wheels and rear view mirrors were neglected in modelling to simplify the simulation. This analysis was based on three different slantwise angles of the back windshield. Aljure et al. [1] studied four different LES models, the QR, the VMS, the SIGMA and the WALE, in the bluff bodies using relatively coarse grids. The SIGMA, QR and VMS models were used for the first time to resolve the flow around simplified vehicle models (the Ahmed and the Asmo models were used as baseline models). Three meshes were used with each car model. Number of nodes for the Asmo model was higher than the Ahmed model. Both cases of cars were simulated using the same boundary conditions. The Reynolds number of 7.68×10^5 based on the height of the body was used for both cases. It was found that coarse grids are useful in LES simulations. Khalighi et al. [3] evaluated Immersed Boundary (IB) and body-fitted methods. The IB method does not require mesh to be conformal to geometry and therefore will speed up the grid generation process. The aerodynamic behaviour of Chevy Tahoe 2006 was studied using the Reynolds-Averaged Navier–Stokes solver. Then, velocity, surface pressure and drag coefficient measurements were used to check the simulation results. The drag coefficients for the IB and the body-fitted methods were within 3% and 3–7% of the experimental measurement, respectively.

The drag coefficient of Sports Utility Vehicles (SUVs) is higher than saloon cars because the size and the rear part design of this kind of vehicles. However, the flow field analysis around SUVs is difficult.
because of the low pressure area behind the car (wake zone). Almost all the previous studies on the aerodynamics of SUVs have focused on the flow characteristics around the car using one turbulence model or one modification of external design [1, 2, and 3]. In this study, four turbulence models and three modifications of external design were used to get all the properties of air around the car and to improve the aerodynamic behaviour.

2. Methodology

The governing equations are solved numerically by finite volume method. The continuity equation and the incompressible Navier-Stokes equation in vector form [5] are given by Eq. (1) and Eq. (2):

\[
\nabla \cdot \mathbf{u} = 0 \tag{1}
\]

\[
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \tag{2}
\]

where \( \mathbf{u} \) is the velocity, \( t \) is time, \( \rho \) is the density, \( p \) is the pressure, \( \nu \) is the kinematic viscosity.

The drag (\( C_D \)) coefficient and lift (\( C_L \)) are calculated based on the following equations in this study [4]

\[
C_D = \frac{F_D}{(\rho V^2 A)/2} \tag{3}
\]

\[
C_L = \frac{F_L}{(\rho V^2 A)/2} \tag{4}
\]

where \( F_D \) is the drag force, \( F_L \) is the lift force, \( \rho \) is the air density, \( V \) is the inlet air velocity, \( A \) is the frontal cross sectional area of the vehicle.

3. Numerical Results

Three modifications of external design were used to improve the aerodynamic behaviour of SUVs. Figure 1 shows the baseline model which is used in this study. The dimensions of the baseline model is Land Rover Discovery. Length, height and width without side mirrors of the baseline model are 4835 mm, 1887 mm and 2510 mm, respectively [6]. Unstructured tetrahedral cells are used throughout the global domain to cope with geometrical complexity. ANSYS 16.0 was used to generate mesh with varying levels of refinement. Mesh optimization was carried out by analysis of the mesh data. The CFD simulations are performed with the ANSYS Fluent 16.0 software. The properties of the flow vary a lot behind the car, so most modifications of external design are in the rear part of the car. Four types of turbulence models are used, Realizable \( k-\varepsilon \), Standard \( k-\omega \), Shear Stress Transport \( k-\omega \) (SST) and Reynolds Stress Model (RSM), in this study. Table 1 illustrates all the drag coefficients of the baseline model. All Numerical modelling provide good agreement with the experimental measurement [6].
Spare tyre on the back door of the car, boattail and vortex generators over the end of the roof of the car are used to improve the aerodynamic behaviour of Land Rover Discovery. The Realizable $k-\varepsilon$ turbulence model was implemented for the simulation. Figure 2 shows the drag coefficient as a function of Reynolds number for three types of modifications in addition to the baseline model of the SUV. The best modification for the SUV with velocity less than 120 km/h ($Re = 1.12 \times 10^7$) is a spare tyre because the minimum drag coefficient and low cost. The drag coefficient of the baseline model is 0.4 while 0.372 for the model with spare tyre. Drag coefficient decreases with increasing of Reynolds number except spare tyre which decreases then slightly increases again.

Figure 3 shows the lift coefficient as a function of Reynolds number for three types of modifications in addition to the baseline model of Land Rover Discovery. Vortex generators at the end of the car roof gives higher downforce than other models. The lift coefficient for spare tyre model is independent on Reynolds number as shown in Figure 3. It was found that placing a spare tyre on the back door of the vehicle is the best modifications regarding drag coefficient, lift coefficient and cost.
4. Conclusions

Realizable $k$–$\varepsilon$, Standard $k$–$\omega$, Shear Stress Transport $k$–$\omega$ (SST) and Reynolds Stress Model (RSM) were utilised to simulate the aerodynamic behaviour of baseline and it was found that all models reasonably predict the experimental measurements. All the modifications to the car provide us with more suitable drag and lift coefficients in comparison with the baseline model. It was found that placing a spare tyre on the back door of the vehicle not only decreases the drag coefficient for a wide range of the Reynolds numbers but also increases the downforce which leads to improvement of aerodynamic behaviour of the vehicle.

Acknowledgements

The first author dedicated his thanks to all who participated in this research, especially the Ministry of Higher Education and Scientific Research (MOHESR) in Iraq and also Al-Qadisiya University in Iraq for sponsoring the first author.

References


FLOW PAST A 3D ELASTIC CANTILEVER BEAM ATTACHED TO A SOLID BLOCK

*M. Al Manthari and P. Nithiarasu

Zienkiewicz Centre of Computational Engineering, College of Engineering, Bay Campus, Fabian Way, Swansea, SA1 8EN, United Kingdom

*683446@swansea.ac.uk

ABSTRACT

This study deals with the subject of fluid-structure interaction between a flexible cantilever beam and incompressible flow using OpenFOAM. The fluid and solid coupling is accomplished through a class of fluidSolidInterface for both weak and strong coupling. The tool applied in the present work to study FSI of elastic cantilever is foam-extend-4.0. Initially, for all calculations presented in this work, the elastic plate attached to the fixed bluff body is assumed to be at rest in an incompressible flow and the vibration of the flexible body is caused by the fluid motion. The 3D elastic cantilever beam example shows the mechanical nature sensitivity for these delicate FSI problems.

Keywords: fluid-structure interaction (FSI); elastic cantilever beam; OpenFOAM; displacement; ALE formulation

1. Introduction

Fluid structure interaction (FSI) remains one of the important research topics across different engineering fields such as structural design, biology and medicine. Flow past a cantilever beam in two- and three-dimensional is prone to flow-induced vibrations. Predicting response of a flexible body to sheared flow is necessary, particularly in marine engineering applications. Different approaches have been employed to model this problem. The contribution represents the specific physical nature in the interaction of incompressible flows and very thin structures such as shells and membranes. Results from these predictions of the flow-induced vibrations help designers and operators in resolving problems in the engineering applications. Generally, the vibration amplitude of a flexible body is dependent on damping. Therefore, measuring damping of a flexible body vibrating in still water or air for both in-line and cross-flow directions is central to response predictions.

In the current work, a partitioned algorithm for fluid-structure interaction solver for large structural deformations and the flow formulation based on an Arbitrary Lagrangian-Eulerian (ALE) are applied.

2. Scope of the work

There are many existing methods and techniques in FSI applications. The FSI solver here is built to simulate the interaction between an incompressible Newtonian flow and St. Venant-Kirchhoff solid. In an Arbitrary Lagrangian-Eulerian (ALE) formulation used, the Navier-Stokes equations are described for the laminar flow while the non-linear momentum equation is modeled for the large solid deformation. The FSI package in OpenFOAM extend version (foam-extend-4.0) has been utilized and a partitioned approach for the fluid-solid coupling is adopted.

It is also important to point out

- the Aitken under-relaxation technique or interface quasi-Newton method based on inverse least squares approximation (IQN-ILS) has been examined in order to accelerate the strong coupling process,
- fsiFoam is the solver used for the strong coupling between the fluid and the solid with the explicit partitioned approach in the FSI package.
3. The governing equations and discretization

For coupling problem of fluid and structure, the Dirichlet-Neumann partitioning solution schemes are presented below.

3.1 The solid domain

For the slender fluid-structure interaction problems, the non-linear geometries are integrated for the large deformation and rotations. However, for the problem considered here small strain of the structure could be considered for the applications. In general, the homogeneous isotropic linear elastic material has been assumed in order to control this contribution.

The solid displacements \( \mathbf{d}_s \) within the Lagrangian description is given by the non-linear elastodynamic equations

\[
\rho_s \ddot{\mathbf{d}}_s = \nabla \times (\mathbf{F} \cdot \mathbf{S}) + \rho_s \mathbf{b}_s,
\]

where \( \rho_s \) is the structure material density and \( \mathbf{b}_s \) represents the body force. \( \mathbf{F} \) and \( \nabla \times \) represent the deformation gradient and the material gradient operator, respectively. The Green-Lagrange strain \( \mathbf{E} \) represents a complete description of the deformation process for a St. Venant-Kirchhoff material by the second Piola-Kirchhoff stress tensor \( \mathbf{S} \) via

\[
\mathbf{S} = \mathbf{C} : \mathbf{E} = \lambda_s \text{tr} \mathbf{E} + 2 \mu_s \mathbf{E},
\]

where \( \mathbf{C} \) represents the constitutive tensor, and the Lame' constants are denoted by \( \lambda_s \) and \( \mu_s \).

For the large deformation, the kinematic equation is given by

\[
\mathbf{E} = \frac{1}{2} (\mathbf{F}^T \cdot \mathbf{F} - \mathbf{I}).
\]

For the Dirichlet-Neumann partitioning of the structural solver of a coupled system, the calculation of the coupling boundary displacement \( \mathbf{d}_{\Gamma, n+1} \) and the coupling forces \( \mathbf{f}_{\Gamma, n+1} \) are given by

\[
\mathbf{d}_{\Gamma, n+1} = \mathbf{S}_{n+1} \left( \mathbf{f}_{\Gamma, n+1} \right).
\]

3.2 The flow domain

Incompressible Navier-Stokes equations are used to describe the Newtonian fluid motion. The fluid domain boundaries are not the same through the simulation, so an ALE description for the flow domain is employed.

For the velocity field \( \mathbf{u}_x \) and the kinematic pressure \( p_x \), the fluid equation is given by

\[
\left. \frac{\partial \mathbf{u}_x}{\partial t} \right|_x + \mathbf{c}_x \cdot \nabla_x \mathbf{u}_x - 2 \nu_f \nabla_x \cdot \mathbf{e}(\mathbf{u}_x) + \nabla_x p_x = \mathbf{b}_f \quad \text{in } \Omega_f \times T,
\]

\[
\nabla_x \cdot \mathbf{u}_x = 0 \quad \text{in } \Omega_f \times T.
\]
\[ \varepsilon(u_x) = \frac{1}{2} \left( \nabla_x u_x + (\nabla_x u_x)^T \right). \] (7)

For the coupling algorithm in Dirichlet-Neumann partitioning of the fluid solver, the calculation for the forces acting on the coupling is combined in the non-linear operator \( F \)

\[ f_{\Gamma,n+1} = F_{n+1} \left( u_{\Gamma,n+1}, d_{\Gamma,n+1} \right). \] (8)

The new mesh position for the fluid-structure interaction is calculated then by the position \( d_{\Gamma,n+1} \) and the velocity \( u_{\Gamma,n+1} \).

4. Description of the Problem and Simulation Parameters

This numerical example follows the two-dimensional approach presented in Wall and Ramm [2]. The problem consists of a light and stiff flexible structure attached to a solid block and fully submerged in a fluid. The uniform velocity \( U_\infty \) over a time leads to the flexible body to be displaced. In this simulation example, the flapping of a plate should be simulated in a light wind. In order to solve this case of fluid-structure interaction numerically, simplifications must be assumed by neglecting the weight of the plate, and only a moderate wind speed up to 100 cm/s is considered.

The fluid and solid properties were set by Dettmer and Perić [1]. The Newtonian fluid parameters are set to viscosity \( \mu_f = 1.82 \times 10^{-4} \text{g/s.cm} \), density \( \rho_f = 1.18 \times 10^{-3} \text{g/cm}^3 \) and uniform flow velocity \( U_\infty = 100 \text{cm/s} \) which were resulting in a Reynolds number \( Re \left( \rho_f D U_\infty / \mu_f \right) \) of 648. This corresponds to the air properties at 20°C.
A plate of size $4 \times 3 \text{cm}$ with the thickness 0.06 cm which attached to a rigid body is examined. The material behaviour of the plate is described according to Wall and Ramm [2] with a St. Venant-Kirchoff model with density $\rho_s = 2.0 \text{g/cm}^3$, Young modulus $E_s = 2.0 \times 10^6 \text{N/cm}^2$ and Poisson's ratio $\nu_s = 0.35$.

In order to be able to take account of the change in the fluid region as a result of the structure movement, an ALE formulation is used for the region $6 \text{cm} \leq x \leq 20 \text{cm}$. For the temporal discretization, the time step $\Delta t = 0.001\text{s}$ is selected in the fluid.

5. Results and Discussions

![Figure 2: Plate in wind: displacement in y-direction at three points on the structure edge](image)

For the investigation of the behaviour of plate in wind, the shifting component in the y-direction for the three points A, B and C shows that there is no iteration over the fields are required due to the symmetrical load from both structure sides and hence does not show any deformation from the beginning of the simulation up to about $t = 2.3\text{s}$. In the further calculations 3-4 iterations over the field, the vortex shedding of the plate is deformed in the positive direction of the y-axis. Then, from $t = 6\text{s}$ the symmetry in the plate deformation and in the vertex shedding is broken.

6. Conclusions

The displacement $d_y$ of the three points at downstream of the plate edge has shown uniform deformation in the positive y-direction after the vortex shedding initiation. The structure length to the thickness ratio is $4/0.06$ (not very thin-walled), but the results from the simulation show high physical sensitivity of the deformation patterns. The interaction of incompressible fluid and thin-walled structures using FSI library in OpenFOAM shows good agreement with other results.

References


AERODYNAMIC IMPROVEMENT OF THE HORIZONTAL AXIS WIND TURBINE BY USING WINGLETS

*A. Farhan¹, A. Hassanpour¹, A. Burns¹ and Y. Ghaffari Motlagh¹

¹School of Chemical and Process Engineering, University of Leeds, LS2 9JT, UK

*pmamf@leeds.ac.uk

ABSTRACT

The aerodynamic behaviour of wind turbine plays a vital role on the wind turbine performance. Over the past decades, many experimental and numerical studies have been carried out to gain a better understanding of the main mechanisms involved in the formation of the vortex on the wing. Wingtip vortices are crucial phenomena in fluid dynamics for their negative effects in many applications particularly wind turbines. Despite many studies on this particular topic, the current understanding is not enough to provide a strong base for the design of effective tip geometry modifications and vortex control devices. One of the alternative solutions to reduce the effect of the wingtip vortices is adding a winglet near-vertical extension of the wingtips. In this work, the influence of winglet planform and winglet airfoil are investigated numerically by the use of Computational Fluid Dynamics (CFD) tools. Couple of turbulence models are used to simulate the turbulent flow around the horizontal axis wind turbine. The CFD results are also validated with the experimental data.

Keywords: aerodynamics; CFD; wind turbine; winglet, wingtip vortices

1. Introduction

In the last few years, many researchers investigated the improvement of wind turbine output by studying the aerodynamic characteristics of wind turbine blades. Winglets are regarded as an extended blades attached to the blade tips. The main aim of adding winglets is to reduce the induced drag that generates due to the spanwise flow by diffusing the wingtip vortices away from the blade tips and thereby increase the wind turbine performance. Unlike non-rotating wing, winglet parameters have not been investigated extensively for rotating wing for instance wind turbine. However, there is a similarity in aerodynamic flow analysis between rotating and non-rotating wing. Maughmer [1] confirmed that, the most important winglet parameters that should be studied to maximize its performance are winglet height, planform shape, sweep, twist, toe and cant angle.

In the literature, the majority of studies used computational fluid dynamics (CFD) methods to solve the governing equations that control flow around wind turbine and winglet parameters have been investigated. Elfarra et al. [2] studied the aerodynamic impacts of the four different winglets by optimizing cant angle and twist angle. The study shows that the wind turbine production is increased by 9% due to use of a winglet that is tilted towards suction side. Gupta and Amano [3] investigated the influence of the winglet height and cant angle on the wind turbine output power. The maximum increase of the output power was 20% which was established by the winglet with cant angle 45° and winglet with 4% height of the blade radius at wind speed 19 m/s. Congedo and Giorgi [4] studied the optimization of the winglet height and winglet curvature radius. The results show that, increase the curvature radius of the winglet by 50% leads to a slight increase in mechanical power by 1.6%, while it increases by 1.7% due to an increase by 25% of the winglet height. Johansen and SØrensen [5] reported the numerical investigation of the winglet influences by using CFD. Different winglet parameters such as winglet height, curvature radius, sweep and twist angle were considered and optimized. The results showed that an increase of the twist angle from 0° to 8° leads to a slight increase in mechanical power (about 1.6%) and thrust (about 1.9%). Moreover, there is no significant increase in mechanical power or thrust unless the curvature radius is equal to 100% of the winglet height. Despite previous studies on the winglet parameters according to Maughmer’s
recommendations the influence of winglet planform and winglet airfoil on its performance has not been investigated in details. Also, extending the baseline rotor by adding a winglet results in an increase in the wetted area penalty and consequently can increase the drag profile. In this paper, the effect of rectangular and elliptical winglet planforms on the winglet performance have been investigated by using CFD. In addition, the effect of two different winglet airfoils S809 and PSU 94-097 on the wind turbine performance are investigated.

2. Methodology

In this work, the Moving Reference Frame (MRF) approach is chosen to simulate the flow around wind turbine. Hence, the computational model is divided into a stationary, that is located away from blades, and rotating frame, close to the blades, while merged by interface boundary conditions. Unstructured mesh is used to discretize the computational model by using a mesh generator (Ansys 17.0). In addition, in order to integrate the partial differential equations from viscous sub-layer without using wall function, $y^+$ less than three is chosen with 10 prism layers created close to the blade surface. The steady state CFD simulation, RANS equations and two different turbulence models including of Spalart-Allmaras and Shear Stress Transport $K$-$\omega$ (SST) are implemented to solve the governing equations using Fluent 17.0. The second order upwind schemes are utilized to discretize the convection terms whereas simple algorithm is implemented for pressure velocity coupling. The convergence criteria are chosen to be $10^{-6}$ for all variables.

3. Numerical results

The two bladed NREL phase VI rotor, Figure 1, is chosen to be a baseline wind turbine to validate the CFD results. The geometrical dimensions of the rotor and the experimental data are taken from [6]. As NREL phase VI rotor blade has a sharp trailing edge, a slight modification is done on the wind turbine trailing edge by reducing the chord length by 1% to avoid the non-orthogonal cell faces. A 3D baseline rotor and modified blades by attaching different winglet planforms that are created by S809 and PSU 94-097 airfoils are shown in figure 2 and figure 3. The validation of the numerical results is done by comparing the experimental output power and pressure coefficient data with the numerical results that are obtained from Spalart-Allmaras and Shear Stress Transport $K$-$\omega$ (SST) at different wind speeds as shown in figure 4. Output power is calculated by monitoring the torque around a rotating axis and multiplying with the angular velocity.
Figure 4 shows the output power of the turbine obtained from the different turbulence models as well as experimental data. Both models are in good agreement with the experimental data at pre-stall region. At the stall region where the wind speed is higher than 10 m/s, the SST predicts more accurate results than Spalart-Allmaras. The reason behind the different prediction is related to capability of the turbulence models. Spalart-Allmaras model is a one-equation model whereas the SST is a two-equation model, a hybrid method, that combines two different turbulence models of K-ω and k-ε by using a blending function that implements the K-ω model near the wall and gradually converting to the k-ε model in the region away from the wall [7]. These features make the SST a robust model to capture the separated flow better than Spalart-Allmaras. Hence, the SST is used to simulate the baseline rotor with all winglet designs. Table 1 displays the rate of increase in output power for different winglet configurations.

Table 1: The rate of increase in power for rectangular and elliptical winglet.

<table>
<thead>
<tr>
<th>Wind Speed(m/s)</th>
<th>Rectangular (S809 airfoil)</th>
<th>Elliptical (PSU 94-097 airfoil)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>h=5cm</td>
<td>h=10cm</td>
</tr>
<tr>
<td>5</td>
<td>2463.77</td>
<td>5.1</td>
</tr>
<tr>
<td>7</td>
<td>6017.44</td>
<td>5.1</td>
</tr>
<tr>
<td>10</td>
<td>9328.94</td>
<td>6.2</td>
</tr>
<tr>
<td>15</td>
<td>8063.57</td>
<td>2.0</td>
</tr>
<tr>
<td>20</td>
<td>6740.53</td>
<td>-3.1</td>
</tr>
<tr>
<td>25</td>
<td>8172.60</td>
<td>0.5</td>
</tr>
</tbody>
</table>

The rectangular planform winglet increases the performance of the wind turbine more than the elliptical planform. In low wind speed range, both winglet with their airfoils show an increasing rate of output power. While in moderate and high wind speeds where stall occurs, there is a reduction in the output power for most of the winglet designs due to flow separation. Furthermore, the rectangular winglet planform with S809 airfoil has more stable performance than elliptical planform when the winglet height is changed.

The rectangular planform winglet provide higher output when the height of winglet is increased, as shown in Figure 5. Unlike the rectangular planform winglet, the elliptical one is not able to offer higher output power in moderate and high wind speeds, as shown in Figure 6.
5. Conclusions

In this study, two different winglet planforms, namely, rectangular and elliptical have been analysed. The results indicate that, the wind turbine output is increased by using the rectangular winglet planform more than elliptical. Moreover, the rectangular winglet shows more stable performance in comparison with the elliptical one.

References

Numerical investigation of particle-fluid flows: formulation, analysis and application

*Y. Ghaaffari Motlagh, A. Hassanpour and A. Bayly

School of Chemical and Process Engineering, University of Leeds, Leeds LS2 9JT, UK

*Y.GhaaffariMotlagh@leeds.ac.uk

ABSTRACT

The technique of coupling Computational Fluid Dynamics (CFD) for continuum fluid and the Discrete Element Method (DEM) for particles has been used to study the complex particle-fluid flows. In this study a four-way coupling, i.e. fluid-particle, particle-particle and particle-wall interactions has been used to simulate particulate flows. Although this approach provides us with high fidelity results, it is computationally expensive, particularly when the number of particles is high. The alternative approach to simulate a large number particles is Multi-Phase Particle-In-Cell (MP-PIC) method. In this method, the Bhatnagar, Gross, and Krook (BGK) model is applied to capture particle-particle interaction. In fluid phase of CFD-DEM and MP-PIC approaches Large Eddy Simulation (LES) techniques are used to capture the turbulence structures. The applicability of CFD-DEM and MP-PIC are demonstrated and discussed for the simulation of the particle-fluid flow problems.

Key Words: CFD-DEM; MP-PIC; multiphase flow; LES; turbulence

1. Introduction

Simulation of dense particulate flows in fluids such as fluidized beds and cyclones has been vastly studied particularly in regards to suitability of well-posed governing equations [1]. These type of particulate flows are normally represented with different flow models to solve different phases. Some terms such as mean fluid pressure gradient, particle viscous stresses, drag and inter-particle stresses are affected by all phases [1]. Various mathematical models have been proposed to solve particulate multiphase flow problems. Gidaspow [2] and Batchelor [1] have applied Eulerian framework for the all phases, whereas William [3] has used a Lagrangian description for the particulate phase, and an Eulerian continuum description for the gas phase. A multiphase particle-in-cell method, (MP-PIC), which provides an accurate and consistent representation of both discrete and continuum multiphase models, has been proposed by Andrew and O’Rourke [4]. O’Rourke et al. [5] has proposed a new mathematical formulation that implements a collision model (similar to that of Bhatnagar, Gross, and Krook [6]), in a particle distribution function transport equation, in order to approximate the rates at which collisions could result in local equilibration of particle velocities and masses, compositions, and temperatures of liquid films on particle bed.

Coupled particle-fluid flow problems can be found in a variety of industries. In order to gain a deeper understanding of the factors influencing the flow, development of suitable mathematical models as well as constitutive laws are crucial [7, 8]. Two common combinations are generally used to describe particle-fluid flow: the two-fluid model (TFM) and computational fluid dynamic- discrete element method (CFD-DEM). In TFM, both fluid and solid phases are treated as continuum media in a computational cell which is much larger than individual particles but still small compared with the size of computational domain of interests, e.g. process equipment [9]. However, its effective use heavily depends on the constitutive or closure relations for the solid phase and the momentum exchange between phases, which are often difficult to obtain within its framework; this is particularly true when dealing with different types of particles that should be treated as different phases. In CFD-DEM, the motion of discrete particles is
obtained by solving Newton’s second law of motion as used in DEM, and the flow of continuum fluid
by solving the Navier-Stokes equations based on the concept of local average as used in CFD, while
CFD and DEM are coupled through particle-particle, particle-fluid; particle-structure and fluid structure
interaction forces [7]. The main advantage of CFD-DEM is that it can generate detailed particle-scale
information, such as the trajectories of and forces acting on individual particles, which is key to under-
stand the mechanisms influencing the complicated flow behaviour. In this paper MP-PIC and CFD-DEM
methods are used to solve various particle-fluid flow problems. The applicability of the methods are
demonstrated and discussed.

2. Mathematical models

2.1. CFDEM formulation

The solid phase is treated as a discrete phase and modelled by the DEM. The translational and rotational
motions of a particle is described by Newton’s law of motion:

\[ m_i \frac{dv_i}{dt} = F_{i,n} + F_{i,t} + F_{i,f} + F_{i,b}, \]

where \( F_{i,n} \) is the normal particle-particle contact force, \( F_{i,t} \) is the tangential particle-particle contact
force, \( F_{i,f} \) is the force that the particle-fluid phase interaction force, e.g. the drag force, pressure gradient
force, viscous force, etc. \( F_{i,b} \) is the body forces like gravity, electrostatic or magnetic forces. \( r_{ic} \) is the
position of particle. \( M_{i,r} \) is an additional torque on the particle that can be used to model non-sphericity
by means of a rolling friction model.

The motion of an incompressible-fluid phase in the presence of a secondary particulate phase is governed
by the volume-averaged Navier-Stokes equations, which can be written as:

\[ \frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f \rho_f u_f) = 0, \]

\[ \frac{\partial (\alpha_f \rho_f u_f)}{\partial t} + \nabla \cdot (\alpha_f \rho_f u_f u_f) = -\alpha_f \nabla (\frac{p}{\rho_f}) - R_{pf} + \nabla \cdot \tau, \]

where \( \alpha_f \) is the volume fraction occupied by the fluid, \( \rho_f \) is the fluid density, \( u_f \) the fluid velocity, and
\( \tau \) is the stress tensor for the fluid phase. \( R_{pf} \) represents the momentum exchange with the particulate
phase. The four-way coupling is considered and the coupling algorithm is the same as one used in [10].

2.2. MP-PIC formulation

The mass and momentum equations for the fluid phase are [2]:

\[ \frac{\partial \alpha_f \rho_f}{\partial t} + \nabla \cdot (\alpha_f \rho_f u_f) = 0, \]

\[ \frac{\partial \alpha_f \rho_f u_f}{\partial t} + \nabla \cdot (\alpha_f \rho_f u_f u_f) = -\alpha_f \nabla p - F + \alpha_f \rho_f g, \]

where \( F \) is the rate of momentum exchange per unit volume from the fluid to the particle phase. The evolution of the particle phase is governed by a Liouville equation for the particle distribution function,
\( f(x, v, m, t) \):

\[ \frac{\partial f}{\partial t} + \nabla_x \cdot (f v) + \nabla_v \cdot (f A) = \frac{f_{eq,v} - f}{\tau^v} + \frac{f_{eq,t} - f}{\tau^t}, \]
where x is the particle position; v is the particle velocity; m is the mass of the particle; \( A = \frac{dv}{dt} \) is the particle acceleration and includes the effects of drag due to particle motion relative to the continuous gas phase, buoyant forces, gravitational acceleration, and an isotropic inter-particle stress [4]; \( f_{eq} \) is the distribution that results if particle velocities are equilibrated, and the remainder of the particle distribution remains unchanged; \( f_{eq,i} \) is the particle distribution when full collisional equilibrium of all particle quantities is achieved [5]; \( \tau^v \) and \( \tau^t \) are collision time scales [5].

3. Numerical results

In this paper numerical 3D simulations of fluidised bed has been carried out using MP-PIC and CFD-DEM methods. Figure 1 shows the snapshot of void fraction of fluidised bed simulated by MP-PIC and CFD-DEM. In these simulations 24,750 particles with the diameter 1 mm and density 2526 kg/m$^3$ have been used and a superficial gas velocity of 1.875 m/s was implemented for fluidised bed which should result in a bubbling regime of fluidisation. The CFD-DEM, Figure 1(a), shows more realistic results in comparison with the MP-PIC, 1(b). The main reason behind the difference between the results from the two methods is accounting for the full particle-particle interactions resulting in more accurate particle motions. Unlike the CFD-DEM, the MP-PIC does not consider the motion of the particles individually and also does not provide particle collision information precisely. As a result the particle information, e.g. positions and velocities from MP-PIC would not be as accurate as the DEM in the CFD-DEM. This is particularly crucial for dense particle-fluid systems, e.g. the transformation from a dense phase to lean phase in fluidised beds, where particle interactions are significant and should be fully taken into account.

4. Conclusions

In this paper the MP-PIC and the CFD-DEM techniques have been presented for solving particulate flow problems. The high fidelity results can be obtained by the use of the CFD-DEM, due to the precise modelling of the discrete phase as well as the four-way coupling approach. For the fluidised bed systems where a dense particle phase will transform to a lean phase at the onset of fluidisation, MP-PIC cannot accurately model the particle motions and concentration due to the intensive particle-particle and particle-structure interactions which is not precisely modelled. However, the MP-PIC may be used as an alternative approach for modelling of lean particle-flow problems. Nevertheless, for particle-fluid systems with large number of particles (billions) where DEM-CFD cannot be practically used due to high computational costs, MP-PIC could be one of the options.
Acknowledgements

The authors gratefully acknowledge the UKs AMSCI scheme for the financial support of the ADDoPT Project: Towards Digital Design and Operation of Robust Manufacturing Processes for the Pharmaceutical Sector (Grant reference 14060).

References


NUMERICAL SIMULATION OF TWO-PHASE FLOW WITH EULERIAN MODEL IN A CHANNEL

*Beatriz Ramos Barboza* and *Chenfeng Li*

1Zienkiewicz Centre for Computational Engineering, College of Engineering, Swansea University, SA2 8PP

*805379@swansea.ac.uk

ABSTRACT

Two-phase flows may be found in many industrial applications, from oil refining processes to sediment transport, so it is relevant to understand how to represent the physics of those problems. In this work, a computational model is being implemented in MATLAB using Euler-Euler method in order to represent the dynamic of a two-phase flow inside a channel. The code is based on the finite volume method and is able to deal with 2D mesh. In addition, an iterative procedure based on SIMPLE algorithm is used to solve the Navier-Stokes equations that characterize the fluid behaviour. To validate the solver, widely studied multiphase flow problems is being simulated and the results compared with ANSYS FLUENT and classical papers.

Keywords: Finite Volume Method, Navier-Stokes, Two-phase fluid flow.

1. Introduction

Multiphase flow systems had been a great interesting in the research community and are encountered in diverse industries. These systems are a key knowledge behind simulations on areas such petroleum engineering, aerospace, chemical engineering, hydraulics and so forth.

A phase can be characterized as distinguishable class of material that has a specific inertial response to and interaction with the flow and the potential field in which it is immersed. Hence, particles of the same material with different sizes can be treated as distinctive phases due to the dynamical response to the flow field [1]. Two-phase systems can be divided into four sets related to the type of the phases: liquid-liquid, gas-liquid, solid-liquid and solid-gas. Those schemes are the most common in multiphase field, however, there are researches dealing with three-phases and four-phases models as in [2].

In this work, a 2D computational model using MATLAB is being developed in the interest of simulates the physical behaviour of a two-phase system flowing inside a channel. Thus, classical Navier-Stokes equations are solved and compared with benchmarks. At this stage, the code is being applied for fluid-fluid systems, though the final aim is apply it on solid-fluid configurations.

2. Governing Equations

The dynamics of many two-phase flows encountered in engineering applications are adequately modelled by the Navier-Stokes equations [7]. Thus, the momentum equation in a conservative form and the continuity equation for incompressible flow are given by Eqs. (1) and (2)

\[
\frac{\partial}{\partial t}(\alpha_k \rho_k \vec{u}_k) + \nabla \cdot (\alpha_k \rho_k \vec{u}_k \vec{u}_k) = -\alpha_k \nabla P + \nabla \cdot (\alpha_k \tau_k) + \alpha_k \rho_k \vec{g} + M_k
\]

(1)

\[
\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \vec{u}_k) = 0
\]

(2)

where the right-hand side (RHS) of Eq. (1) are the pressure gradient, viscous and turbulent stress forces, body force, and interfacial momentum transfer, respectively, and RHS of Eq. (2) is zero due to the incompressibility. The phase volume fraction is \( \alpha_k \).
In this code, an Euler-Euler approach used for the numerical representation of two-phase flow, consequently the different phases are treated as interpenetrating continuum. Thus, the conservation equations are derived for each phase, e.g. a set of momentum and continuity equations is solved for each phase. The pressure and interfacial momentum transfer are responsible for the coupling in this case. More details about the Eulerian model can be find on [5].

3. FVM Code

The discretization method behind the Finite Volume Method involves the integration of the partial differential equations over an element, which changes the surfaces and volumes integrals into discrete algebraic relations over elements [4]. This gives flexibility as a discretization method. Hence, there are powerful commercial CFD packages that use FVM as discretization procedure, e.g. Fluent ANSYS. After discretize momentum and continuity equations, the SIMPLE [6] (Semi-Implicit Method for Pressure Linked Equations) algorithm is applied to solve the equation system. In this algorithm the solution is found iteratively by generating pressure and velocity fields that satisfy both the momentum and continuity equations.

4. Results

The Lid-Driven Cavity Flow is a benchmark in Computation Fluid Dynamics simulation and was used to validate the code for single-phase flow. The Figure 1 illustrates the geometry and boundary conditions for the case.

![Figure 1: Lid-Diver Cavity configuration.](image)

The case was reproduced with the same conditions on both Fluent ANSYS and the FVM code from this work. In the Figure 2 is possible to see that the curves are similar. Thus, the validation to single-phase problem was concluded.

![Figure 2: Comparison between experimental data from Ghia et al., Fluent ANSYS and the FVM code.](image)
Results from two-phase flow simulations will be presented orally during the conference.

5. Conclusion

A FVM code using MATLAB has been developed to simulate two-fluid dynamics present in engineering problems, more specifically in proppant transport simulations. Thus, until this stage, the research is during validation process to two-phase flow and the results will be presented orally in the conference.

Acknowledgements

The author gratefully acknowledges CNPQ/Brazil and Science Without Borders Program for the financial support.

References


CFD Investigation of Transitional Separation Bubble Characteristics on NACA 63415 Airfoil at Low Reynolds Numbers

*Iham F. Zidane¹, **Greg Swadener¹, Khalid M. Saqr², Xianghong Ma¹, Mohamed F. Shehadeh²

¹ School of Engineering and Applied Science, Aston University, Aston Triangle, Birmingham, B4 7ET, U.K
² Mechanical Engineering Department, College of Engineering and Technology, Arab Academy of Science. Technology and Maritime Transport, 1029 Abu Kir, Alexandria – Egypt

*zidanifh@aston.ac.uk ** j.g.swadener@aston.ac.uk

ABSTRACT

The wind turbine blades performance is strongly influenced by transitional separation bubbles, which may occur at low Reynolds numbers. Such a separation bubble is caused by a strong adverse pressure gradient, which makes the laminar boundary layer to separate from the curved airfoil surface. In the present paper, a CFD investigation is conducted to document the structure and behaviour of transitional separation bubbles at different Reynolds numbers. A two-dimensional incompressible Navier-Stokes equation and the transition SST turbulence model are used. The wind-tunnel tests of the NACA 63415 airfoil at Reynolds number 1×10⁶ are used to compare with the time-averaged results of the present steady computations. The simulations were carried out at Reynolds number range of 150×10³ - 460×10³ at different angle of attacks. This study presents the effects of angle of attack and Reynolds number on the separation characteristics and airfoil performance.

Keywords: Wind Energy; Low Reynolds Number; Wind Turbine Blade; Transitional Separation Bubble

1. Introduction

Wind energy is one of the most important renewable energy resources [1, 2]. The performance of wind turbine blades operating in low Reynolds number, incompressible flows has been of increasing interest. Many significant aerodynamic problems appear to occur at small Reynolds number ranges. Most of the previous research studies concentrated on the behavior of the boundary layer, such as, transitional separation bubble, transition, turbulent reattachment, etc., due to its significant influence on the performance of devices based on lifting bodies such as the wind turbine blades [3]. The transitional separation bubble has been studied for many years. Most of these studies have focused on angle of attack, Reynolds number, and freestream turbulence effects on bubble characteristics and length [4-9]. Transitional separation bubble was classified into short and long separation bubbles. For a short bubble, the length of the turbulent separation shear layer is about the same as the laminar shear layer and the bubble usually extends for only a few percent of the airfoil chord. The long bubble has a turbulent shear layer that extends over most of the airfoil chord with a correspondingly large interaction with the external flow [10].

This paper studies the effects of angle of attack and Reynolds number on the separation characteristics and airfoil performance. Thus, the wind turbine designers have an accurate prediction of transitional separation bubble existence and extent for airfoils operating at low Reynolds number.

2. Model Description and Simulation Details

2.1. Governing Equations

The flow past the airfoil NACA 63415 was modelled by the Full Navier-Stokes equation for two-dimensional, viscous, incompressible flow. The continuous equation and Momentum equation based on Reynolds averaged N-S equations are as follows:

\[
\frac{\partial u}{\partial x} = 0
\]
\[ \rho (\nabla \cdot \mathbf{V}) \mathbf{V} = -\nabla p + \nabla \cdot \tau + \rho \mathbf{u}' \mathbf{u}' \]  

(2)

2.2. Mesh Refinement Investigation

The whole computational zone consists of a semicircle with the radius of 12.5m and a rectangle with the length of 25m as shown in Figure 1(a). The chord length of numerical airfoil which locates near the center of the semicircle is 1m. The number of the grid nodes is 120,878. The height of the grid near the airfoil surface is 7 x 10^{-6} m as shown in Figure 1(b). The range of values of the dimensionless wall distance \( Y^+ \) through the airfoil were less than 1. Coupled algorithm was used to solve the coupling problem between velocity components and pressure in momentum equations. Turbulence kinetic energy was taken as third-order MUSCL scheme in Calculation. However, momentum and specific dissipation rate were solved using second-order upwind scheme.

![Figure 1: (a) C-H Computational Domain (b) General Mesh with Boundary Adaptation](image)

2.3. Turbulence Model and Validation Method

The numerical simulation of the 2D NACA 63415 was made using the CFD software Fluent to compare with the wind tunnel experimental data taken from Bak et al [11] to ensure that the numerical model is available for the free-stream flow past the airfoil. The experiment was performed at Reynolds number 1.6 x 10^6. The lift and pressure coefficients of the NACA 63415 airfoil were computed under the angle of attack (AOA) between 0 and 10 degree. The governing equations were Navier-Stokes equations, and turbulence models were applied. The calculation results of Transition SST model of four equations [12] were closest with the experimental data. The comparison between numerical results and experimental data is shown in Figure 2. It was obvious that the numerical results at Reynolds number 460 x 10^3 had a good consistency with the experimental data. After this validation works, the continuing works uses the same model but the analyses were for airspeeds such that the Reynolds Numbers are 150 x 10^3, 300 x 10^3 and 460 x 10^3.

![Figure 2: Numerical Validation Results](image)
3. **Results and Discussion**

Transitional separation bubble occurs when the boundary layer separates from the airfoil surface due to an adverse pressure gradient. Figures 3 and 4 describe the flow separation phenomenon occurred at the three Reynolds number values \(150 \times 10^3\), \(300 \times 10^3\) and \(460 \times 10^3\) at AOA 2° and 10° respectively. The pressure rise is related to the velocity drop towards the trailing edge of the airfoil. The fluid particles in the inner part of the boundary layer is slower, it is more affected by the increasing of the pressure gradient. As a result, this fluid may slow to zero velocity. After the laminar boundary layer separation, a highly unstable detached shear layer forms and transition to turbulence takes place in the detached shear layer. The enhanced momentum transport in the turbulent flow enables reattachment and a turbulent boundary layer develops downstream. In contrast, as shown in both figures, the height and length of the transitional separation bubble at Reynolds number \(460 \times 10^3\) is quite small. Thus, the transitional separation bubble effect on the aerodynamic performance of the airfoil is very limited. However, as the Reynolds number decreases, the height and length of the transitional separation bubble increases. This could be observed in the figures 3 and 4 at Reynolds number \(150 \times 10^3\).

Increasing angle of attack causes boundary layer separation to occur further upstream and produce a shorter transitional separation bubble. The separation bubble thickens the boundary layer and thus increases the pressure drag of the airfoil. The drag increase can be several times the drag of the airfoil without a separation bubble. In addition, lift is influenced by a transitional separation bubble, which can lead to problems with the aerodynamic performance of the airfoil. Figure 5 shows the lift and drag coefficients degradation due to the increase of transitional separation bubble length. Comparing the lift and drag coefficients at both Reynolds number values \(150 \times 10^3\) and \(460 \times 10^3\), there was a decrease in lift (20% reduction at 10° AOA) and an increase in drag that exceeded 80%.

![Figure 3: Transitional separation Bubble at AOA 2° for the Three Reynolds Number Values](image)

![Figure 4: Transitional separation Bubble at AOA 10° for the Three Reynolds Number Values](image)

![Figure 5: Drag and Lift Coefficients vs AOA for the Three Reynolds Number Values](image)

172
4. Conclusion

A four-equation steady incompressible turbulence Transition SST model is applied in this study to simulate the flow around a two-dimensional wind turbine airfoil NACA 63415 in three Reynolds number values. The angle of attack range was from 0° to 10°. The effects of angle of attack and Reynolds number on the transitional separation bubble characteristics and airfoil performance were investigated and studied. Results showed that the decrease in lift could exceed 20 percent and the increase in drag could exceed 80%.

References

Parallel Performance of an Open Source Fluid Structure Interaction Application

*Sam Hewitt�, Lee Margetts� and Alistair Revell�

�School of Mechanical, Aerospace and Civil Engineering, University of Manchester

*Sam.Hewitt@Manchester.ac.uk

ABSTRACT

This paper describes the coupling of two pieces of software Foam-Extend and ParaFEM, to model fluid structure interaction problems. The two applications are open source and scale well on HPC systems. The motivation behind such a coupling is to enable the solution of large complex fluid structure interaction problems, that previously would have been too time consuming, by utilising HPC systems. The coupling uses Foam-Extend as the master application with ParaFEM being used as a back end plugin, this results in problems being run in a manner consistent with Foam-Extend. The two packages pass data between each other directly through subroutine calls, which is significantly quicker than file sharing based methods. Initial validation and scaling results have been positive with a factor of 7.7 speed up on 16 cores. Foam-Extend has a comprehensive level of CFD functionality which is complemented by the growing list of solid mechanics capabilities of ParaFEM. Such as multi-scale modelling of non linear deformation in solids. This paper and application will be of value to those engineers and academics wishing to improve simulations and model complex fluid structure interaction phenomenon.

Key Words: Fluid-Structure Interaction; High Performance Computing; Simulation and Modelling

1. Introduction

Fluid-Structure Interaction (FSI) is a growing topic of interest in a number of fields, it has been used to study a range of problems; the deflection of a wind turbine blade[1] and the analysis of aortic aneurysms[2]. Recently the improvement in both the numerical models to solve single field physics and the increase in level of computational resources available to academics has seen a rise to the number of studies developing FSI algorithms and numerical models.

The motivation behind this paper is to develop highly parallel FSI software that is capable of running on a large number of cores, which is often difficult with commercial packages. This will enable the complexity and size of problems being solved to increase.

Solving FSI problems can be done using a monolithic approach, where the governing equations of the solid and fluid are combined into as single set of equations or in a partitioned approach where each set of governing equations is solved individually. Partitioned approaches offer a greater level of flexibility when compared to their monolithic counter parts and allow the reuse of well established existing codes.

The application was developed by coupling Foam-Extend[3] and ParaFEM[4] in a black box, partitioned manner. In doing so the pre-existing models and solution algorithms that have been well validated for CFD and FEM solvers can be used independently of the coupling strategy, offering greater levels of fidelity and flexibility in the modelling. With the possibility to include more advanced and parallelised structural assessment methods to the solid side of the problem, such as plasticity[5], geometric nonlinearity[6], multi-scale fracture[7], thermomechanical analysis[8] and stochastic Monte Carlo[9] capabilities, that are already available in ParaFEM.

2. Method

An FSI problem is defined by three important sets of equations, those governing the fluid domain, those governing the solid domain and those which describe the interface. These individual domains, along with appropriate boundary conditions define the problem.
2.1. Fluid Dynamics

Equations in 1 represent the Newtonian, laminar and incompressible form of the conservation of mass and momentum for the fluid, which are used in the initial scaling test case shown in Section 4.

$$\nabla . U_f = 0, \quad \rho_f \frac{\partial U_f}{\partial t} + \rho_f U_f \nabla U_f + \nabla P - \mu_f \Delta U_f = \rho_f b_f$$

(1)

Where $U_f$ represents the velocity vector $[u \ v \ w]^T$, $\rho_f$ the density of the fluid, $P$ the pressure, $\mu_f$ the viscosity and $b_f$ the body forces.

2.2. Solid Mechanics

The structural domain is modelled using the equations for forced vibration of an elastic solid, described by Equation 2:

$$[M][\dddot{U}_s] + [C][\ddot{U}_s] + [K][U_s] = \{f_t\}$$

(2)

Where $\{U_s\}$ represents the displacement vector $[u_x \ u_y \ u_z]^T$ of the solid, with $\dddot{U}_s$ and $\ddot{U}_s$ being the second and first derivative with respect to time, or acceleration and velocity respectively. $[M]$, $[C]$ and $[K]$ represent the mass, damping and stiffness matrices of the structure respectively.

2.3. Interface

The interface describes the coupling between the two sets of equations and domains. FSI problems have two key interface conditions shown in Equation 3:

$$\sigma_f.n = \sigma_s.n, \quad U_f = \frac{dU_s}{dt}$$

(3)

These equations state that the traction and displacement at the boundary must be in equilibrium between the solid and fluid.

3. Implementation

The two packages used to solve the equations above are Foam-Extend and ParaFEM. Foam-Extend is an open source Computational Fluid Dynamics(CFD) package based on the finite volume method. It is a mature CFD solver with capabilities in meshing, pre-processing and post-processing. ParaFEM is an open source library of tools and driver programs, based on the finite element method, used to solve structural mechanics problems. It is highly parallel and has been shown to scale well to around 32,000 cores for certain problems[4]. Coupling these two pieces of software in a partitioned approach has resulted in an application capable of modelling FSI phenomena using well established numerical methods.

In the implementation, Foam-Extend is considered the master application with ParaFEM the slave. Foam-extend contains an external library[11] that wraps and partitions the components required for a FSI problem, such as convergence accelerators, weak and strong coupling algorithms, interpolation and mesh motion libraries. The ParaFEM driver program used to solve the forced vibration of an elastic solid using implicit integration in time, was coupled to this library. The driver program was first decomposed into two subroutines that are called to initialise ParaFEM and solve ParaFEM. Figure 1 shows the FSI algorithm used in the application along with how ParaFEM is called during run time.

The initialisation is called once at the start of the program, it builds and distributes the arrays required for the “Solve Solid” subroutine. The “Solve Solid” subroutine is called whenever a solution to the structural domain is needed. The inputs are an external force vector, calculated from the traction of the fluid on the structure, and outputs are displacement, velocity and acceleration vectors used to move the fluid domain.
3.1. MPI Coupling

MPI is used by both applications to run in parallel, however Foam-Extend decomposes the domain as a preprocessing step based on a specified method, whilst ParaFEM decomposes the domain at run time on an element by element basis. The interface or boundary between the two domains is considered global, in order to simplify the passing of information between the two applications. This was deemed suitable for current applications where the interface often represents a small proportion of the total domain.

4. Validation and Scaling

The validation and scaling case used is the benchmark developed by Hron and Turek[12]. It involves the flow around a cylinder with an elastic flag attached behind. The results for the validation will be shown at the conference. Initial scaling tests have been run on the Computational Shared Facility at the University of Manchester. These tests considered the validation case with an over refined mesh, and ran for one time step with 30 sub-iterations between the fluid and solid domains. Figure 2 shows the speed up and reduction in execution time achieved using 16 cores.

Further analysis of the scalability of the software will be shown at the conference along with the outlook and possibilities to solve large FSI problems on different HPC systems.
5. Conclusion

This paper has discussed and introduced a new open source application that couples a popular and well known CFD solver Foam-Extend to a highly scalable finite element package, ParaFEM, used to solve structural mechanics problems. The paper has shown some initial scaling results of the software on the Computational Shared Facility at The University of Manchester, with positive results. The consequences of this software will enable the introduction of more complex multi scale solid models into FSI simulations.

Acknowledgements

The authors acknowledge the support of EPSRC and General Electric through grant EP/M507969/1.

References


Geomechanics
Stability analysis of geometrically non-homogeneous stratified slopes

*R. Sauffisseau¹, A. Ahangar Asr¹

¹School of Computing, Science and Engineering (CSE), University of Salford, Salford, M5 4WT

*r.sauffisseau@edu.salford.ac.uk

ABSTRACT

Due to ongoing construction of cities and development of new buildings and infrastructures, many natural slopes in and around urban areas are often subjected to cuts. These excavations result in dramatic changes in the geometry of slope faces mostly by the slope angle to the ground level increasing which could potentially develop levels of risks of slope failures with catastrophic consequences. As most natural slopes are of non-homogeneous layered nature it will be of utmost importance to understand the stability behaviour of such slopes. The current practice in analysing slopes of complicated nature, geometrically and materially, is mostly to apply simplifications which could sacrifice accuracy resulting in application of large factors of safety which could question analytical and also economic feasibility of projects. In this research limit equilibrium and finite element methods are implemented by employing commercial software in order to empirically and numerically model and analyse stratified slopes with the aim of understanding effects of non-homogeneity of geometry and materials on stability. The analysis included determination of factors of safety as well as a sensitivity analysis looking into the combined effects of contributing parameters such as slope angle and non-homogeneity in stability analysis.

Keywords: natural slopes, non-homogeneity, numerical modelling, stability analysis

1. Introduction

Slope failures are a major problem everywhere in the world because of their hazardous and costly consequences which cause thousands of deaths every year [4][9]. Most slopes are natural and engineers must often cut through them in order to construct new transportation routes, buildings and infrastructures [1]. Therefore, the slope stratification must be known to obtain the factor of safety of the slope for the desired face angle using data from ground investigations[8].

Natural ground is extremely variable from one location to another, even on a same relatively small area which is why knowing the ground conditions is highly important before starting any design and construction. Some factors such as the presence of water [6], the rainfall intensity [4], the soil properties and the overall geometry of the slope [10] have an impact on slope behaviour when subjected to additional loads. However little attention was given to the direction of the layers within the slope itself which is what this research focuses on. Nowadays, computers and softwares are used to obtain quicker results: OASYS Slope uses the Limit Equilibrium Method [7] and PLAXIS 2D uses the Finite Element Method [3] to analyse slopes considering the appropriate input parameters [5]. In this research, the aim is to observe the effect of the soil layers’ direction on the general stability of a slope before and after cut using and comparing limit equilibrium and finite element methods.

2. Modelling process

Guo and He [2] used a stratified slope model in their research which is used again here with Limit Equilibrium (LE) and Finite Element (FE) methods as a good representation of natural slopes. In LE and FE, a Mohr-Coulomb shear strength model was used to fulfil the aim: to observe the impact of the stratification of the ground on the stability of slopes. Layered slopes were analysed and the layer
orientation was modified, keeping the same layer thicknesses and properties (Figure 1 (a) and (b)). With the main focuses being the slope geometry and stratification effects, the water table was placed very deep and its effects were not considered (drained conditions). Initially, the slope face rests at an angle of 18°, then 56° after the cut (Figure 1 (a) and (b)) to observe any change in behaviour of the slope when increasing the steepness. PLAXIS 2D with FE was used to automatically generate a “very fine” 15-noded mesh. The calculation phases were defined as Initial (initial stress conditions) and Safety (factor of safety using the c-phi reduction method).

Figure 1: Presentation of the models: Case 1 (original) (a) and Case 2 (b)*

* C: crest location of the slope; Numbering corresponds to a material type as presented in Table 1.

![Figure 1: Presentation of the models: Case 1 (original) (a) and Case 2 (b)*](image)

**C: crest location of the slope; Numbering corresponds to a material type as presented in Table 1.

Figure 2: Slip surface results with Limit Equilibrium (orange curved line) and Finite Element (colour shading): Case 1 (a) before and (b) after cut and case 2 (c) before and (d) after cut

Table 1: Slope soil parameters

<table>
<thead>
<tr>
<th>Soil Type</th>
<th>Elastic Modulus (MPa)</th>
<th>Poisson's ratio</th>
<th>Unit Weight (kN/m³)</th>
<th>Cohesion (kPa)</th>
<th>Friction angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filling Soil (6)**</td>
<td>15.1</td>
<td>0.3</td>
<td>18.1</td>
<td>18</td>
<td>20.3</td>
</tr>
<tr>
<td>Brown Coal (4)</td>
<td>23.1</td>
<td>0.27</td>
<td>23</td>
<td>16</td>
<td>12</td>
</tr>
<tr>
<td>Carbonaceous Mudstone (5)</td>
<td>16.3</td>
<td>0.28</td>
<td>22.5</td>
<td>30</td>
<td>23.2</td>
</tr>
<tr>
<td>Mudstone (3)</td>
<td>12.7</td>
<td>0.29</td>
<td>21.2</td>
<td>16.9</td>
<td>16.6</td>
</tr>
<tr>
<td>Ophitic (9)</td>
<td>200</td>
<td>0.21</td>
<td>26.2</td>
<td>200</td>
<td>28.35</td>
</tr>
<tr>
<td>Dirty Sandstone (2)</td>
<td>120</td>
<td>0.22</td>
<td>27.3</td>
<td>100</td>
<td>33</td>
</tr>
<tr>
<td>Soil (1)</td>
<td>80.6</td>
<td>0.26</td>
<td>19.3</td>
<td>18</td>
<td>10.2</td>
</tr>
<tr>
<td>Cobble-stones (7)</td>
<td>2000</td>
<td>0.21</td>
<td>21.5</td>
<td>0</td>
<td>24</td>
</tr>
<tr>
<td>Clay (8)</td>
<td>40</td>
<td>0.29</td>
<td>19.4</td>
<td>18.3</td>
<td>16</td>
</tr>
</tbody>
</table>

***(1): Material ID number linked to Figure 1 and Figure 2.

3. Observation of the results

Initially, the case study used in this research had a layer of cobblestones (Layer 7 in Figure 1) which was replaced in the analysis by a different material because (i) while running the limit equilibrium analysis a factor of safety of 0.064 was found (very low factor of safety) for the “after cut” case
(Figure 2 (b) and (d)) and (ii) it was also observed that this failure was local in the cobblestones at the very top of the slope rather than a general failure. Unlike OASYS Slope, PLAXIS 2D doesn’t allow the user to observe the local failure cause by the cobblestones as the overall lowest factor of safety (generally in the slope) was calculated. Cobble-stones is a cohesionless material (c=0 kPa) and increasing the c value led to a converging factor of safety of 1.865 when c=10 (FoS=1.527 when c=2 kPa) which proved that this material was the source of misleading results. With a factor of safety being close to 0 a good representation of the general factor of safety could not be obtained using this model. As the aim of this paper is focused on general failures linked to the geometry of the slope, cobblestones layer was replaced by filling material to address the issue.

### Table 2: Factors of Safety for cases 1 and 2 and comparison ratios

<table>
<thead>
<tr>
<th>Condition</th>
<th>LE</th>
<th>FE</th>
<th>LE/FE ratio</th>
<th>Condition</th>
<th>LE</th>
<th>FE</th>
<th>LE/FE ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Before/After ratio</td>
<td>2.62</td>
<td>3.52</td>
<td></td>
<td>Before/After ratio</td>
<td>3.45</td>
<td>3.68</td>
<td></td>
</tr>
<tr>
<td>Case 1</td>
<td></td>
<td></td>
<td></td>
<td>Case 2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Before Cut</td>
<td>2.201</td>
<td>1.877</td>
<td>1.17</td>
<td>Before Cut</td>
<td>2.131</td>
<td>2.003</td>
<td>1.64</td>
</tr>
<tr>
<td>After Cut</td>
<td>0.839</td>
<td>0.533</td>
<td>1.57</td>
<td>After Cut</td>
<td>0.618</td>
<td>0.545</td>
<td>1.14</td>
</tr>
</tbody>
</table>

### a. Limit Equilibrium Method

The slope was modelled to observe its stability and failure mechanisms prior and following a cut. In its natural environment, the slope (case 1; Figure 1) had a factor of safety of 2.201 (stable; Figure 2 (a)), which was observed to drop significantly after the removal of the soil down to 0.839 (unstable; Figure 2 (b)). Regarding the slip surface before the cut (Figure 2 (a)), the high point ‘m’ was located at 7m away from the crest to the left and the lower point of the failure surface ‘n’ at ¼ down the slope with a maximum normal depth to the slope surface of 10m. After the cut (Figure 2 (b)), the slip surface was 6m to the left of point C (point ‘m’, closer than previously) and reaches the very bottom of the slope where slope and horizontal ground meet (point ‘n’) showing a full slope failure. The failure plane was shallower at a depth of 7m.

Then, case 2 (Figure 1 (b)) was modelled and analysed. Prior any excavation, the stratified slope had a factor of safety of 2.131 (stable; Figure 2 (c)), then 0.618 after the removal of the soil (unstable; Figure 2 (d)). Regarding the slip surface before the cut (Figure 2 (c)), the high point ‘m’ was located at 2m away from the crest ‘C’ to the left to half way down the slope with a maximum normal depth to the slope surface of 5m. Following the cut (Figure 2 (d)), the slip surface at ‘m’ followed the interface of the dirty sandstone and mudstone layers (approximately the same as before the cut) and like in case 1, it reached the bottom of the slope ‘n’. The failure plane was shallower at a depth of 5m.

### b. Finite Element Method

The FE method resulted in differences in the factor of safety, the location and shape of the failure line. In case 1, the factor of safety was 1.877 (stable; Figure 2 (a)) before the cut then 0.533 (unstable; Figure 2 (b)); lower than LE (Table 2). Before the excavation (Figure 2 (a)), the slip surface was located at a lower depth than using LE (6.5m-7m) and a non-circular abnormality was observed at the location of the dirty sandstone where the slip surface depth was even lower which can be explained by the shear strength parameters of the soil type (c=100 kPa; phi=30°) which were higher than the average layer. After the cut (Figure 2 (b)), (compared to LE), it was observed that the bottom end of the slip surface was not located at the toe of the slope but at approximately 2.5m above this location.

In case 2, a factor of safety of 2.003 (stable; lower than LE, Table 2) was obtained before the slope cut (Figure 2 (c)). Compared to case 1, the top of the slip surface was located 2m to the left of point C (same as LE in case 2) but the bottom end of the slip was located at the very bottom of the slope with a slip located at 10m depth. After the removal of the soil, the factor of safety was 0.545 (unstable; Figure 2 (d); lower than LE, Table 2). As observed in case 2 with LE, an even more significant meeting line between the slip surface and the interface of the dirty sandstone and mudstone layers was observed demonstrating the impact the verticality of the layers has on the location of the slip surface.
The top of the slip had the same location as in LE but the bottom end was located at 2m above the horizontal ground (same difference as in case 1 between LE and FE methods).

c. Combined Observations
Before the cut, the bottom of the slip surface in case 1 was located at the interface of two layers at a given depth whereas in a vertically stratified slope, the slip surface depths through each layer was depending on their respective shear strength (the higher ‘c’ and ‘phi’, the shallower). This first same phenomenon was observed after the cut in case 2 where a part of the slip surface followed the vertical interface of two layers. It appeared that after the cut, the arrangement of the layers had some effects on the factor of safety and that the shear failure in vertically stratified slopes followed a circular pattern (Figure 2 (d)) against a linear pattern in the horizontal case (Figure 2 (b)). When a stratified slope problem is modelled before construction, simplifications regarding the stratification should be avoided to use a good representation of the reality. Indeed, if any stratified slope (most natural slopes) was simplified into a homogeneous slope (with adequate soil properties), the impact that the layer orientation and interface would have on the stability would be ignored to some extent, which would lead to misleading results especially when observing the location of the slip surface at failure.

4. Conclusions
Limit Equilibrium and Finite Element Methods were used to assess the factor of safety and location of the failure of two stratified slopes and enable the assessment for the need of slope reinforcement or other slope stabilisation methods to avoid landslides. It was observed that in fact, the orientation of the soil layers show a higher factor of safety when layers are as original compared to rotated. The factors of safety using the FE method are lower than the ones from the LE method. This makes the use of the FE method safer for designs of structures or excavations of stratified slopes. Indeed, FE method looks at elements within the generated mesh which provides a better accuracy. If the certainty about the slope behaviour is increased, the applied factor of safety within a design could be reduced leading to more economically viable designs. Attention must be paid to local failures when using the FE Methods as these may not be always of high concern.

References
NUMERICAL INVESTIGATION OF THE BEDDING FACTORS ASSOCIATED WITH THE DESIGN OF BURIED CONCRETE PIPES SUBJECT TO TRAFFIC LOADING

*Saif Alzabeebee1, David N. Chapman1 and Asaad Faramarzi1

1School of Engineering, University of Birmingham, Edgbaston, Birmingham, UK
2College of Engineering, University of Al-Qadisiyah, Al-Diwaniyah, Iraq

*Saif.Alzabeebee@gmail.com; Sia392@student.bham.ac.uk

ABSTRACT

Buried pipelines, and in particular concrete pipelines, are a vital element in maintaining modern life as they provide a convenient way to transport sewage and storm water. These buried structures have to resist the external forces due to soil weight and traffic loading. The current design practice for these pipelines is based on an empirical methodology linking the laboratory pipe capacity to the in-place pipe capacity utilising an empirical factor known as the load factor or bedding factor. This bedding factor is the ratio of the maximum bending moment in the laboratory pipe wall to the maximum bending moment in the in-place pipe wall. The British Standard (BS) bedding factors were derived assuming a uniform and equal soil pressure above the top half of the buried pipe. However, the rigour of this assumption, and hence the resulting bedding factors, has never been investigated before. This paper uses validated three-dimensional finite element analyses to rigorously investigate the bedding factors for a buried concrete pipe with an inside diameter of 1.2 m buried at different backfill heights, and provided with good support in the haunch zone and subjected to the BS traffic loading. The study examined the impact of the backfill height and the traffic loading on the maximum bending moment developed in the pipe wall. Furthermore, the bedding factors are calculated utilising the maximum bending moment calculated from the finite element analysis and are compared with that given in the BS for the good support condition to investigate the robustness of the BS bedding factor for good haunch support. The study showed that the traffic load no longer affects the bending moment in the pipe wall for a backfill height of 3.0 m. The BS bedding factor is shown to be overly conservative by a factor of up to 3.4 depending on backfill height, indicating that the current design methodology is not economic.

Keywords: Indirect Design Method, Bedding factor, Reinforced concrete pipes, British Standard.

1. Introduction

Buried pipelines, and in particular concrete pipelines, are a vital element in maintaining modern life as they provide a convenient way to transport sewage and storm water. Buried concrete pipes are often buried beneath roads, where these pipes have to resist forces due to backfill soil weight and traffic loads. Buried concrete pipes are designed based on an empirical methodology linking the field capacity of the buried pipe to the laboratory capacity using an empirical factor known as the bedding factor or the load factor [1]. The laboratory capacity of the pipe is obtained from a test called the three-edge bearing test. In this test, the pipe is supported at the invert zone (the critical locations on a pipe are shown in Figure 1a) and loaded at the pipe crown by a line load [1] as shown in Figure 1b. The pipe capacity is equal to the force which corresponds to a crack width of 0.254 mm [2]. The bedding factor is used because the support condition of the buried pipe in the field is different from the laboratory pipe [1]. The bedding factor is therefore a fundamental parameter in the design of buried concrete pipes. However, it has received little attention from researchers in the literature, where the thorough review of the literature only showed two studies on bedding factors [2, 3]. MacDougall et al. [2] and Petersen et al. [3] investigated the bedding factor of buried concrete pipes under the AASHTO traffic loading requirements (one axle load with a nominal tyre load of 72 kN). However, these previous studies cannot be used to examine the British Standards (BS) bedding factors because the traffic loading requirements of the BS (two axle loads with an axle load of 450 kN for the main road traffic loading) is significantly different from the AASHTO traffic loading requirements (one axle load with a nominal axle load of
Moreover, the BS bedding factors were derived assuming a uniform and equal soil pressure above the top half of the buried pipe. However, the rigour of this assumption, and hence the resulting bedding factors, has never been investigated before. This paper therefore investigates the robustness of the BS bedding factor for the case of good haunch support by studying the maximum bending moment in a buried concrete pipe with an inside diameter of 1.2 m and a thickness of 0.127 m under the effect of the main road BS traffic loading, using a validated three-dimensional finite element model. The maximum bending moment was used to calculate the bedding factor as the bedding factor equals to the maximum bending moment in the laboratory test to the maximum bending moment in the field [3]. The effect of the backfill height on the bending moment developed in the pipe wall was also examined in this study.

2. Details of numerical modelling

A three-dimensional finite element model has been developed to achieve the objectives of this study. The development and validation of the numerical model can be found in Alzabeebee et al. [4]. The model was developed using MIDAS GTS/NX, a three-dimensional finite element software. The model is shown in Figure 2 (dimensions 12 m long, 15 m wide, and 10 m high). The soil was modelled using four-noded tetrahedron solid elements, while the pipe was modelled using three-noded shell elements. The Duncan-Chang hyperbolic soil model [5] was used to simulate the behaviour of the soil. This model has the ability to include the effect of the stress level on the soil stiffness, improving the predictions from this soil-pipe interaction problem [6]. The pipe was modelled using a linear elastic model.

The main road BS traffic loading was simulated by applying a static load to the top surface of the model (Figure 2). The main road BS traffic loading comprises two axles spaced by 1 m. Each axle has four wheels with a centre to centre spacing of 1 m between each of the wheels [1]. The total wheel load is equal to 112.5 kN [1]. The tyre footprint was assumed to be of length 0.5 m and width 0.25 m [2, 3]. The numerical modelling was done in four steps. Step 1 involved calculating the in-situ soil stresses assuming a coefficient of a lateral earth pressure of 1.0 [7]. The trench was excavated in the step 2, which was then filled with the bedding soil, the pipe, and the backfill soil in step 3. Well-graded sandy soil with a degree of compaction of 90% (SW90) was used as the bedding and backfill soil. This meant that a good support was provided to the pipe in the haunch zone. The main road BS traffic loading was applied in step 4 using 25 equal loading increments. The properties of the in-situ soil, the SW90 soil, and the pipe can be found in Alzabeebee et al. [4].
3. Results and Discussions

Figure 3a shows the maximum bending moment obtained due to the backfill soil weight only and the combined backfill soil weight and traffic load (total load) for a backfill height ranging from 1.0 m to 3.0 m. It can be seen that the maximum bending moment linearly increases as the backfill height increases for the case of soil weight only. In addition, the figure shows a significant increase of the maximum bending moment due to the application of the traffic load, where the bending moment increased by 119% for a backfill height of 1.0 m. As expected, the effect of the traffic load decreases as the backfill height increases, with the traffic load not affecting the maximum bending moment at a backfill height of 3.0 m. This means that in this case, the effect of traffic load can be neglected if the pipe buried with a backfill height of 3.0 m or higher. However, additional studies for buried pipes with different diameters are required to examine the combined effect of the pipe diameter and backfill height under the action of traffic load.

Figure 3b shows the bedding factors ($BF$) calculated using Equation 1, i.e. obtained by dividing the maximum bending moment obtained from the laboratory test based on the BS method to calculate the force applied on the pipe (further details can be found in the BSI [1]) by the maximum bending moment obtained from the finite element analysis. Comparing these factors with the BS bedding factor for the good support condition (1.9 [1]) indicates that the BS bedding factor is very conservative, where the ratio ranges from 3.1 to 3.4 for backfill heights of 1.0 m to 3.0 m. Hence, it can be concluded that the BS design bedding factor for the good support condition does not produce an economic design and the BS should be updated to improve the design methodology and make it more economic and robust.

$$BF = \frac{0.318 \times W_t \times r}{BM}$$

(1)

Where, $W_t$ is the force applied on the pipe calculated based on the BSI [1] (refer to BSI [1] for details), $r$ is the radius of the pipe measured to the centre of the pipe wall, and $BM$ is the maximum bending moment obtained from the finite element analysis (Figure 3a).
4. Conclusions

The present study has employed a three-dimensional finite element analysis to study the maximum bending moment and the bedding factor of a buried concrete pipe with an inside diameter of 1.2 m under the effect of traffic loading. The study has shown that the traffic load no longer affects the maximum bending moment in the pipe wall for a backfill height of 3.0 m. In addition, the paper has demonstrated that the bedding factor adopted in the BS for the good support condition is overly conservative, with the ratio of the obtained bedding factor to the design bedding factor ranging from 3.1 to 3.4, depending on the backfill height. It is therefore recommended that additional work is required to update the design procedure in the BS to make it more economic and robust.

Acknowledgment

The first author thanks the financial support for his PhD study provided by the higher committee for education development in Iraq (HCED).

References


AN EFFICIENT LARGE-SCALE DEM MODEL INITIALIZATION PROCEDURE

*Matteo O. Ciantia¹ and Tom Shire¹

¹ Dept. Civil and Environmental Engineering, Geotechnics Section, Imperial College London, UK

*m.ciantia@imperial.ac.uk

ABSTRACT

In civil engineering, the discrete element method (DEM) is a numerical tool often used to reproduce soil behaviour at the elementary level. In general, small cubic or cylindrical samples are generated in a representative elementary volume (REV) to assess the micromechanical behaviour of the virtual soil. As the response of particulate media is strongly dependent on the initial state (stress and porosity), sample generation is the most crucial part of a DEM model and different procedures have been established to prepare homogeneous REVs. Thanks to the technological improvement of both hardware and software, in recent years the DEM has started to be used to simulate large-scale boundary value problems (BVPs). However, the use of any of the existing procedures employed to prepare REV samples is unsatisfactory in terms of computational cost and sample homogeneity. In this work a simple but very efficient procedure to initialize large-scale DEM models is presented. Periodic cells are first generated with a sufficient number of particles (enough to consider the cell an REV) matching the desired particle size distribution (PSD) and equilibrated at 100 kPa isotropic stress state at the desired porosity. Once the cell is in equilibrium, it is replicated in space in order to fill the problem domain. Once the BVP’s model is filled, only a small number of mechanical cycles are needed to equilibrate the large domain. The result is an equilibrated homogeneous sample at the desired porosity in a large volume. Results of shearing test simulations on such samples are presented and compared to simulations using the smaller REVs alone.

Keywords: DEM; Periodic Cells; Sample preparation; BVP

1. Introduction

The discrete element method (DEM), first proposed by [1], is a numerical approach widely used to study fundamental aspects of soil response [2-5]. In particular, small cubic or cylindrical samples are generated in a representative elementary volume (REV) to assess the micromechanical behaviour of the DEM specimen. As the response is strongly dependent on its initial state (stress and porosity), attaining a specified initial state is a crucial part of a DEM model. Different procedures of controlled sample generation have thus been established to prepare homogeneous REV’s. These include the Fixed Point Method [5], the Radius Expansion Method [1], the Isotropic Compression Method [7] the Modified Isotropic-compression Method [8] and the multi-layer Under Compaction Method [9]. Applying the latter procedures to large scale DEM models is inefficient in terms of computational cost and challenging in terms of sample homogeneity [10]. In the following a simple but efficient procedure to initialize large-scale DEM models is presented. Periodic cells are first generated with a sufficient number of particles (enough to consider the cell an REV) matching a desired particle size distribution (PSD). The cells are then equilibrated at low-level isotropic stress at the wanted porosity. Once the cell is in equilibrium, it is replicated in space in order to fill the model domain. After the domain is thus filled only a few thousand mechanical cycles are needed to re-equilibrate the large domain. The result is a large, homogeneous sample, equilibrated under prescribed stress at the desired porosity. In section 2 the cell generation procedure and the choice of the size of the reference cell to replicate is described while in section 3 the cell replication method (CRM) approach is extended to larger domains that could be used for DEM models of boundary value problems.

2. REV and unit cell generation

Four samples, enclosed by different sized periodic boundaries (PB) were created using a modified version of the open-source code Granular LAMMPS [11]. All simulations were carried out with 20
cores on the CX1 cluster at Imperial College London. The particle size distribution (PSD) were such that the mean radius was 0.2 mm and the ratio of the largest to smallest particle diameter is 2.25 (Figure 1(e)). A Hertzian contact model was used with shear modulus (G) of 25 GPa a Poisson’s ratio (ν) of 0.2. In DEM modelling the representative elementary volume (REV) size is usually selected to be as small as possible to ease computation, but big enough so that the observed mechanical response does not change with further size increases. Four samples are hence prepared and, by using isotropic compression [12] and by setting the contact friction coefficient to μ = 0.05, a dense sample (void ratio of 0.58) at 100 kPa of isotropic pressure was obtained, following which the μ was set to 0.3 to match the experimental value for glass beads. The samples required a small number of cycles to equilibrate back to 100 kPa [5]. The time taken to reach an equilibrated state for each sample is given in Figure 4.

Figure 1: a-d) Periodic cell sample of 625, 5k, 40k and 320k spherical particles (figures not in scale), e) corresponding PSD of the four samples.

The four samples are then sheared in drained triaxial conditions until the axial strain reaches a value of 30%. The results, which show the classic behaviour of a dense granular material (namely a peak of deviator stress followed by a softening behaviour until critical state is attained whereby the void ratio reaches a plateau), are shown in Figure 2. As is clear from the figure, the response of the four samples is similar in terms of global trends. Nevertheless, the 625 sample response is too irregular to consider it as an REV while for this work the 5k sample, despite fluctuations are still visible, can be considered as the smallest REV.

Figure 2: Deviatoric stress (q=σ₁-σ₃) (a) void ratio (b) and coordination number (c) evolution with axial strain of the sheared 625, 5k, 40k and 320k DEM models.
3. Triaxial response of the cell replicated samples (CRS)

After the REV minimum dimension has been identified, to exploit the idea of the CRM, the 625, 5k and 40k equilibrated samples are replicated 512, 64 and 8 times in space in order to fill a cubic cell with the dimensions of the large model. The time required to replicate and re-equilibrate this new cell replicated samples (CRS) is around 40 minutes for each sample using 20 cores on the CX1 cluster (note that the 320k REV sample took around 83 h to equilibrate). The three CRS are now tested in triaxial conditions and the results are shown in Figure 3 along with the 320k particle REV sample. Although one may expect the 625-CRS sample (now made up of 320k particles) to behave as a REV sample this does not occur. The response of the 625-CRS model does lose the local fluctuations but inherits a smoothed general trend of the 625 sample as a sort of best line fit. On the other hand, the 5k-CRS loses the local fluctuations and because the 5k initial cell is an REV it gives practically the same response as the 320k sample. The same response is also observed in the 40k-CRS sample. The time needed to generate the DEM models in an equilibrated condition at the initial porosity are reported in Figure 4. As it would be highly efficient to prepare a large DEM sample starting from a non-REV cell, a parametric analysis testing a procedure aimed at disturbing the 625-CRS. The diameter of each particle was randomly multiplied by a factor between 1±ΔD and re-equilibrated before the shear test. This re-equilibration required only a few minutes run time. As clear from Figure 3c factors of ΔD = 0.1% and 0.0001% of the particle diameter were not sufficient to disrupt the 625-CRS inherited behaviour. Larger ΔD factors were found to significantly change the initial coordination number.

![Figure 3](image1.png)
**Figure 3**: Deviatoric stress (q=σ1−σ3) (a) void ratio (b) and coordination number (c) evolution with axial strain of the sheared CRS models.

![Figure 4](image2.png)
**Figure 4**: Time required to prepare the 7 samples (625, 5k, 40k, 320k, 625-CRS, 5k-CRS and 40k-CRS) used in this work.
4. Conclusions

In this paper a novel approach to reduce the computational time needed to obtain initial conditions for large scale DEM models is presented. The cell repetition method (CRM) builds upon a simple idea which is the in space repetition of small equilibrated periodic samples (CRS). The advantages of the method are its computational efficiency, control of initial conditions and quality of the sample in terms of desired porosity and homogeneity. It was observed that when the CRM is used on a non-REV cell, the CRS sample, despite being formed by large number of particles does not behave as a REV. A random small change of the particle radii was used as an attempt to destroy the periodic inherited pattern, but this proved ineffective.

Acknowledgements

This study was undertaken as part of an Imperial College London Junior Research Fellowship Research Grant.

References


Energy dissipation in granular materials in triaxial tests

*R.A. Mukwiri\textsuperscript{1}, Y. Ghaffari Motlagh\textsuperscript{2}, W.M. Coombs\textsuperscript{1} and C.E. Augarde\textsuperscript{1}

\textsuperscript{1}School of Engineering and Computing Sciences, Durham University, Durham, DH1 3LE, UK
\textsuperscript{2}School of Chemical and Process Engineering, University of Leeds, Leeds LS2 9JT, UK

*r.a.mukwiri@durham.ac.uk

ABSTRACT

The triaxial test is used in a laboratory to investigate the behaviour of geotechnical materials (e.g. clays and sands). The difficulty in measuring some properties of granular media such as energy changes throughout the test have motivated the current numerical simulations of this test. This paper presents a description of a series of triaxial tests using LIGGGHTS open source Discrete Element Modelling software in a study of how energy is dissipated in granular media. The simulated triaxial tests are being carried out on cube shaped samples with six mesh walls enclosing the particles. Three of the walls (i.e. bottom, left and back walls) are fixed in position while the other three walls are allowed to move. Energy dissipation will be investigated by tracing changes of the energy terms at various time steps and applying the principle of energy conservation. The relationship between confining pressure, particle size distribution, friction coefficient and the voids ratio with energy dissipation will be investigated during the analysis of the results from the simulations. It is hoped that understanding the relationship between grain scale parameters and energy dissipation will help in the formulation of constitutive relationships within, for instance, the hyperplasticity framework. It is envisioned that relating grain scale parameters to constitutive models will allow the formulation of models that are purely based on the micro mechanics of granular media.

Key Words: DEM; energy dissipation; compression; triaxial test; hyperplasticity

1. Introduction

The Discrete Element Method (DEM) introduced by Cundall and Strack \cite{1} has been used in numerous numerical modelling studies over the past few decades. It models individual particles by considering the laws of motion. In civil engineering, it has been used to study geotechnical materials (mainly sands). DEM modelling is a numerical tool that is able to capture physically difficult to measure details about granular media such as particle rotations, displacements and energy evolutions. As such, it has been used to model geotechnical laboratory tests (e.g. direct shear and triaxial tests), and used them to study the behaviour of granular media closely. Examples of such modelling can be found in \cite{2} and \cite{11}. This paper focuses on the simulation of triaxial tests to study energy dissipation in granular media.

Energy dissipation in granular media has been a subject of interest in recent years. The relationship between energy dissipation and particle crushability, grain roughness, and energy dissipation response to seismic loading are some examples of many studies on energy dissipation in granular media \cite{10, 6, 9}. Mukwiri et al. \cite{7} recently highlighted an area of research in which grain scale parameters could potentially be linked to constitutive models by gaining a deeper understanding of energy dissipation in granular media. The simulations presented in this paper will hopefully build on that work by using triaxial tests to obtain relationships between grain scale parameters and energy dissipation.

2. Numerical simulations

The triaxial tests are being carried out using an open source DEM particle simulation software, LIGGGHTS developed by Kloss et al. \cite{5}. Unlike the commercial DEM software, LIGGGHTS has no user interface. Simulations are driven using text-based input scripts containing a series of commands to conduct the simulation.
The scripts that drive the simulations for the present study are broken down into four parts: initialisation, setup, general settings, and execution. In the initialisation part, the simulation geometry is specified and any required memory settings are declared. Within the setup part, the material properties of the particles are declared. The simulation procedures are also stated in this part. The general settings part of the scripts is where settings that corresponded to speed and memory utilisation are specified and the output options also generated. Each script is then supplied with execution commands to be carried out at various stages of the simulation. Throughout the simulations, files are output for later post processing.

The triaxial test simulations model spherical particles each of density $2650 \text{ kg/m}^3$, Poisson’s ratio of 0.25, and Young’s modulus of 70 GPa. Each simulation sample size is a cube of 0.1 m length. With these details, the simulations are set up such that three enclosing walls (i.e. top, right and front walls) would be allowed to move while the rest are fixed. The walls allowed to move are inserted into the sample as servo walls and set to compress the particles until a target total force corresponding to a desired pressure on the wall is achieved. Each wall is a mesh discretised into triangular elements.

For each triaxial test, the particles are inserted at half the target particle diameter and then grown in size. This is done to speed up the particle insertion stage of the simulation. Once this stage is completed, the particles are then allowed to settle before the consolidation stage. A hydrostatic confining pressure ($\sigma$) is then applied to the servo walls during consolidation. Front and right walls are then maintained at this pressure and the top wall is allowed to move at a maximum set velocity of 0.001 m/s downwards during shearing. To ensure that the desired pressure is accurate, the target total force on the walls is updated at every time step by evaluating the product of $\sigma$ and the current wall contact area with the particles.

Four parameters will be varied during this study: the confining pressure ($\sigma$), particle-particle friction coefficient ($\mu$), initial voids ratio before consolidation ($e_{ini}$), and the coefficient of uniformity ($C_u$). The particle-wall coefficient of friction for each simulation is kept at zero. $C_u$ is a particle size distribution measurement given by

$$C_u = \frac{d_{60}}{d_{10}}$$

where $d_{60}$, $d_{30}$, and $d_{10}$ are equivalent to grading sieve sizes used in a laboratory to determine the particle size distribution of soils. 60, 30 and 10 values are the percentage of particles that go through the sieve size considered. These $d$ values correspond to particle diameters when modelled using DEM.

<table>
<thead>
<tr>
<th>Parameter/No.</th>
<th>1</th>
<th>2</th>
<th>2</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma$ (kPa)</td>
<td>100</td>
<td>100</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>800</td>
<td>800</td>
<td>800</td>
<td></td>
</tr>
<tr>
<td>$\mu$</td>
<td>0.2</td>
<td>0.3</td>
<td>0.5</td>
<td>0.2</td>
<td>0.3</td>
<td>0.2</td>
<td>0.3</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>$C_u$</td>
<td>1</td>
<td>3</td>
<td>6</td>
<td>3</td>
<td>6</td>
<td>1</td>
<td>6</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$e_{ini}$</td>
<td>0.4</td>
<td>0.6</td>
<td>0.8</td>
<td>0.8</td>
<td>0.4</td>
<td>0.6</td>
<td>0.8</td>
<td>0.4</td>
<td></td>
</tr>
</tbody>
</table>

The intended number of simulations to run was obtained using the Taguchi experimental design technique [8]. This analysis involves defining a suitable orthogonal two dimensional array matrix that defines all the variable settings required for each experiment. The technique helped to reduce the number of simulations that would be required to vary all four variable parameters in this study at three levels each. If one parameter is changed at a time, 81 simulations would have been required. However, using the Taguchi method reduced this number to the nine simulations shown in Table 1. The meaning of orthogonality in this context is "statical independence" [8]. In Table 1, each row has each level of a parameter appearing an equal number of times. Further more, statical independence also means that the relationship between one row and another is such that each level in any other row will occur an equal number of times as well.
To facilitate the study of energy dissipation for the triaxial tests, energy monitoring will be done by post processing the files output during the simulations using Matlab. The energy equation used is

$$dE_p + dW = dE_k + dE_\mu + dE_\zeta + dU,$$  \hspace{1cm} (2)

where $dE_p$ is the change in potential energy, $dW$ the change in boundary work, $dE_k$ the change in kinetic energy, $dE_\mu$ is the dissipated frictional energy, $dE_\zeta$ the change in dissipated energy through damping, and $dU$ is the change in stored work.

The total change in dissipated energy, $dE_\eta$ during the simulations comes from the $dE_\mu$ and the $dE_\zeta$ terms of (2). Since the simulations are pseudo-static, it has been found that the potential and kinetic energies are usually each $\approx 10^6$ times smaller than either of the boundary work or the stored elastic energy. We can therefore re-write (2) as

$$dE_\eta \equiv dW - dU$$ \hspace{1cm} (3)

The change in boundary work is calculated as:

$$dW = \sum_{j=1}^{m} \sigma^i_j A_s^i \delta x^i,$$  \hspace{1cm} (4)

where $\sigma^i_j$ is the normal stress on mesh $j$, which is the sum of all the individual stress values from each triangular mesh element, $i$ composing it. $A_s$ is the surface area of the mesh considered and is obtained by summing up the areas of each triangular mesh element, $i$ as

$$A_s = \frac{1}{2} \sum_{i=1}^{n} |\text{AB}_i \times \text{AC}_i|,$$  \hspace{1cm} (5)

where the area of each triangular element with vertices A, B and C is calculated using cross product between vectors $\text{AB}$ and $\text{AC}$.

Changes in the stored energy are due to the evolution of normal and tangential contact forces. The summation of strain energy for all the contacts is equal to the stored energy, $dU$ and is calculated as

$$dU = dU^n + dU^t,$$  \hspace{1cm} (6)

where $dU^n$ and $dU^t$ are the contributions from normal and tangential contact forces and are equal to

$$dU^n = \int_0^{\delta_n} \frac{1}{3} E^* \sqrt{R^* \delta_n} \delta_n \frac{4}{3} \left(\frac{d_1}{d_1 + d_2}\right)^{1/2} d_1 n,$$  \hspace{1cm} (7)

and

$$dU^t = \int_0^{\xi_t} \frac{8G^* \sqrt{R^* \delta_n} \xi_t d\xi_t}{F^t},$$  \hspace{1cm} (8)

respectively. $F^n$ and $F^t$ are in turn the normal and tangential contact forces and $K_n$ and $K_t$ are the corresponding stiffness parameters from the Hertzian contact model, which governs how spherical particles interact at contact. Two particles 1 and 2 will have an effective radius, $R^* = R_1 R_2 / (R_1 + R_2)$, which is the geometric mean of radii $R_1$ and $R_2$, $\delta_n = R_1 + R_2 - d_{12}$ and is the overlap at contact between the two particles in the normal direction where $d_{12}$ is the distance between their centres. The effective Young’s modulus, $E^* = 0.5E / (1 - \nu^2)$, is derived from the particles’ material Young’s modulus, $E$ and Poisson’s ratio, $\nu$. In Equation (7), $\text{n}$ is the normal vector for the particles in contact. The term $\xi_t$ in Equation (8) is the tangential displacement and is calculated by integrating the tangential relative velocity over the contact time [3].
4. Further analysis

Sections 2 and 3 have described the simulation procedures and the method used to post process for energy dissipation. Currently, these simulations are being done and the results will be used to investigate the relationship between grain scale parameters and energy dissipation in triaxial tests. The influence of particle size distribution, initial voids ratio, friction coefficients, and the confining pressure will in particular be studied. The present plan is to only have the nine simulations described in Section 2, however, more simulations can be conducted if required.

It is hoped that the observations made from this analysis will facilitate the development of energy dissipation functions that are purely based on grain scale parameters.

The energy dissipation functions formed would then be used to formulate yield surfaces and plastic flow rules which would describe the inelastic behaviour of these materials (sands in particular) based on the hyperplasticity framework [4]. This would potentially facilitate the formation of constitutive models informed by grain scale parameters. This method of formulating constitutive models could then be further extended to all granular media.

References


ENHANCING EFFICIENCY OF DEM MODELING OF PARTICLE BREACKAGE

*Matteo O. Ciantia¹, Ningning Zhang² and Marcos Arroyo²

¹ Dept. Civil and Environmental Engineering, Geotechnics Section, Imperial College London, UK
² Department of Geotechnical Engineering and Geosciences, Technical University of Catalonia (UPC), SPAIN

*m.ciantia@imperial.ac.uk

ABSTRACT

In geotechnical practice, the discrete element method (DEM) is gaining wide acceptance as a powerful modelling tool. One field for which DEM is well adapted is that of crushable soils. Grain crushing has been modelled in DEM employing two alternative approaches: the multigenerational approach, in which single particles break and are replaced by new, smaller fragments; or by using agglomerates. The latter, despite being very helpful for the understanding of the micromechanics occurring in a single particle, becomes impractical when applied for modelling large scale problems. This work focuses on the enhancement of model efficiency from code-specific issues, as indicated in a series of simulation of high pressure isotropic compression of crushable sands. A recently developed model for crushable soils using multigenerational approach is adopted. It is shown that the advantageous code implementation adopted allows a considerable savings in computational cost with little influence on the accuracy in terms of grain size distribution evolution and mechanical behaviour.

Keywords: DEM; Grain Crushing; User defined model; Efficiency

1. Introduction

The mechanical effects of grain crushing are important for several geotechnical problems, such as side friction on driven piles [1] railway ballast durability [2] and slaking induced irreversible deformations [3]. These, and other applications, have motivated efforts to experimentally investigate the mechanical consequences of particle breakage [4] to incorporate grain crushing into constitutive models for soils [5] and to model soil crushing using DEM [6]. To model particle fragmentation using DEM two alternative approaches may be used: replacing the breaking grains with new, smaller fragments; or by using bonded agglomerates. The latter, despite being very helpful for the understanding of the micromechanics occurring to a single grain [7], becomes an unpractical tool if larger scale problems are intended to be modelled. On the other hand, the former is more practical and has been adopted intensively for large scale 2D problems [8] and recently in a 3D case [9]. The crushing model was used to simulate cone penetration tests using the commercial PFC3D code [10] in crushable soil giving very good results [11]. However, the failure criterion was coded by means of FISH (short for FLACish, a PFC built-in programming language) functions. FISH functions result in communication overheads that might be avoided if the contact model source code is directly modified. In this work the efficiency of using a user defined contact model (UDCM) instead of FISH functions for the modelling of grain crushing is tested. In particular, the numerical investigation concentrates on a series of simulation of high pressure isotropic compression of crushable particles.

2. Crushing Model description

The numerical models applied here are built using the PFC3D code [10]. This code implements the DEM in a similar form to that originally described by Cundall and Strack [12]. For completeness an overview of the DEM model for crushable soil proposed by Ciantia et al. [9] is given here. Coulomb friction and the simplified Hertz-Mindlin contact model were used. The failure criterion is based on the work of Russell and Muir Wood [13]: a two-parameter material strength criterion is used along with consideration of the elastic stresses induced by point loads on a sphere. A particle subject to a set
of external point forces reaches failure when the maximum applied force reaches the following limit condition:

\[
F \leq \sigma_{\text{lim}} A_F \Rightarrow F \leq \sigma_{\text{lim}} f(\text{var}) \left( \frac{d}{Nd_0} \right)^{2/3} \left( \frac{1-v_1^2}{E_1} + \frac{1-v_2^2}{E_2} \right)^{2/3} \left( \frac{1}{r_1} + \frac{1}{r_2} \right)^2 \]

(1)

where \( \sigma_{\text{lim}} \) is the limit strength of the material and \( A_F \) is the contact area. \( f(\text{var}) \) is a function used to incorporate the natural material variability into the model. The limit strength, \( \sigma_{\text{lim}} \), is assumed to be normally distributed for a given sphere size. The coefficient of variation of the distribution, \( \text{var} \), is taken to be a material parameter. The mean strength value \( \langle \sigma_{\text{lim}} \rangle \) depends on the particle diameter \( d \) where \( m \) is a material constant, \( d_0 \) is the reference diameter (2 mm) and \( N \) is the scaling factor. The latter is used to model large scale problems and particle size scaling is required [11] in order to reduce the number of particles of the model. \( A_F \) depends on the contact force and the particle’s elastic properties. \( r_1 \) and \( r_2 \) are the radii of the contacting spheres and \( E_i, \nu_i \) are the Young’s Moduli and Poisson’s ratio respectively. Once the limit condition is reached, the spherical particle will split into smaller inscribed tangent spheres. The crushed fragments assume the velocity and material parameters of the original particle. Ciantia et al [13] concluded that a 14-ball crushed configuration can adequately represent macroscopic behaviour.

3. DEM Model numerical implementation

Particle crushing can be implemented in PFC by using either FISH algorithms or within a C++ coded user defined contact model (UDCM). The main difference between the FISH and UDCM crushing algorithms schemes is that the FISH implementation requires a time-consuming loop through all the contacts that the UDCM does not need. In fact, in PFC5, there is a loop over all the contacts during the force-displacement law, no matter which contact model is used. The contact model force-displacement method is executed for each contact, and in the case of this UDCM it emits a signal if the crushing criterion is met. The UDCM then uses another FISH function that performs the 14-ball substitution by listening to this signal, and is therefore automatically triggered anytime the criterion has been met in a contact. Therefore, differently from the FISH crushing formulation, there is no need for an extra loop over the contacts using FISH functions.

![Figure 1 a) Initial uncrushed particle, b) Particle splitting configuration](image)

Figure 1 a) Initial uncrushed particle, b) Particle splitting configuration

In the FISH implementation, the failure criterion is evaluated every \( n_{\text{crush}} \) mechanical time-steps. Figure 1 shows preliminary simulation results used to validate the correct implementation of the UDCM. To test ball-wall contacts the compression of a sphere between two rigid walls is simulated. On the other hand, to test ball-ball contacts, the compression of two spheres is modelled.
4. High pressure isotropic compression and computational efficiency

To test the computational efficiency of using a UDCM crushing model with respect to FISH crushing algorithms an isotropic compression test on 10,000 crushable spheres is performed. The DEM specimen was created by filling a 4-cm sided cube with spheres having a particle size distribution (PSD) with particle diameters ranging from 1.44 to 2.16 mm (Figure 2a). Gravity was set to zero and the specimen boundaries were defined using “wall” elements. Target stress values were attained by using a servo-control to adjust the wall positions. Following [9] a stress control isotropic compression test was run. A logarithmic control of the load increment was used

\[ L_{\text{R}} = L_{\text{ref}} + \log \left( \frac{p'}{p_{\text{ref}}} \right) \]

where \( L_{\text{R}} \) is a load increase coefficient, \( i \) indicates the step of the calculation and \( p'_{\text{ref}} \) is a reference stress of 1 kPa. The model parameters and some model characteristics are summarized in Table 1.

In Figure 2 comparisons between the UDCM and the FISH crushing implementation are reported in terms of PSD and porosity evolution. It is interesting to observe the influence \( n_{\text{crush}} \) may have on the mechanical response. In particular, choosing a high value of \( n_{\text{crush}} \) may lead to a non-realistic response. In this work and for the \( L_{\text{R}} \) used, it is clear that a \( n_{\text{crush}} \) value of 100 is too high to capture all the expected crushing events, while the FISH-10 model has an \( n_{\text{crush}} \) value \((n_{\text{crush}} = 10)\) that is small enough to give the same response of the \( n_{\text{crush}} = 1 \) (FISH-1) model. This means that for this set of analyses the highest \( n_{\text{crush}} \) that can be used to obtain the correct mechanical response is 10. The UDCM isotropic compression response is very similar to the one of the FISH-10 and FISH-1 models and, as detailed in Table 1, it results to be more efficient. In particular, the UDCM simulation results 2.14 and 11 times faster than FISH-10 and FISH-1 models respectively.

![Figure 2](image)

**Figure 2** Comparison of (a) Initial and final PSDs and (b) porosity evolution with mean effective stress \((p')\) for the 4 DEM models.

<table>
<thead>
<tr>
<th>Test-ID</th>
<th>( \mu_w ) [-]</th>
<th>( E_w ) [MPa]</th>
<th>( \mu_b ) [-]</th>
<th>( E_b ) [MPa]</th>
<th>( v )</th>
<th>( \sigma_{\text{lim,0}} ) [MPa]</th>
<th>( m )</th>
<th>variance</th>
<th>( n_{\text{crush}} )</th>
<th>( L_R )</th>
<th>( Np,0 )</th>
<th>( Np,\text{end} )</th>
<th>Time* [h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>FISH-100</td>
<td>0.4</td>
<td>866</td>
<td>0.4</td>
<td>866</td>
<td>0.3</td>
<td>116</td>
<td>5</td>
<td>0.0</td>
<td>100</td>
<td>0.01</td>
<td>10k</td>
<td>72,101</td>
<td>3:15</td>
</tr>
<tr>
<td>FISH-10</td>
<td>0.4</td>
<td>866</td>
<td>0.4</td>
<td>866</td>
<td>0.3</td>
<td>116</td>
<td>5</td>
<td>0.0</td>
<td>10</td>
<td>0.01</td>
<td>10k</td>
<td>86,388</td>
<td>8:04</td>
</tr>
<tr>
<td>FISH-1</td>
<td>0.4</td>
<td>866</td>
<td>0.4</td>
<td>866</td>
<td>0.3</td>
<td>116</td>
<td>5</td>
<td>0.0</td>
<td>1</td>
<td>0.01</td>
<td>10k</td>
<td>85,868</td>
<td>17:39</td>
</tr>
<tr>
<td>UDCM</td>
<td>0.4</td>
<td>866</td>
<td>0.4</td>
<td>866</td>
<td>0.3</td>
<td>116</td>
<td>5</td>
<td>0.0</td>
<td>-</td>
<td>0.01</td>
<td>10k</td>
<td>83,905</td>
<td>3:46</td>
</tr>
</tbody>
</table>

* performed using the same hardware (Intel® Xeon® CPU E5-2637 v3 at 3.50 GHz with 64.00 GB of Ram)
5. Conclusions

In this paper, the computational efficiency of using an inbuilt C++ crushing contact law using the commercial PFC3D code [10] is tested. The correct implementation of the failure criterion is first tested on simple ball-wall or ball-ball models. The computational efficiency of using a user defined contact model (UDCM) is then evaluated by simulating a high pressure isotropic compression of a 4-cm sided cube containing 10,000 crushable spheres. The UDCM results to be at least 2 times faster than the failure criterion coded by means of FISH (short for FLACish, a PFC built-in programming language) functions. The efficiency of using a UDCM is expected to increase with increasing number of contact in the DEM model as the FISH implementation requires a time-consuming loop through all the contacts that the UDCM does not need. It is also shown that the FISH coded crushing model is highly sensitive to $n_{\text{crush}}$ the parameter that regulates the number of mechanical time steps after which the failure criterion is evaluated.

Acknowledgements

This study was undertaken as part of an Imperial College London Junior Research Fellowship Research Grant.

References

Numerical investigation into the effect of cavity size and location on stability of earth dams

H. Al-Ateya*, A. Ahangar Asr
School of Computing Science and Engineering (CSE), University of Salford
Salford, Greater Manchester, M5 4WT
H.Alateya@edu.salford.ac.uk

ABSTRACT

Numerical investigations performed to study the effect of the presence of cavities on stability of slopes considering rapid draw down conditions. The aim of the investigation is was to study the influence of different factors (such as diameter and location of the cavities in horizontal and vertical directions). Numerical models were used to estimate slope stability of earth dam considering the effect of cavities in subsoil using PLAXIS 2D software. The results of the analysis indicated that the presence of cavities decreases the stability of upstream facer extremely for all considered locations for the cavities in both directions (horizontal and vertical). The numerical results also demonstrated that increasing the size of cavities lead to decreasing the value of safety factor, until it drops to values less than the required value for the earth dam under rapid drawdown conditions to be considered stable.

Keywords: cavities, stability analysis, numerical modelling

1. Introduction

Presence of cavities in the soil is problematic in the field of geotechnical engineering, which can lead to considerable losses of life and properties. In particular, when cavities exist under hydraulic structures where these cavities could form channels for motion of groundwater and then extend in the size until amount to a stringent size then collapse [1]. Susceptible structures, such as earth dams, demand continuous investigations and information to ensure their stability. The rapid drawdown condition is one of the most dangerous loading conditions which could influence the stability of earth dams. This case arises when the water level rises during a flooding season and remain stable for an interval of time, then most of the flood water can pass away comparatively in short intervals of time. In such condition, the pore water pressure in the body of dam may stay high and do not take the adequate time to dissipate [2].

Extensive study was introduced to use the finite element method with shear strength reduction technique to analysis the stability of an earth dam under rapid drawdown conditions. A comparison was conducted between the factor of safety of soil slopes which acquired by shear strength reduction technique and the limit equilibrium method [3]. The stability of an earth dam was studied utilizing finite element method after filling a reservoir. It was achieved using the modified finite element computer program (Nonlinear Finite-element Analysis Program). In the study, the initial stress state in an earth dam before the filling of the reservoir was assessed [4]. A numerical mode was developed to analyse the stability of the Tieng main dam in rapid drawdown condition for two cases before and after rehabilitation, using limit equilibrium and finite element methods. Changes of stress-strain behaviours and pore pressure, failure mechanism, and factor of safety of the upstream slope were investigated [5]. Slope stability was analysed by adopting a numerical procedure for integrating a commercial finite difference method into a probabilistic analysis of slope stability. Given that the limit state function cannot be expressed in an explicit form, an artificial neural network (ANN)-based response surface was adopted to approximate the limit state function, thereby reducing the number of stability analysis calculations [6]. In this investigation a finite element model is developed and implemented to look into the effect of presence of cavities in subsoil of an earth dam on the stability of the upstream (reservoir) slopes.
2. Numerical Modelling

The slope stability analysis was performed using a numerical model developed in PLAXIS 2D software relying on conventional strength reduction method, where the safety factor is determined through the lowering of the shear strength parameters. PLAXIS 2D software is dependent on finite element method, used to analysis the stability of upstream slope considering rapid drawdown condition for the state of 8-m lowering of reservoir level in 8 days. In the model, fifteen-node triangular elements were applied for the finite element mesh considering plane strain analysis condition [7]. The behavior of the embankment materials and subsoil were deemed elastic-plastic on the basis of the Mohr-Coulomb failure criteria. A numerical model of an earth dam, which was deemed to simulate slope stability, was 15-m in height with side slope 1 V: 2.5 H for both upstream and downstream faces, with subsoil depth of 30-m depth and 6-m crest width was used. The initial considered water level of upstream reservoir was 12-m. Figure (1) depicts the earth dam geometry and the finite element mesh.

3. Material Parameters

To analyse the numerical models using PLAXIS 2D code, the implemented parameters included γ, unit weight of soil, ν’, Poisson’s ratio, C’, cohesion, ψ, angle of dilatancy, ϕ’, internal angle of friction, kx, & ky, coefficients of permeability in X and Y direction, and E’, the Young's modulus. Table (1) presents the implemented input parameter values.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Embankment</th>
<th>Subsoil</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>Mohr-Coulomb</td>
<td>Mohr-Coulomb</td>
<td></td>
</tr>
<tr>
<td>Type</td>
<td>Drained</td>
<td>Drained</td>
<td></td>
</tr>
<tr>
<td>γ unsaturated</td>
<td>16.0</td>
<td>17.0</td>
<td>kN/m3</td>
</tr>
<tr>
<td>γ saturated</td>
<td>20.0</td>
<td>21.0</td>
<td>kN/m3</td>
</tr>
<tr>
<td>ν’</td>
<td>0.33</td>
<td>0.3</td>
<td></td>
</tr>
<tr>
<td>C’</td>
<td>30</td>
<td>5.0</td>
<td>kN/m2</td>
</tr>
<tr>
<td>ψ, ϕ’</td>
<td>1.0, 20</td>
<td>5.0, 35.0</td>
<td>Degrees</td>
</tr>
<tr>
<td>kx, ky</td>
<td>10⁻⁴</td>
<td>0.01</td>
<td>cm/s</td>
</tr>
<tr>
<td>E’</td>
<td>2.0×10⁴</td>
<td>5.0×10⁴</td>
<td>kN/m2</td>
</tr>
</tbody>
</table>

4. Parametric study

Cavities were placed into the foundation of the earth dam under upstream face in the model. The investigation consisted of two parts; a parametric study for numerical models with and without cavities to simulate the influence of presence of cavities. In this part, the influence of changes in cavity locations in horizontal (X) and vertical (Y) directions were considered. The second part was to study the effect of various values of cavity diameter (D) on the stability of earth dams. All stability analyses were performed considering rapid drawdown condition and presence of a single cavity under the upstream reservoir in subsoil.

5. The results of analysis

In the first section of analysis: two sets of numerical models were used to investigate the effect of location of cavity horizontally and vertically on stability upstream of slope. The first numerical set (CL-X), conducted for models with cavities in different locations horizontally, while the location of cavity remained unchanged in Y-direction. The second numerical set (CL-Y), performed for models with cavities in different locations vertically without any change in the location of cavity horizontally. L1, L2, L3 and L4 (Figure 2): are the locations of cavities in X-direction and Y-direction. Table (2) contains the input and output parameters showing effect of the location and size of cavities. The horizontal location of cavity is the distance between vertical centerline of the earth dam and centerline.
of each cavity, while the vertical location is the distance between the base of embankment of dam and the centerline of cavity, as displayed in Figure (2). In all these analyses the diameter of cavity was equal to 100 cm. The results of stability analysis are exhibited in Figure (3) for various locations of cavities in both directions. In the second section, the present study involves an investigation to estimate the effect of cavity size on stability of dam. Cavities of various diameters 20, 60, 100 and 140 cm were considered in the software analysis. Figure (4) represents the stability analysis results obtained from the model for different values of cavity sizes. Table (3) shows the effect of diameters of cavities on value of safety factor.

Table 2: Input and output parameters showing effect of the location of cavities

| Location of cavity | The coordinates of points | F.S MN, without cavities | 2.129 |
|--------------------|---------------------------|--------------------------|
|                    | CL-X*                     | CL-Y**                   | CL-X | CL-Y |
| L1                 | (-18,-2)                  | (-25,-1)                 | 1.396| 1.597|
| L2                 | (-25,-2)                  | (-25,-2)                 | 1.480| 1.480|
| L3                 | (-30,-2)                  | (-25,-3)                 | 1.557| 1.387|
| L4                 | (-40,-2)                  | (-25,-4)                 | 1.720| 1.413|

*CL-X: Change of the location of cavities in X-axis.
** CL-Y: Change of the location of cavities in Y-axis.

Table 3: Input and output parameters showing effect of the size of cavities

<table>
<thead>
<tr>
<th>Diameter of cavity, cm</th>
<th>F.S</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.787</td>
</tr>
<tr>
<td>60</td>
<td>1.580</td>
</tr>
<tr>
<td>60</td>
<td>1.480</td>
</tr>
<tr>
<td>140</td>
<td>1.004</td>
</tr>
</tbody>
</table>

Figure 1: The earth dam geometry and finite element mesh

Figure 2: locations of cavities

Figure 3: Safety factor for models with and without cavities, for different location of cavities

Figure 4: Safety factor for models with and without cavities, for different sizes of cavities
6. Discussions and conclusions

All the investigations were conducted under rapid drawdown conditions. The analysis results pointed out that the presence of cavities reduces the stability of upstream slope dramatically, as shown in Figure (3), where for instance the safety factor lowered from (2.129) for the model without cavities, to (1.387) for the model with cavity at location L3 (-25,-3). It means that the stability of earth dam got close to the critical condition, which is the minimum factor of safety of 1.3 for rapid drawdown condition [8]. This behaviour may attribute to decreasing strength of subsoil as a result of the presence of cavities. It can be observed that the factor of safety increases with the increasing distance between centerline of dam and centerline of cavity for the CL-X set (Table 2), from (1.396) to (1.720) for locations L1 (-18,-2) to L4 (-40,-2), as the cavity gets further away from the centre of the dam. Whereas, in the case of the CL-Y set, safety factor decreases with the increase of the cavity depth from (1.597) to (1.413), for locations L1 (-25,-1) to L3 (-25,-3) with an exception of L4 (-25,-4) where a small rebound in the factor of safety can be observed which could contributed to the fact that the cavity starts to fall out of the zone affected by the stress and seepage distribution. The results of stability analysis looking into the effect of the size of the cavities have also indicated that increasing the diameter of cavities results in significant reduction in the safety factor values changing from (1.787) to (1.004), for models with cavities of diameters of 20 cm to 140 cm, respectively (Table 3). The results also showed that the earth dam becomes unstable when, the subsoil contains a cavity of size equal to 140 cm.

Acknowledgements

The research has been financed by the Government of Iraq via Kufa University as part of a PhD scholarship for the lead author.

References


LAYOUT OPTIMIZATION OF SOIL REINFORCEMENT

Javier González-Castejón¹ and Colin Smith²

¹LimitState Ltd, Sheffield, S1 4DP
²Department of Civil and Structural Engineering, University of Sheffield, Sheffield, S10 2TN

*j.g castejon@limitstate.com

ABSTRACT

Discontinuity layout optimization (DLO) is a numerical limit analysis procedure which provides a powerful alternative to other numerical methods such as finite element limit analysis approaches. In its core form it uses optimization techniques to identify the critical collapse mechanism in the form of discrete slip-lines for any problem geometry, enabling the engineer to identify the factor of safety for a system. In geotechnical engineering this can for example be applied to model a reinforced soil slope/wall and find the critical collapse mode.

To date soil reinforcement can be modelled by many software packages but few address the optimal layout of reinforcement needed for a specific problem, leaving the engineer the task of achieving the optimal solution. The approach proposed herein automates the process, giving a rapid and sensible solution. In this extended abstract a novel modification of the DLO optimization process is outlined that enables it to find the minimal amount of reinforcement required to ensure stability. This provides a promising new approach to optimal geotechnical design. An example scenario is presented to illustrate the practicality of the method.

Keywords: Limit Analysis; DLO; Soil Reinforcement; Optimization

1. Introduction

Discontinuity layout optimization (DLO) is an upper bound numerical limit analysis procedure which provides a powerful alternative to other numerical methods such as finite element limit analysis approaches. In its core form it is able to identify the critical collapse mechanism in the form of discrete slip-lines for any problem geometry, enabling the engineer to identify the factor of safety for the system. Rather than being formulated in terms of elements, the method is based on nodes and the lines connecting these nodes. The method is typically presented in its primal kinematic form (Smith and Gilbert [1]) where a regular square grid of nodes is typically utilized in the solution. The basic principles of the analysis are presented in Figure 1.

![Figure 1: Stages in DLO procedure (after Gilbert et al. [2]): (a) initial problem definition (surcharge applied to block of soil close to a vertical cut); (b) discretization of soil using nodes; (c) interconnection of nodes with potential discontinuities; (d) identification of critical subset of potential discontinuities using optimization (giving the layout of slip-lines in the critical failure mechanism).](image)

The dual equilibrium form can also be used to achieve the same solution: in general terms, its aim is to maximize the live load while determining equilibrium shear and normal forces acting on every slip-line or potential slip-line connecting any pair of nodes and ensuring they do not violate yield. Due to
space requirements of the present abstract, details on the formulation have been omitted; the reader can find a full explanation in Smith and Gilbert [1]. The current study aims to provide an optimization tool for soil reinforcement layout by means of the modified original dual DLO formulation.

2. Soil Reinforcement Modelling.

Soil reinforcement modelling has been successfully addressed by several commercial software packages using different approaches (Clarke et al. [3]), however it is worth revisiting herein some of the fundamental principles for a planar reinforcement, used to extend the DLO formulation:

- There is continuity of normal stress across the reinforcement.
- There may be discontinuity of shear stress across the reinforcement. Any difference results in a change in tension in the reinforcement itself.
- Reinforcement is assumed to possess a finite rupture or tensile strength $R_M$.
- The shear strength of the soil/reinforcement interface may be lower than the shear strength of the adjoining soil by a factor $\alpha$.

Figure 2 shows a simplified representation of the soil reinforcement model where the variables $S$ and $N$ indicate the shear and normal forces on the slip-lines modelled on the upper and lower surfaces of the reinforcement and the variables $T$ represent the tensile force in the reinforcement at a given node $i$.

![Simple sketch of an isolated piece of reinforcement with the correspondent internal variables.](image)

From the model the following relations can be deduced:

$$T_{i+1} = T_i + S_u - S_l \quad ; \quad N_u = N_l$$
$$S_u \leq (N_u \tan \phi + cL)\alpha \quad ; \quad S_l \leq (N_l \tan \phi + cL)\alpha$$
$$T_i \leq R_M \quad ; \quad T_{i+1} \leq R_M$$

Where $c$ and $\phi$ are the cohesion and angle of shearing resistance of the soil respectively and $L$ is the length of the reinforcement element. For simplicity, in this extended abstract, the analysis will be restricted to a weightless undrained cohesive soil where $c = c_u$ and $\phi = \phi_u = 0$.

3. Optimized reinforcement layout.

To date, engineers are able to model soil reinforcement for the design of reinforced slopes or retaining walls, for example. However the optimization of the layout via an automated procedure has been addressed by only a few authors (Pucker and Grabe [4]) and iterative hand methods or rules of thumb are normally used instead. Figure 3 shows an example, hand-optimized using the software Limit State GEO [5], for a vertically sided ‘embankment’ with properties given in Table 1. For simplicity, and to illustrate the process, unit strength soil and reinforcement is modelled. The hand optimization followed the below procedure:
Start with full width reinforcement for the required number of layers.

- Starting with the top layer of reinforcement, reduce the width symmetrically until the load capacity starts to decrease.
- Fix the reinforcement width for that layer and repeat for the next layer down.

This is a heuristic and time-consuming procedure which does not assure an optimal layout. Due to discretisation the reinforcement width is reduced in 1m sections in this simple example. The initial scenario utilised a total length of reinforcement of 55m. The hand optimised solution uses 25m total length of reinforcement.

Figure 3: Optimisation achieved by hand for a vertically sided ‘embankment’ with central load of 5kN/m (a) First step of the hand procedure removing the extremes of the first layer (b) final optimised problem with a slightly lower factor of safety. Reinforcement is depicted by red lines. Pale red profile above reinforcement indicates distribution of tensile force along the reinforcement.

An alternative automated procedure can be carried out by means of Linear Programming (LP) formulated as a modification of the dual DLO formulation. In this modified form each node along the reinforcement is assigned a linear programming variable rupture strength \( R_i < R_M \) and the objective function is altered to minimise \( \sum R \) over all the modelled reinforcement while still fulfilling equilibrium and yield conditions subject to the specified external load.

Table 1: Parameters for reinforced embankment problem depicted in Fig 3 and Fig 4.

<table>
<thead>
<tr>
<th>Problem type</th>
<th>Short term (undrained conditions)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Problem Dimension ((X \times Y = m \times m))</td>
<td>11 x 6</td>
</tr>
<tr>
<td>Nodal spacing (m)</td>
<td>1</td>
</tr>
<tr>
<td>(c_u ) (kPa)</td>
<td>1</td>
</tr>
<tr>
<td>(\phi_u ) (°)</td>
<td>0</td>
</tr>
<tr>
<td>Unit weight (kN/m3)</td>
<td>0</td>
</tr>
<tr>
<td>Applied Load (kN/m)</td>
<td>5</td>
</tr>
<tr>
<td>Reinforcement tensile strength, R (kN/m)</td>
<td>1</td>
</tr>
<tr>
<td>Compressive Rupture Strength (kN/m)</td>
<td>0</td>
</tr>
<tr>
<td>Load Application Coordinates ((X_1, Y_1)-(X_2, Y_2) ) (m x m)</td>
<td>(4,6) - (7,6)</td>
</tr>
</tbody>
</table>

The analysis proposed has been tested and verified using a specially written MATLAB code coupled with the MOSEK [6] interior point solver. It runs in 2 stages. First the optimization is carried out on a model with full width reinforcement modelled in each layer as shown in Fig. 4a, generating results for the required values of \( R \) at each node (Fig. 4b). An empirical refinement is then applied where any reinforcement element with values of \( R < 0.2R_M \) on both nodes bracketing the element are removed, followed by a re-running of the optimization process giving a new set of results for the required values of \( R \) (Fig. 4c). The final layout (Fig 4d) is determined placing reinforcement where non-zero values of \( R \) were calculated. This gives a 22m total length of reinforcement.

It is noted that while the objective function of the LP is to minimise the sum of all the \( R \) variables, the algorithm shows consistent results with values of \( R \) monotonically reducing toward the edges of the modelled reinforcement as would be intuitively expected. Research is ongoing to identify a more
A promising computational approach for reinforcement layout optimization has been presented. The approach is still under development and research is ongoing in order to extend the method to frictional self-weighted soils and to develop a robust procedure for obtaining refined solutions. Nevertheless, the results obtained up to now are positive.

Acknowledgements

The authors wish to express their gratitude to the support provided by the European Union through its EU Horizon 2020 programme.

References


DYNAMIC RESPONSE OF IMPROVED SEABED SOIL - CAISSON FOUNDATION UNDER EARTHQUAKE LOADING

*Esra Tatlıoğlu1,4, M. B. Can Ülker2 and M. Ayşen Lav3

1 Graduate School of Science, Engineering and Technology, Istanbul Technical University, Istanbul, Turkey
2 Institute of Earthquake Engineering and Disaster Management, Istanbul Technical University, Istanbul, Turkey
3 Faculty of Civil Engineering, Istanbul Technical University, Istanbul, Turkey
4 Faculty of Engineering, Ömer Halisdemir University, Nigde, Turkey

*esratatlioglu@gmail.com

ABSTRACT

In this study, dynamic behaviour of a liquefiable seabed soil under caisson foundation is studied. Plane strain numerical analyses are performed and the deformations and pore pressures of the soil skeleton and the caisson foundation are calculated. Caisson foundation sitting on a gravel layer is considered and the seabed-gravel-caisson foundation system is modeled using classical finite elements. The dynamic response of the porous seabed-caisson system is assumed to be governed by the Biot’s equations of coupled flow and deformation. Earthquake loading is applied as a harmonic loading along the bottom of the seabed. Spatial and temporal variations of pore water pressure as well as horizontal and vertical displacements are presented. A number of parametric analyses investigating the effect of hydraulic conductivity of seabed and peak ground acceleration of earthquake loading on the dynamic response are carried out.

Keywords: Earthquake excitation; dynamic response; finite elements; poroelasticity; soil improvement

1. Introduction

Many geotechnical engineering problems require solving coupled processes of flow of pore water and deformation of solid skeleton. That is, development of internal forces and resulting deformation behaviour along with pore water pressure rise under transient loading in the soil are dependent upon dynamic consolidation which is studied through time-dependent numerical analyses. In this study, dynamic response of seabed soil which is under the pier foundation system of Osman Gazi Bridge in the Gulf of Izmit, Turkey is investigated conducting plane strain analyses. The foundation system used in the analyses consists of a caisson and a compacted granular bedding layer placed below the caisson. Underlying the bedding is an improved seabed soil. Also, the system is kept under 15 m of hydrostatic water pressure.

2. Mathematical Formulation

Dynamic response of the porous seabed-caisson system is assumed to be governed by the Biot’s equations of coupled flow and deformation. The equations governing the response of saturated porous media incorporating the fluid–solid skeleton interaction was first established for the QS case in 1941 by Biot [1] who then extended the formulation to include dynamics [2, 3].

For a unit total volume, the overall equilibrium of the system can be written as:

\[ \sigma_{ij,j} + \rho g \ddot{w} + \rho \ddot{u} = 0 \]  

where \( \sigma_{ij} \) is total stress, \( \rho \) and \( \rho_f \) are the densities of the mixture and fluid, \( \dot{u} \) is the acceleration of the soil skeleton, \( \ddot{w} \) is the average fluid acceleration relative to the solid skeleton. Using the Darcy’s Law, the equation of the pore fluid equilibrium can be written as:

\[ -p_x + \rho_f g_i - \frac{\dot{w}_i}{k_i} \rho_f g_i - \rho_f \ddot{u}_i - \frac{\rho_f}{n} \ddot{w}_i = 0 \]
\( n \) is the porosity and \( k_i \) is the permeability coefficient of porous medium. The equation representing the mass balance completes the system as:

\[
\dot{\varepsilon}_i + \dot{W}_{i,i} = -\frac{n}{K_f} \dot{p}
\]

(3)

where \( K_f \) is the bulk modulus of the pore fluid [5] and \( \dot{\varepsilon}_i \) is the rate of change of volumetric strain. Also, ‘,’ shows the partial derivatives of respective quantities with respect to coordinate axes.

3. Finite Element Analysis of the Seabed–Gravel–Caisson Foundation System

In this study, displacements and pore water pressures of seabed soil under caisson foundation are calculated by using finite element (FE) method [4]. Figure 1 presents the physical model. Analyses are conducted in temporal domain and numerical values of the parameters used in analyses can be seen in Table 1.

![Figure 1: Model of the Seabed–Gravel–Caisson Foundation System as used in Osman Gazi Bridge, Izmit](image)

As for boundary conditions, displacements are constrained at the bottom which is shaken by a harmonic load having a 1 sec wave period and applied for a duration of 300 sec.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Unit</th>
<th>Seabed Soil</th>
<th>Gravel Layer</th>
<th>Caisson Foundation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height</td>
<td>( h )</td>
<td>m</td>
<td>30</td>
<td>3</td>
<td>15</td>
</tr>
<tr>
<td>Elasticity modulus</td>
<td>( E )</td>
<td>kPa</td>
<td>35000</td>
<td>70000</td>
<td>(3 \times 10^6)</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>( v )</td>
<td>-</td>
<td>0.35</td>
<td>0.33</td>
<td>0.2</td>
</tr>
<tr>
<td>Vertical Permeability</td>
<td>( k_z )</td>
<td>m/s</td>
<td>(10^{-4})</td>
<td>0.01</td>
<td>(10^{-9})</td>
</tr>
<tr>
<td>Horizontal Permeability</td>
<td>( k_x )</td>
<td>m/s</td>
<td>(10^{-4})</td>
<td>0.01</td>
<td>(10^{-9})</td>
</tr>
<tr>
<td>Bulk modulus</td>
<td>( K_f )</td>
<td>kPa</td>
<td>(2 \times 10^6)</td>
<td>(2 \times 10^6)</td>
<td>(2 \times 10^6)</td>
</tr>
<tr>
<td>Porosity</td>
<td>( n )</td>
<td>-</td>
<td>0.3</td>
<td>0.33</td>
<td>0.05</td>
</tr>
<tr>
<td>Density</td>
<td>( \gamma )</td>
<td>t/m³</td>
<td>1.8</td>
<td>1.9</td>
<td>2.4</td>
</tr>
<tr>
<td>Length</td>
<td>( L )</td>
<td>m</td>
<td>726</td>
<td>87</td>
<td>66</td>
</tr>
<tr>
<td>Density of fluid</td>
<td>( \gamma_w )</td>
<td>t/m³</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Acceleration of gravity</td>
<td>( g )</td>
<td>m/s²</td>
<td>9.81</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Period</td>
<td>( T )</td>
<td>s</td>
<td>1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
In the FE model, 8-node poro-elastic quadrilateral elements are used. The horizontal and vertical displacements, $u_h$ and $u_z$ as well as pore pressure, $p$ are specified as degrees of freedom (DOF) at the nodal points. Pore pressure values are approximated with bilinear shape functions at corner nodes, while the displacements are obtained at each node. The results are presented in terms of the absolute values of DOF distributions in the domain.

4. Numerical results

All the results along the sections 1-1 and 2-2 (see Figure 1) are presented in Figures 2–5. According to these graphs, although the permeability values do not have a significant effect on the dynamic responses of seabed, the effects of the changes in the peak ground acceleration are found to be more significant.

Figures 2 and 3 show the results in terms of the effect of different seabed permeability values on the dynamic response. When the permeability of seabed decreases, horizontal and vertical displacements in 1-1 and 2-2 sections of seabed increase. Especially in section 2-2, high values of pore pressure are observed for higher values of permeability at the bottom of the caisson foundation.

![Figure 2: Effect of permeability on the horizontal and vertical displacements cyclic responses in 1-1 and 2-2 sections of seabed, $k=10^{-3}, 10^{-4}, 10^{-6}$ m/s](image)

![Figure 3: Effect of permeability on the pore pressure cyclic responses in 1-1 and 2-2 sections of seabed, $k=10^{-3}, 10^{-4}, 10^{-6}$ m/s](image)

Figures 4 and 5 show the effect of peak ground acceleration of earthquake loading on the dynamic response. When the acceleration of earthquake load rises, horizontal and vertical displacements in 1-1 and 2-2 sections of seabed significantly increase. In section 1-1 along depth, pore pressure also increases with peak ground accelerations but in section 2-2 such an increase is only observed under the caisson foundation. The reason of this is attributed to the pore pressure being equal to hydrostatic pressure at the seabed surface.
5. Conclusions

In this study, a caisson-seabed system built at the Gulf of Izmit in Turkey is studied in terms of its seismic response under harmonic wave. Poroelasticity formulation is used to evaluate the coupled pore pressure and deformation response and the effect of the changes in the soil permeability and the peak ground acceleration are studied. The latter is found to be more considerable than the former as far as the dynamic response of the entire system is considered. According to current results, when the permeability of the soil decreases, deformations increase in the seabed and peak accelerations have an important role in the development of strains and hence, the change in the pore pressures around the caisson foundation. It should be mentioned here that more parametric studies are currently being considered investigating the effects of other parameters such as the soil rigidity and quality of improvement, the results of which will be subsequently presented.

References


The modelling of soil-tool interaction using the material point method

*Michael Cortis¹, William Coombs¹, Charles Augarde¹, Scott Robinson², Andrew Brennan² and Michael Brown²

¹School of Engineering and Computing Sciences, Durham University, South Road, Durham, DH1 3LE
²Civil Engineering, University of Dundee, Fulton Building, Dundee, DD1 4HN

*michael.cortis@durham.ac.uk

ABSTRACT

The material point method (MPM) is a numerical tool able to model very large deformations in solid mechanics such as geotechnical problems. To date, soil-tool interaction modelling in the MPM is somewhat difficult, especially when the tool position is not stationary. Usually, the tool’s boundaries do not coincide with the MPM grid and therefore boundary conditions cannot be imposed directly on the grid nodes. An implicit approach based on a penalty type method to impose essential boundary conditions in the MPM has been developed and used in the paper to demonstrate how to model frictionless soil-tool interaction mechanism [3]. This approach assumes that the tool is a rigid body as the deformation of the tool boundaries are insignificant. The same approach can also be used to model the interaction between structures and soil such as foundations.

Key Words: material point method; essential boundary conditions; soil-tool modelling; offshore geotechnics

1. Introduction

Since the development of the material point method (MPM) by Sulsky et al. [9] in 1994, it has been widely promoted as the next generation of numerical methods to model large deformations in materials such as soils. The method has two components: the material points which represent the volume of the solid, and the background grid that is used to solve the discretised linear system using same approach as the finite element method (FEM). While the MPM was developed in an explicit form [9], an implicit approach was later presented in [8] making it easy to transfer finite element analysis (FEA) technology to the MPM. After every load step, the material points’ positions are updated and the background grid is reset to its original configuration. This means that the grid remains regular without any skewness, distortion and any associated numerical error.

The MPM has been successful in modelling large deformation problems such as landslides [1] and other geotechnical problems where boundary conditions are likely to coincide with the background grid nodes. When modelling soil-tool or soil-structure interaction in the MPM, it is often the case that the boundary of the tool or structure is arbitrary and does not coincide with the background grid nodes, so that it is not possible to impose these essential boundary conditions in the standard FEM approach. To overcome this problem, one can adopt the “moving mesh concept” [8], generally used when the boundary movement is known a priori and therefore the background grid nodes are moved simultaneously, but this unfortunately loses the advantageous regular grid concept of the MPM. The problem of imposing arbitrary essential boundary conditions on non-matching meshes, or so-called “embedded domains” (e.g. [5]), has been widely discussed with attempts to impose such boundary conditions (e.g. [4]) by using penalty, Lagrange multiplier or Nitsche methods. A simple penalty approach developed by Kumar et al. [7] to impose essential boundary conditions on a non-conforming grid FEA (called the implicit boundary method (IBM)), has been adopted in the MPM [2, 3] to impose both homogeneous and inhomogeneous Dirichlet boundary conditions. That means that arbitrary inclined fixed, rollers and non-zero displacement boundary conditions can be applied in the MPM to represent frictionless soil-tool interaction.

In this paper, we summarise the essential components for implementing the of IBM in the MPM, and demonstrate its effectiveness to model soil-tool interaction using an elastic domain pushed over a wedge-like tool.
2. Essential boundary conditions in the material point method

The IBM proposed for the structured grid FEM is based on a penalty approach proposed by Kantorovich and Krylov [6] during the 1950s, but only for orthogonal arbitrary positioned essential boundary conditions in the FEM[7]. The main concept of the IBM is to use Dirichlet step functions

\[ d_\phi = \begin{cases} 
0, & \phi < 0 \\
1 - \left(1 - \frac{\phi}{\delta}\right)^2, & 0 \leq \phi \leq \delta \\
1, & \phi > \delta 
\end{cases} \quad (1) \]

to identify the area inside/outside the solid region which are then used to activate/deactivate the standard approximation for displacement \( \{u\} \) in the finite element sense and impose the essential boundary condition \( \{u^a\} \). The displacement solution \( \{u'\} \) is therefore obtained as follows,

\[ \{u'\} = [D]\{u\} + \{u^a\}, \quad (2) \]

where \([D] = \text{diag}(d_x, d_y)\) in 2D. \(d_\phi\) is set to unity to free the degrees of freedom in the \(\phi\)-direction [3]. When Equation 2 is substituted in the standard FEM weak form, the strain-displacement matrix \([B]\) is now expanded and includes not only the finite element shape functions derivatives, but also the values of Dirichlet functions and their derivatives. Therefore the element stiffness matrix \(k^E\) with a volume \(V_e\) is expressed in four terms, i.e.

\[ [k^E] = \int_{V_e} [B_1]^T[D^e][B_1]dV + \int_{V_e} [B_1]^T[D^e][B_2]dV + \int_{V_e} [B_2]^T[D^e][B_1]dV + \int_{V_e} [B_2]^T[D^e][B_2]dV, \quad (3) \]

where the first term is denoted as the standard finite element stiffness matrix \([K_1]\), while the second, third and fourth term of the implicit part are denoted as \([K_2]\), \([K_2]^T\) and \([K_3]\) and expressed as

\[ [K_2] = \int_T [\tilde{B}_1]^T \left( \int_0^\delta [\tilde{D}_1]^T[D^e][\tilde{D}_2][T]dn \right) [\tilde{B}_2]dt, \quad (4) \]
\[ [K_3] = \int_T [\tilde{B}_2]^T \left( \int_0^\delta [T]^T[D_2]^T[D_2][T]dn \right) [\tilde{B}_2]dt, \quad (5) \]

where \([\tilde{B}_2]\) is a diagonal matrix contain the shape functions, \([\tilde{B}_1]\) is identical to the finite element strain-displacement matrix \([B]\), \([\tilde{D}_1]\) and \([\tilde{D}_2]\) are expressed as

\[ [\tilde{D}_1] = \begin{bmatrix} D_1 & 0 & 0 & 0 \\
0 & D_2 & 0 & 0 \\
0 & 0 & D_1 & D_2 \end{bmatrix} \quad \text{and} \quad [\tilde{D}_2] = \begin{bmatrix} \frac{\partial D_1}{\partial x} & 0 \\
0 & \frac{\partial D_2}{\partial y} \\
\frac{\partial D_1}{\partial y} & \frac{\partial D_2}{\partial x} \end{bmatrix}, \]

\([D^e]\) is the tangent stiffness matrix and \([T]\) is a rotation matrix in the Cartesian coordinate system used to transform the inner integrals of \([K_2]\) and \([K_3]\) by a rotation angle \(\theta\) to achieve an inclined boundary condition as shown in Figure 1. Non-zero prescribed displacement boundaries are imposed by calculating the equivalent reaction force as

\[ \{f^E_R\} = [[K_2] + [K_2]^T + [K_3]]\{u^a\} \quad (6) \]

caused by a nodal displacement \(\{u_a\}\), and are included in the linear system to be solved.

Another important step to impose arbitrary essential boundary conditions in the MPM is the discretization of the continuum into a set of material points. In the initial pre-processing step, the background grid is usually populated with a set of material points with associated domains and volumes. If the material point domain lies complete inside the solid region, this point is retained, while if the material point domain
lies completely outside the solid region, this point is removed. If a material point domain lies on the
boundary of the problem, the material point domain is truncated to reflect the new solid region only, and
the volume is adjusted accordingly. In the MPM, the material points are used similar to Gauss points in
the standard FEM to evaluate the stiffness matrix \([K]\), and therefore grid elements are omitted from the
system of equations if they containing material points with a tiny fraction of volume measured to a given
tolerance. The implementation of the IBM in the MPM has now been successfully benchmarked [2, 3],
and is used in the next section on a soil-tool interaction problem.

![Figure 1: Essential boundary through a grid element](image)

3. Penetration of a wedged-like tool

In this section, a wedge-like tool penetrating an elastic domain is used to demonstrate how soil-tool
interaction can be modelled by using the IBM in the MPM. The problem consists of a solid elastic
continuum confined between two horizontal and an inclined roller boundary conditions, while the elastic
domain (shaded area) is being pushed toward the wedge as shown in Figure 2 (a). The stationary inclined
boundary is used to represent a frictionless wedge onto which the elastic domain will be compressed
while moving horizontally to the left. The problem is solved on 2mm x 2mm background grid and a single
material point in every grid element is used, as shown in Figure 2 (b). The elastic body has a Young’s
Modulus of 1000 MPa and a Poisson’s ratio of 0.3. The bandwidth \(\delta\) was set to \(\delta = 5 \times 10^{-6} \ h\), where
\(h\) is the background grid size. An incremental displacement of 6mm per load step was used to push the
elastic domain toward the wedge. The deformations of the body at the 1st, 3rd, 5th and 6th load steps
are shown in Figures 2 (c-f) respectively, where the contour plots represent the \(x\)-displacement of the
material points. Despite large load steps, that the material points clearly move along the wedge without
crossing the boundary, causing the elastic domain to “funnel” through the space between the wedge and
top horizontal roller boundary conditions. Such wedge type problem can be easily used to represent a
frictionless soil-tool interaction such as ploughing schemes and other similar problems.

4. Conclusions

In this paper we have described how an implicit boundary method has been used to model roller and
other boundaries in the MPM. This allows the modelling of frictionless soil-tool interaction problems.
In future work, the IBM will be developed to account for friction when this is important to the overall
mechanism of the problem.

Acknowledgements

The work presented in this paper is part of a study of seabed ploughing for offshore energy infrastructure
and is funded by Grants EP/M000397/1 and EP/M000362/1 of the UK EPSRC.
Figure 2: Rigid body penetration into an elastic domain: (a) problem dimensions, (b) initial MP discretisation and (c) through (h) deformed material point positions coloured according to their $x$-displacement.

References


SOIL CONDITIONS AND PIPING CRITERION DURING SUCTION CAISSON INSTALLATION IN LAYERED STRATA

*M. Mehravar¹, O. Harireche², A. Faramarzi³, S, Dirar³

¹School of Engineering and Applied Science, Aston University, Birmingham, B4 7ET
²Department of Civil Engineering, Faculty of engineering, University of Medina, KSA
³Department of Civil Engineering, School of Engineering, University of Birmingham, Birmingham, B15 2TT

ABSTRACT

Suction-induced seepage has a key role to the installation of caisson foundations in sand. Indeed, the upward pore water flow on the inner side of the caisson wall causes a release of a fraction of soil resistance due to the reduction of the lateral effective stress, and facilitates the installation process. A safe caisson installation requires a reliable prediction of soil conditions, especially soil resistance and critical suction for piping. This study is motivated by the fact that in some environments, there is a thin layer of low permeable soil (e.g. clay) in homogenous sand that can affect the installation process of suction caisson foundations at some stages. In this paper, soil conditions as well as critical suction for piping in sandy soils with clay layer substratum are investigated. An in-house developed finite element tool is employed to simulate the normalised seepage problem at different stages of installation taking into account the actual pressure gradient distribution on both sides of caisson wall. The results revealed how the pressure gradient, and hence soil resistance, are affected by the existence of a clay layer. It was concluded that considering the actual variation of pressure gradient within the caisson depth leads to the prediction of more accurate critical suction for piping condition.

Keywords: caisson foundation; installation in sand with clay layer, normalised geometry; piping condition

1. Introduction

A suction caisson is an upturned ‘bucket’ of cylindrical shape made from steel. This type of foundation has been very popular in the oil and gas industry and the current trend is to extend its use in the developing industry of wind farms [1]. Installation of these foundations is achieved by pumping out the water trapped inside the caisson cavity after initial penetration under self-weight. Seepage produced in permeable soils during suction caisson installation causes an overall reduction in soil resistance and facilitates caisson penetration [5]. Nevertheless, during caisson installation in sand, suction must be controlled to avoid the formation of piping channels which would prevent further penetration and may cause the installation process to fail. The role of porewater seepage has been extensively investigated in the development of design procedures for the installation of suction caissons in sand [1, 3]. However, specific soil conditions such as the existence of low permeability soil layers which may affect seepage and consequently the installation design procedures has received less attention [2-4]. In the aforementioned literature, the hydraulic gradient on both sides of caisson wall has been described in terms of an overall value based on the pressure difference between the mudline and caisson tip [1,3]. However, due to the importance of the variation of pressure gradient over the caisson penetration depth, it is important to investigate the gradient distribution over the penetration depth through the installation process. In this paper, an in-house developed finite element (FE) model [5] is employed to study whether the presence of a clay layer in sand would affect the installation process of suction caisson foundations or not. In addition, critical soil condition due to piping will be investigated in sandy soil with a low permeable soil layer such as clay. The results are compared to those obtained from installation in homogenous sand as well as other existing method to calculate critical piping condition in such soils.

2. Formulation for the Normalised Seepage Problem and Permeability Profiles

In order to draw conclusions that are not related to the problem dimensions, any length measure is scaled with respect to the caisson radius ($R$) and pressure is normalised by the magnitude of the
applied suction. The caisson height, penetration depth into the seabed and the height of the clay layer are denoted as \( L \), \( h \), and \( h_c \) respectively. Hence, the following normalised variables are adopted:

\[
p^* = \frac{p}{s}, \quad h^* = \frac{h}{R}, \quad h_c^* = \frac{h_c}{R}
\]

where \( p^* \), \( h^* \) and \( h^*_c \) represent normalised applied suction, caisson penetration depth and the height of the clay layer, respectively. Figure 1 shows a vertical section through the meridian plane of the caisson soil system where a cylindrical system of coordinates \( z^*=z/R \) and \( r^*=r/R \) is used. Four different soil profiles identified as Case A (\( h^*_c=0 \)), B (\( h^*_c=3h^* \)), C (\( h^*_c=2h^* \)) and D (\( h^*_c=h^* \)) are considered. The first soil profile, case A, represents a homogenous sandy soil with permeability \( k \) (Fig 1a). The permeability of the sand (upper layer) is taken as 10 times higher than that of the clay layer. The other three seabed profiles (Case B, C and D) correspond to the cases where clay (impermeable layer) is at a closer distance to the caisson tip. In case D (\( h^*_c=h^* \)) the caisson tip touches the top of the clay layer (Fig 1b).

The excess pore water pressure \( p^* \) must satisfy the dimensionless equation (1)

\[
\nabla^2 p^* = \frac{1}{r} \frac{\partial p^*}{\partial r} + \frac{\partial^2 p^*}{\partial z^*^2} = 0
\]

(1)

and the boundary conditions \( p^*=-1 \) on OC, \( p^*=0 \) on C’F, FH, BH and \( \frac{\partial p^*}{\partial r} = 0 \) on CD and OB (Fig 1).

3. Results and Discussion

3.1. Soil Condition during Suction Installation

The FE results of normalised excess pore water pressure \( p^* \) distribution for values of \( h^*=0.6 \) are shown in figure 2. This figure corresponds to a homogeneous sand (fig 1a) as well as to a sand with a layer of clay placed at \( h_c=2h^* \) (fig 1b) and \( h_c^*=h^* \) (fig 1c). These figures clearly indicate that the pressure distribution is affected by the low permeability layer. Water seepage produced by suction creates a hydraulic gradient which varies with depth on both sides of the caisson wall. Figure 3 shows the vertical component of the normalised hydraulic gradient \( g^* = \frac{\partial p^*}{\partial z^*} \) on both sides of the caisson wall as a function of normalised depth \( z^* \) for normalised penetration depth \( h^*=0.2 \) and 1 in four different soil seabed profiles (case A-D). In this study the vertical component of the pressure gradient on the inner and outer side of the caisson wall are denoted as \( g_i(R, \zeta) \) and \( g_o(R, \zeta) \), respectively. It can be seen that the pressure gradient on both sides of the caisson wall is higher at early stages of penetration. Maximum values of the gradient occur at the caisson tip regardless of soil seabed profile. By comparing the normalised gradients for all soil profiles, it can be observed that the effect of the low permeability layer is more pronounced inside the caisson cavity and becomes more noticeable where the caisson tip touches the low permeability layer (Case D: \( h^*_c=h^* \)). The difference in gradient magnitude for the first three soil permeability profiles (case A to C) is not significant on
both sides of the caisson wall. However, such a difference increases and becomes significant for soil profile D, which is likely to affect soil resistance through the increase in soil effective stress. In this case (case D) up to 3/4 normalised penetration depth, the magnitude of pressure gradient is lower compared to the soil permeability profiles A to C. Below such a depth the opposite trend is observed. This behaviour suggests that the soil is less prone to piping in those sandy soil profiles where a low permeability layer exists at a close distance to the caisson tip. In terms of soil resistance to caisson penetration, it can be anticipated that soil seabed profiles with a low permeability layer located around the caisson tip, are likely to be subject to less reduction in soil resistance due to seepage.

![Figure 2: Normalised excess pore water pressure distribution for normalised penetration depth $h^*=0.6$ at (a) $h_c^*=0$ (homogeneous sand), (b) $h_c^*=2h^*$ and (c) $h_c^*=h^*$](image)

![Figure 3: Dimensionless pressure gradient as a function of normalised depth for $h^*=0.2$ and $h^*=1$, at four different soil profiles](image)

### 3.2. Critical Suction for piping condition

During caisson installation in sand, suction must be controlled to avoid the formation of piping channels around the caisson wall, which may cause the installation procedure to fail (Ibsen & Thilsted, 2010). At a generic material point of normalised coordinates $r^*$, $z^*$ within the soil inside the caisson cavity, piping takes place when the vertical effective stress becomes zero. This is expressed by the equation 2:

$$\sigma_\zeta = \gamma z - \int_0^{\zeta} g_i(R, \zeta') d\zeta' = 0$$

Hence, the suction magnitude that causes such condition is given by:

$$\frac{\bar{s}}{\gamma R} = \frac{\zeta}{L_i(1, \zeta')}$$

where $L_i(1, \zeta') = \int_0^{\zeta'} g_i(1, \zeta') d\zeta'$. 

217
Houlsby and Byrne (2005) have proposed the piping criterion: $\tau / (\gamma R) = h^*/(1 - a)$ where $a$ is the magnitude of the normalised pressure at the caisson tip on the inner side and known as pressure factor. An expression of the pressure factor $a$ as a function of the penetration depth in sand with a clay layer, was proposed by Leblanc-Bakmar [3]. The proposed piping criterion by Houlsby and Byrne (2005) assumes a constant pressure gradient on each side of the caisson wall. In this study, based on the numerical solution for the normalised seepage problem, condition (3) is an expression of the same criterion that takes into account the actual variation of the pressure gradient as a function of depth. To account for the actual variation of the pressure gradient on the caisson wall in sand overlying a clay layer, the coefficient $a$ used by Cotter (2009) is to be replaced by the coefficient $(1-L_i^*)$. Figure 4 shows a comparison of parameters $a$ and $(1-L_i^*)$ at soil seabed profiles A and D. The difference between these two parameters is negligible in homogenous sand, but it is pronounced in case D where the caisson tip touches the clay interface. The magnitude of this difference becomes relatively high at a higher penetration depth. The result of Figure 4 justifies that the use of the parameter $a$ in piping criteria underestimates the suction magnitude that causes soil piping to initiate inside the caisson cavity in multi-layered soils, especially in the presence of low permeability clay layers.

![Figure 4: Comparison of parameter $a$ and $(1-L_i^*)$ for critical piping condition](image)

4. Conclusion

In this study, the effect of suction-induced seepage on soil conditions during caisson installation in multi-layered soils and the critical suction that causes piping were investigated. Firstly, the numerical solution of the normalised model problem for seepage around the caisson foundation was developed. The present analysis takes into account the actual variation in pressure gradient on both sides of the caisson wall over the caisson penetration depth. Four different soil permeability profiles were considered in which the low permeability layer were moved towards the caisson tip. It was concluded that soil seabed profiles with a low permeability layer located close to the caisson tip, are likely to have less reduction in soil resistance due to seepage. In addition, the results revealed that taking into account the actual variation of the pressure gradient leads to a more accurate estimation of the critical suction for piping in multi-layered soil seabed with relatively less restriction on the magnitude of the applied suction during the installation process.

References:


Solids and Structures
ISOGEOMETRIC ANALYSIS OF SMALL-SCALE PLATES WITH NONLINEARITY

Hoang X. Nguyen and Thuc P. Vo

1Faculty of Engineering and Environment, Northumbria University, Newcastle upon Tyne, NE1 8ST, UK

*thuc.vo@northumbria.ac.uk

ABSTRACT

This study aims to investigate the geometrically nonlinear behaviour of functionally graded (FG) microplates with size-dependent effects using isogeometric analysis (IGA) approach. While modified couple stress theory (MCST) is introduced to account for small-scale effects, the displacement fields are described based on the four-variable refined plate theory (RPT). The MCST, which has advantages of including asymmetric couple stress tensor and using only one material length scale parameter, would be able to effectively capture the size-dependent effects in nano/micro structures. The RPT, which requires $C^1$ elements, not only is able to improve the accuracy of the analysis but also helps to describe the nonlinear distribution of shear stress through plate thickness without using shear correction factors. The geometrically nonlinear behaviours of rectangular and circular FG microplates based on these two theories are studied in the platform of IGA. This recently developed method utilises the non-uniform rational B-splines (NURBS) functions to establish approximation functions and describe geometry domains simultaneously. In addition, NURBS functions, by its nature, could satisfy high-order continuity which is essentially required in RPT theory without any difficulty. While the governing equations and weak forms are directly derived using Hamilton’s principle, the Newton-Raphson iterative algorithm is employed to solve the nonlinear problems. A number of numerical examples conducting for FG microplates reveal that the consideration of small-scale effects is followed by the increase in plates’ stiffness.

Key Words: Functionally graded microplates; Isogeometric analysis; Geometrical nonlinearity

1. Introduction

Functionally graded materials (FGMs) are composite materials formed of two or more constituent phases in which material properties vary smoothly from one surface to the other. With the rapid development of technology, FGMs have been increasingly used in micro electromechanical systems (MEMS/NEMS), electrically-actuated MEMS devices, atomic force microscopes, etc. Mechanical properties of such small-scale structural devices including Young’s modulus, flexural rigidity are size-dependent [1]. However, classical continuum elasticity which is scale-free theory fails to predict these size effects. Modified couple stress theory [1, 2] appears to be one of the size-dependent theories in which only one material length scale parameter is employed. Based on the MCST, a couple of research works using various plate models have been carried out to investigate the size-dependent effects of micro FG plates, one of them is to use refined plate theory (RPT) [3]. However, RPT requires $C^1$-continuity of general displacements causing significant challenge to derive second derivative of deflection in the platform of finite element analysis (FEA) where $C^0$ elements are frequently used. Recently, a new numerical method so-called Isogeometric Analysis (IGA) which is able to deal with $C^1$-continuity problem without using any additional variables has been introduced by Hughes and his co-workers [4]. This method bridges the gap between Computer Aided Design (CAD) and FEA in which same basis functions generated by B-splines or non-uniform rational B-splines (NURBS) shape functions are employed to describe exact geometry and unknown variables. Since modelled geometry is exact and the number of unknown terms is not increased, it is expected that IGA would yield more accurate results with lower computational cost for RPT problems in the comparison with regular FEA [5].

In this study, the size-dependent nonlinear bending behaviours of FG microplates will be investigated. While the size effects are captured using the modified couple stress theory, the four-variable refined plate theory is employed to describe displacement field. The nonlinear problems are solved in the platform of the isogeometric analysis and Newton-Raphson iterative procedure.
2. Theoretical Formulation of FG Microplates

Assuming that the functionally graded microplates are made of metal and ceramic varying continuously through the plates’ thickness, the effective material properties of the plates are obtain following the rule of mixture or Mori-Tanaka scheme. Detail of those expressions could be found from existing works in the literature [5].

According to the modified couple stress theory, the strain energy is defined as a combination of strain tensor and curvature tensor [3]. The components of the deviatoric part of the symmetric couple stress tensor $m_{ij}$ and symmetric curvature tensor $\chi_{ij}$ are given by

$$m_{ij} = 2G\ell^2 \chi_{ij}, \quad \chi_{ij} = \frac{1}{2} \left( \frac{\partial \theta_i}{\partial x_j} + \frac{\partial \theta_j}{\partial x_i} \right),$$

(1)

where $G$ and $\ell$ are shear modulus and material length scale parameter, respectively, and the rotation vector $\theta = \frac{1}{2} \text{curl}(u)$ where $u$ is the displacement vector.

In order to take into account the shear deformation effects, the $C^1$ plate displacement field is presented with respect to the refined plate theory as

$$u(x, y, z) = u_0(x, y) - zw_{b,x}(x, y) + g(z)w_{s,x}(x, y),$$

(2a)

$$v(x, y, z) = v_0(x, y) - zw_{b,y}(x, y) + g(z)w_{s,y}(x, y),$$

(2b)

$$w(x, y, z) = w_b(x, y) + w_s(x, y),$$

(2c)

where $u_0, v_0$ are membrane displacements, $w_b$ and $w_s$ represent bending and shear components of transverse displacement, $g$ is the distribution function. The rotation vector and curvature vector are obtained by substituting the above displacement expressions into Equation 1 [3].

The general nonlinear strains can be derived from the displacement fields as

$$\varepsilon_{ij} = \frac{1}{2} \left( u_{i,j} + u_{j,i} \right) + \frac{1}{2} u_{k,i}u_{k,j},$$

(3)

Then the nonlinear von Kármán strains are obtained with the assumptions of moderate rotations. Consequently, $(w_{s,x})^2, (w_{s,y})^2, w_{s,x}w_{s,y}$, are not negligible.

3. NURBS-based Formulation of FG Microplates

By using the NURBS basis functions, the displacement field $u$ of the FG microplates based on the RPT and MCST could be approximated as follow [4, 5]

$$u^h(\xi, \eta) = \sum_{A}^{n \times m} R_A(\xi, \eta)q_A,$$

(4)

where $n \times m$ is the number of basis functions, $R_A$ represents two-dimensional NURBS basis functions and $q_A$ denotes the vector of degrees of freedom associated with the control point $A$. The nonlinear isogeometric finite element formulation of the bending analysis is defined as

$$K(q)q = F,$$

(5)

where $F$ is the force vector and $K$ is the global stiffness matrix. The inclusion of the solution $q$ in the global stiffness matrix makes the problem nonlinear, consequently, the Newton-Raphson iterative procedure is employed to solve for the nonlinear solutions in this study.
4. Numerical Examples

In this section, the nonlinear bending analysis of FG microplates will be conducted based on the RPT, modified couple stress theory, and the proposed IGA approach. The Al/Al$_2$O$_3$ is chosen to be the metal-ceramic FG material whose properties are of $E_m = 70$ GPa, $E_c = 380$ GPa, $\rho_m = 2707$ kg/m$^3$, $\rho_c = 3800$ kg/m$^3$, and $\nu_m = \nu_c = 0.3$.

The fully simply-supported (SSSS) microplates subjected to uniformly distributed load are parametrically studied considering various values of the aspect ratio $a/h$, material length scale ratio $\ell/h$, and material index $n$. The numerical results of normalised central deflection, $\bar{w} = \frac{w}{h}$, and normal stress, $\bar{\sigma} = \frac{\sigma_x a^2}{E_m h^2}$, of FG microplates subjected to the external load $P = \frac{q_0 a^4}{E_m h^4}$ are presented in the Table 1.

Figure 1 illustrates the effects of the material length scale ratio $\ell/h$ on the nonlinear displacement of the Al/Al$_2$O$_3$ microplates. As can be seen, the increase in the material length scale ratio $\ell/h$ causes the gain in structures stiffness. Consequently, the displacement and stresses are declined correspondingly. On the contrary, the increase of material index $n$ leads to completely different trend in which the displacement is also increased as a result of stiffness lost.

Table 1: Normalised nonlinear deflection and normal stress of simply-supported square Al/Al$_2$O$_3$ microplates, load parameter $P = 100$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\ell/h$</th>
<th>Deflection</th>
<th></th>
<th>Normal stress</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.0</td>
<td>0.7575</td>
<td>0.7007</td>
<td>0.685</td>
<td>0.6805</td>
</tr>
<tr>
<td>0.2</td>
<td>0.6857</td>
<td>0.6322</td>
<td>0.6174</td>
<td>0.6131</td>
<td>0.6125</td>
</tr>
<tr>
<td>0.4</td>
<td>0.5215</td>
<td>0.477</td>
<td>0.4651</td>
<td>0.4617</td>
<td>0.4612</td>
</tr>
<tr>
<td>0.6</td>
<td>0.3603</td>
<td>0.3288</td>
<td>0.3205</td>
<td>0.3182</td>
<td>0.3178</td>
</tr>
<tr>
<td>0.8</td>
<td>0.2473</td>
<td>0.226</td>
<td>0.2205</td>
<td>0.219</td>
<td>0.2188</td>
</tr>
<tr>
<td>1.0</td>
<td>0.1753</td>
<td>0.1606</td>
<td>0.1568</td>
<td>0.1557</td>
<td>0.1555</td>
</tr>
<tr>
<td>1</td>
<td>0.0</td>
<td>1.1161</td>
<td>1.0656</td>
<td>1.0521</td>
<td>1.0482</td>
</tr>
<tr>
<td>0.2</td>
<td>1.0342</td>
<td>0.9874</td>
<td>0.9745</td>
<td>0.9707</td>
<td>0.9702</td>
</tr>
<tr>
<td>0.4</td>
<td>0.8359</td>
<td>0.7901</td>
<td>0.7774</td>
<td>0.7738</td>
<td>0.7732</td>
</tr>
<tr>
<td>0.6</td>
<td>0.6069</td>
<td>0.5657</td>
<td>0.5547</td>
<td>0.5516</td>
<td>0.5511</td>
</tr>
<tr>
<td>0.8</td>
<td>0.4235</td>
<td>0.3919</td>
<td>0.3837</td>
<td>0.3814</td>
<td>0.381</td>
</tr>
<tr>
<td>1.0</td>
<td>0.3006</td>
<td>0.2775</td>
<td>0.2716</td>
<td>0.2693</td>
<td>0.2697</td>
</tr>
</tbody>
</table>

5. Conclusions

The geometrically nonlinear bending behaviours of the functionally graded microplates have been investigated. The size effects are captured by the modified couple stress theory. The four-variable refine plate theory is employed to describe the displacement field of the plates. The formulation of the microplates using the proposed theories which require $C^1$-continuity element is then successfully integrated and solved in the platform of isogeometric analysis. The numerical results reveal that the size-dependent investigation using modified couple stress theory results in an increase in the plates’ stiffness. Consequently, the nonlinear deflection and stresses are both decreased.
Figure 1: Effect of material length scale ratio $\ell/h$ on the nonlinear central deflection of simply supported Al/Al$_2$O$_3$ square microplates, with $a/h = 5$, $P = 100$.

Acknowledgements
The authors acknowledge the financial support from the Northumbria University via the Researcher Development Framework.

References


OBJECTIVE FIXED-POLE APPROACH IN GEOMETRICALLY EXACT 3D BEAMS: IMPLEMENTATIONAL ASPECTS

*Maja Gaćeša\(^1\) and Gordan Jelenić\(^1\)

\(^1\)Faculty of Civil Engineering, University of Rijeka, Radmile Matejčić 3, 51000 Rijeka, Croatia

*maja.gacesa@uniri.hr

ABSTRACT

The 6D representation of the configuration tensor was used to develop a geometrically non-linear beam finite element of an arbitrary order with Lagrangian (additive) interpolation of the configurational parameters. Analogously to the 3D case, where additive interpolation of the rotational parameters results in non-objective formulation, as shown by Crisfield and Jelenić, the proposed elements exhibit even worse non-objective behaviour, evident even in planar cases! A remedy for this problem was to develop and implement the so-called generalised shape functions (given by Jelenić and Crisfield for a 3D case) for the configurational parameter (which is a 6D vector). This successfully solved the problem of objectivity, but decreased formulation robustness significantly. We assume that the cause of this are not the shape functions themselves, but the significant numerical instability of the transformational matrices they contain. In this paper we pinpoint the terms in those matrices which we assume to be responsible for loss of robustness and analyse them with respect to computational precision and propose a remedy.

Key Words: 3D beams; objectivity of strain measures; fixed-pole approach; numerical stability

1. Introduction

When dealing with 3D rotations, the orientation matrices at two configurations are related via \( \Lambda = \exp \hat{\psi} \Lambda_{\text{old}} \), where \( \psi \) is the rotational parameter. The exponentiation \( \exp \hat{\psi} \) is defined via well known Rodrigues formula \( \exp \hat{\psi} = I + \alpha_1 \hat{\psi} + \alpha_2 \hat{\psi}^2 \) \[1\]. By taking the directional derivative of the rotation matrix in the direction of a superimposed infinitesimal perturbation \( \delta \psi \) the relationship between the spin vector \( \delta \vartheta \) and the variation of the rotational vector \( \psi \) is obtained via \( \delta \vartheta = \mathbf{H}(\psi) \delta \psi \), where \( \mathbf{H}(\psi) = I + \beta_1 \hat{\psi} + \beta_2 \hat{\psi}^2 \). The coefficients appearing in aforementioned functions are

\[
\alpha_1 = \frac{\sin \psi}{\psi}, \quad \alpha_2 = \frac{1 - \cos \psi}{\psi^2}, \quad \beta_1 = \frac{1 - \cos \psi}{\psi^2}, \quad \beta_2 = \frac{\psi - \sin \psi}{\psi^3}.
\]

The aforementioned functions \( \exp \) and \( \mathbf{H} \) are used when implementing beam finite-elements to compute the orientation matrix and curvature at integration points. Additionally, \( \mathbf{H}'(\psi) = \delta_1 (\psi \cdot \hat{\psi}') \hat{\psi} + \alpha_2 \hat{\psi}' + \beta_2 (\hat{\psi} \hat{\psi}' + \hat{\psi}' \hat{\psi}) + \delta_2 (\psi \cdot \hat{\psi}') \hat{\psi}^2 \) is used as an ingredient of the generalised shape functions in the objective approach given by Jelenić and Crisfield [2], where

\[
\delta_1 = \frac{\alpha_1 - 2\alpha_2}{\psi^2} = \frac{\psi \sin \psi + 2 \cos \psi - 2}{\psi^4}, \quad \delta_2 = \frac{3\alpha_1 - 2 - \cos \psi}{\psi^4} = \frac{3 \sin \psi - \psi (\cos \psi + 2)}{\psi^5}
\]

are the two additional coefficients multiplying the matrices.

Bottasso and Borri in [3] proposed an integral approach, which treats rotations and displacements in a unified manner. This is achieved by means of a configuration tensor which shares many analogies with the rotation matrix \( \Lambda \). This means that, analogously to the rotation case, using \( \mathbf{C} = \exp \hat{\nu} \mathbf{C}_{\text{old}} \), two configurations can be related, with \( \nu = (\rho^T \cdot \hat{\psi})^T \) as the parameter of complete motion where \( \hat{\psi} \) is the rotational vector and \( \rho \) is a quantity which is a combination of both position and rotation vectors (see
(3) for details) but its norm does not appear in any of the trigonometric coefficients. The exponential \( \exp \vec{v} \) takes the form

\[
\exp \vec{v} = \begin{bmatrix}
\exp \vec{\psi} & Q(\nu) \\
0 & \exp \vec{\psi}
\end{bmatrix}, \quad Q(\nu) = H(\vec{\psi})\rho \exp \vec{\psi}.
\]

At this point it is worth noticing that no new trigonometric coefficients are introduced. By taking the directional derivative of \( C \) in the direction of a superimposed infinitesimally small perturbation \( \delta \zeta = (\delta \xi^T \delta \theta^T)^T \) which we term the configurational spin vector we obtain the relationship between the configurational spin vector \( \delta \zeta \) and the variation of the configuration vector \( \nu \) as \( \delta \zeta = H_6(\nu)\delta \nu \), where \( H_6(\nu) \) is a 2 by 2 matrix containing blocks \( H(\vec{\psi}) \) on the main diagonal, a zero matrix in the lower-left block and \( \mathbf{B}(\nu) = \alpha_2 \hat{\rho} + \delta_1 (\rho \cdot \vec{\psi}) \hat{\psi} + \delta_2 (\rho \cdot \vec{\psi}) \hat{\psi}^2 + \beta_2 (\vec{\psi} \hat{\rho} + \hat{\rho} \vec{\psi}) \) in the upper right block. The generalised shape functions may be generalised to this 6D case \([4]\). Such an approach were only relative configurations are interpolated results in an objective formulation. Analogously to the 3D case, the derivative of the function \( H_6 \) is one of the ingredients of these shape functions. Taking the derivative of the block matrix \( H_6 \), the out-of-diagonal block is

\[
\mathbf{B}'(\nu) = \delta_1 \left[ (\vec{\psi} \cdot \vec{\psi}) \hat{\rho} + (\vec{\rho} \cdot \vec{\psi}) \hat{\psi} + (\rho \cdot \vec{\psi}) \hat{\psi} \right] + \alpha_2 \hat{\rho}' + \zeta_1 (\vec{\psi} \cdot \vec{\psi})(\rho \cdot \vec{\psi}) + \\
+ \zeta_2 (\vec{\rho} \cdot \vec{\psi})(\rho \cdot \vec{\psi}) \hat{\psi}^2 + \delta_2 \left[ (\vec{\rho} \cdot \vec{\psi} + \rho \cdot \vec{\psi}) \hat{\psi}^2 + (\rho \cdot \vec{\psi}) \left( \hat{\psi} \hat{\psi} + \hat{\psi} \hat{\psi} \right) + (\vec{\psi} \cdot \vec{\psi}) \left( \hat{\psi} \hat{\rho} + \hat{\rho} \hat{\psi} \right) \right] + \beta_2 (\vec{\psi} \hat{\rho} + \hat{\rho} \vec{\psi} + \vec{\rho} \hat{\psi} + \hat{\rho} \hat{\psi}),
\]

where

\[
\zeta_1 = \frac{\cos \psi - 5a_1 + 8a_2}{\psi^4} = \frac{\psi^2 - 8}{\psi^6}, \quad (3)
\]

\[
\zeta_2 = \frac{a_1 - 7a_2 + 15\beta_2}{\psi^4} = \frac{\psi^2 - 15}{\psi^6} \sin \psi + 8\psi + 7\cos \psi. \quad (4)
\]

2. Motivation: a generalised fixed-pole beam finite element

In our recent work we developed a family of finite elements based on the combination of the fixed-pole approach and objective interpolation of the iterative configuration vectors (more detailed analysis of these as well as some other interpolations was given in \([4]\), with respect to element accuracy). The proposed formulation is indeed objective (strain-independent), however it is less robust (ie. it cannot converge unless the load or displacement is applied in small increments) than its non-objective counterpart. Considering that the formulation of Jelenić and Crisfield is more robust than the iterative formulation of Simo and Vu-Quoc \([5]\), we assumed that this analogy (like many others) will hold. Our guess is that the cause of this is numerical instability of the coefficients \((3), (4)\) appearing only in the 6D generalised shape functions.

3. Numerical analysis of \( \zeta_1 \) and \( \zeta_2 \)

During the Newton-Raphson solution procedure, the nodal displacement increments and spin vectors (iterative) approach zero with quadratic convergence. Consequently, the argument of all trigonometric coefficients \((1)-(4)\) approaches zero, which means that their values should approach their respective limits, \( \lim_{\psi \to 0} \zeta_1 = \frac{1}{90} \approx 0.01111 \) and \( \lim_{\psi \to 0} \zeta_2 = \frac{1}{630} \approx 0.00158730 \), which is demonstrated in Figure 1. When evaluating \( \zeta_1 \) and \( \zeta_2 \) for \( \psi \in [-0.1, 0.1] \) spurious results are obtained as shown in Figure 2. It is worth noting, though, that smooth graphs may be obtained by increasing \$WorkingPrecision\ variable to 100 (all computations were executed using \textit{Wolfram Mathematica}). However, our idea is to see would it be possible to get smooth results without manually changing the precision settings, which is not as straightforward in other programming languages. Setting the computing precision to 16, 20 and 50 digits respectively, we evaluate \( \zeta_1 \) and \( \zeta_2 \) (see Tables 1 and 2). We also evaluate \( \zeta_1 \) and \( \zeta_2 \), the first six terms of Taylor series expansion for \( \zeta_1 \) and \( \zeta_2 \) using default precision.

225
Figure 1: Plots of $\zeta_1$ and $\zeta_2$, $\psi \in [-10, 10]$

Figure 2: Plots of $\zeta_1$ and $\zeta_2$, $\psi \in [-0.1, 0.1]$ using default computing precision

Table 1: Numerical results for $\zeta_1(10^{-i})$ obtained using 16, 20 and 50 digit computation precision compared to $\overline{\zeta_1}$

<table>
<thead>
<tr>
<th>i</th>
<th>16</th>
<th>20</th>
<th>50</th>
<th>$\overline{\zeta_1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.010528935</td>
<td>0.010528935</td>
<td>0.010528935</td>
<td>0.010528935</td>
</tr>
<tr>
<td>1</td>
<td>0.011105159</td>
<td>0.01110516</td>
<td>0.01110516</td>
<td>0.01110516</td>
</tr>
<tr>
<td>2</td>
<td>0.010657491</td>
<td>0.011111052</td>
<td>0.011111052</td>
<td>0.011111052</td>
</tr>
<tr>
<td>3</td>
<td>32.64549682</td>
<td>0</td>
<td>0.011111111</td>
<td>0.011111111</td>
</tr>
<tr>
<td>4</td>
<td>-220540221.5</td>
<td>0</td>
<td>0.011111111</td>
<td>0.011111111</td>
</tr>
<tr>
<td>5</td>
<td>4.13785E+13</td>
<td>0</td>
<td>0.011111111</td>
<td>0.011111111</td>
</tr>
<tr>
<td>6</td>
<td>4.44503E+20</td>
<td>0</td>
<td>0.011111111</td>
<td>0.011111111</td>
</tr>
<tr>
<td>7</td>
<td>-2.62008E+26</td>
<td>0</td>
<td>0.011111111</td>
<td>0.011111111</td>
</tr>
<tr>
<td>8</td>
<td>-5E+32</td>
<td>0</td>
<td>0</td>
<td>0.011111111</td>
</tr>
<tr>
<td>9</td>
<td>-5E+36</td>
<td>0</td>
<td>0</td>
<td>0.011111111</td>
</tr>
</tbody>
</table>
Table 2: Numerical results for $\zeta_2(10^{-i})$ obtained using 16, 20 and 50 digit computation precision compared $\zeta_2$

<table>
<thead>
<tr>
<th>$i$</th>
<th>16</th>
<th>20</th>
<th>50</th>
<th>$\zeta_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.001522354</td>
<td>0.001522354</td>
<td>0.001522354</td>
<td>0.001522354</td>
</tr>
<tr>
<td>1</td>
<td>0.00158664</td>
<td>0.00158664</td>
<td>0.00158664</td>
<td>0.00158664</td>
</tr>
<tr>
<td>2</td>
<td>0.002775558</td>
<td>0.001587295</td>
<td>0.001587295</td>
<td>0.001587295</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>0.001587302</td>
<td>0.001587302</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>0</td>
<td>0.001587302</td>
<td>0.001587302</td>
</tr>
<tr>
<td>5</td>
<td>2.71051E+15</td>
<td>0</td>
<td>0.001587302</td>
<td>0.001587302</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>0</td>
<td>0.001587302</td>
<td>0.001587302</td>
</tr>
<tr>
<td>7</td>
<td>2.11758E+27</td>
<td>0</td>
<td>0.001587302</td>
<td>0.001587302</td>
</tr>
<tr>
<td>8</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.001587302</td>
</tr>
<tr>
<td>9</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.001587302</td>
</tr>
</tbody>
</table>

4. Conclusions

The numerical instability of trigonometric coefficients $\zeta_1$ and $\zeta_2$ was demonstrated. As their argument approaches zero, the values of these functions do not approach their respective limits. If using double precision floating point computation, we are not able to compute (sufficiently) exact results for arguments smaller than 0.1. Increasing the computational precision in Wolfram Mathematica we can get better results. We propose using the first six terms of the Taylor series expansions instead when argument is smaller than 0.1. In this way, there is no need for adjusting the computing accuracy and the code may be used even for programming languages where precision setting is not as straightforward as in Wolfram Mathematica.

Acknowledgements

Research resulting with this paper was made within the scientific project No 1631: “Configuration-dependent approximation in non-linear finite-element analysis of structures” financially supported by the Croatian Science Foundation.

References


An adapted artificial compressibility algorithm for nearly and truly incompressible large strain solid dynamics

*Osama I. Hassan¹, Antonio J. Gil¹, Chun Hean Lee¹, F. Auricchio² and Javier Bonet³

¹Zienkiewicz Centre for Computational Engineering, College of Engineering, Swansea University
Bay Campus, SA1 8EN, United Kingdom
²Department of Civil Engineering and Architecture (DICAR), Università di Pavia, Via Ferrata 1, 27100 Pavia, Italy
³University of Greenwich, London, SE10 9LS, United Kingdom

*o.i.i.hassan@swansea.ac.uk

ABSTRACT

This paper presents an adapted artificial compressibility algorithm for large strain problems in the field of computational solid dynamics. The proposed methodology builds on a recent Updated Lagrangian framework presented by the authors, by introducing an efficient iterative algorithm aiming at extending the range of applications to nearly and truly incompressible materials. The well-known artificial compressibility method is adapted by adding pseudo time derivative terms to the conservation laws and the solution is advanced in pseudo time. The algorithm proves very useful in problems with Poisson’s ratio approaching the incompressibility limit (i.e. \( \nu \approx 0.5 \)) where typically the time step would be severely restricted in a purely explicit scheme. A series of numerical examples are presented in order to assess the robustness and the applicability of the proposed framework.

Key Words: finite volume; upwind; artificial compressibility; locking

1. Introduction

Current commercial codes (e.g. PAM-CRASH, ANSYS AUTODYN, LS-DYNA, ABAQUS) used in industry for the simulation of large-scale solid mechanics problems are typically based on the use of classical low-order finite element displacement-based formulations. However, these formulations present a number of shortcomings, namely, (1) reduced order of convergence for strains and stresses in comparison with displacements; (2) high-frequency noise in the vicinity of shocks or sharp spatial gradients; and (3) numerical instabilities associated with shear locking, volumetric locking and pressure checker-boarding. To circumvent these drawbacks, a system of first order hyperbolic conservation laws for large strain solid dynamics was introduced [1, 2, 4]. Essentially, the formulation was established in terms of the linear momentum and the deformation gradient tensor written in a Total Lagrangian formalism. The mixed-based system can be alternatively expressed in the Updated Lagrangian framework. This paper introduces an adapted artificial compressibility algorithm widely used in the field of CFD with the purpose of increasing the computational efficiency of the framework and handling truly incompressible materials.

2. Governing equations

In this section, the motion of a continuum body is considered. The body assumes an initial reference configuration at time \( t = 0 \) and occupies a volume denoted as \( \Omega_0 \). As the body undergoes a deformation process it occupies a volume \( \Omega \) in the deformed configuration. The motion of a body is governed by the following set of \( p \cdot F \cdot J \) mixed-based system expressed in terms of Updated Lagrangian formalism [3]:

\[
\frac{d}{dt} \int_{\Omega_0} p \, d\Omega_0 = \int_{\partial \Omega} t \, da + \int_{\Omega} f \, d\Omega; \tag{1a}
\]

\[
\frac{d}{dt} \int_{\Omega_0} F \, d\Omega_0 = \int_{\partial \Omega} \left( \frac{p}{\rho_0} \otimes H^{-1} \right) n \, da; \tag{1b}
\]

\[
\frac{d}{dt} \int_{\Omega_0} J \, d\Omega_0 = \int_{\partial \Omega} \frac{p}{\rho_0} \cdot n \, da; \tag{1c}
\]
where \( p := \rho_0 v \) is the linear momentum, \( \rho_0 \) is the material density, \( v \) is the velocity field, \( f \) is the body force per unit current volume, \( F \) is the deformation gradient (or fibre map), \( H := J F^{-T} \) is the cofactor of the deformation gradient (or area map), \( J \) is the Jacobian of the deformation (or volume map) and \( t \) represents the nominal traction related through the Cauchy stress tensor \( \sigma \) and the spatial unit outward normal vector \( n \). For closure, appropriate initial and boundary conditions, as well as a constitutive model, are supplemented.

3. Finite volume spatial discretisation

The set of hyperbolic conservation laws (1) is spatially-discretised using the vertex–centred finite volume method. Specifically, the use of Upwind Riemann solver introduces sufficient (consistent) numerical viscosity to the mixed-based system. This can be achieved by making use of the Rankine-Hugoniot jump conditions, which gives the following:

\[
\Omega_0^a \frac{dp_a}{dt} = \sum_{b \in \Lambda_a} t_C ||c_{ab}|| + \sum_{\gamma \in \Gamma_a^\alpha} \frac{1}{\rho_0} \left( p_a \otimes p_b \right) + \frac{1}{\rho_0} \left( p_a^\gamma \otimes N^\gamma \right) \frac{A^\gamma}{3}; \quad (2a)
\]

\[
\Omega_0^a \frac{dF_a}{dt} = \sum_{b \in \Lambda_a} \frac{1}{2\rho_0} \left( p_a + p_b \right) \otimes C_{ab} + \sum_{\gamma \in \Gamma_a^\alpha} \frac{1}{\rho_0} \left( p_a^\gamma \otimes N^\gamma \right) \frac{A^\gamma}{3}; \quad (2b)
\]

\[
\Omega_0^a \frac{dJ_a}{dt} = \sum_{b \in \Lambda_a} \frac{1}{\rho_0} p_C \cdot c_{ab} + \sum_{\gamma \in \Gamma_a^\alpha} \frac{1}{\rho_0} p_a^\gamma \cdot n \frac{a^\gamma}{3}; \quad (2c)
\]

where

\[
t_C = \frac{1}{2} \left( \sigma^- + \sigma^+ \right) n + \frac{1}{2} \left[ \frac{1}{c_p} (n \otimes n)(\sigma^+ - \sigma^-) n + \frac{1}{c_s} (I - n \otimes n)(\sigma^+ - \sigma^-) n \right] ; \quad (3a)
\]

\[
p_C = \frac{1}{2} (p^+ + p^-) + \frac{1}{2c_p} (\sigma^+ - \sigma^-) n; \quad \sigma_{\text{dev}} = \sigma_{\text{dev}}^+ + k(J_{\text{dev}} - 1)I. \quad (3b)
\]

Here, \( \sigma_{\text{dev}} \) is the deviatoric part of the stress tensor, \( k \) is the bulk modulus of the material and \( c_p, c_s \) are the volumetric and the shear wave speeds respectively. The above equations are integrated from time step \( t^n \) to \( t^{n+1} \) using an explicit one-step two-stage Total Variation Diminishing Runge Kutta (TVD-RK) time integrator [2] for its excellent TVD properties. The conservation of angular momentum is guaranteed through the use of Lagrange multiplier method as described in [4].

4. The artificial compressibility scheme

Alternatively, expression (1c) can also be expressed in terms of the pressure, \( p \):

\[
\frac{1}{\kappa} \frac{d}{dt} \int_{\Omega_0} p \, d\Omega_0 = \int_{\partial\Omega} \frac{p}{\rho_0} \cdot n \, da. \quad (4)
\]

The above equations (1a), (1b) and (4) could then be solved via a predictor-corrector algorithm. The conservation variables are first predicted based on the shear modulus of the material, \( \mu \):

\[
p^+ = p^n + \Delta t \left( J_x \nabla \cdot \sigma(F^n) \right); \quad (5a)
\]

\[
F^+ = F^n + \Delta t \left( \frac{p^n}{\rho_0} \right) \nabla \cdot (\frac{p^n}{\rho_0}); \quad (5b)
\]

\[
p^+ = p^n + \Delta t \mu J_x \nabla \cdot (\frac{p^n}{\rho_0}). \quad (5c)
\]
For the satisfaction of incompressibility constraints, the above predicted variables will then be projected through an iterative algorithm. The iterative projection is given as follows:

\[
p_{k+1}^{n+1} = \frac{1}{1 + 2r} \left( p_{k}^{n+1} + r \Delta t J_{x} \left[ \nabla \cdot \sigma' (F^{*}) + \nabla \cdot p_{k}^{n+1} I \right] + r \left( p^{n} + p^{*} \right) \right); \tag{6a}
\]

\[
F^{n+1} = \frac{1}{2} \left[ F^{n} + F^{*} + \Delta t \nabla_{0} \left( \frac{p_{k}}{\rho_{0}} \right) \right]; \tag{6b}
\]

\[
p_{k+1}^{n+1} = \frac{1}{1 + 2r \beta} \left( p_{k}^{n+1} + r \beta \Delta t J_{x} \nabla \cdot \left( \frac{p_{k}^{n+1}}{\rho_{0}} \right) + \frac{r \beta}{\kappa} \left( p^{n} + p^{*} \right) \right). \tag{6c}
\]

where \( \beta \) is an artificial compressibility parameter, and \( r \) is the ratio between a pseudo time step and the physical time step.

5. Numerical examples

This section presents a series of numerical examples in order to assess the validity of the proposed algorithm. The material is modelled as a hyperelastic neo-Hookean material with Young's modulus \( E = 1.7 \times 10^7 \) Pa, and density \( \rho_0 = 1.1 \times 10^3 \) kg/m\(^3\). In order to show the robustness of the proposed algorithm, a short column with a unit square cross section is subjected to an angular velocity field \( \omega = \left[ 0, \Omega \sin(\pi Z/2L), 0 \right] \) where \( \Omega = 105 \) rad/s and \( L = 6 \) m. The problem has been solved using a library of in-house numerical methodologies (Figure 1). The Poisson’s ratio is taken to be \( \nu = 0.495 \). The results show a smooth pressure distribution and excellent agreement with other schemes.

The same column is subjected to an initial diagonal velocity along its height given by \( v_0 = \frac{V Z}{L} \left[ \frac{\sqrt{3}}{2}, 1/2, 0 \right] \) where \( V = 10 \) m/s. Figure 2 shows a comparison between the results obtained using the proposed artificial compressibility algorithm, the Total Lagrangian explicit solver [4] and the Updated Lagrangian explicit solver [3]. For benchmarking purposes, the Poisson’s ratio is limited to a value of \( \nu = 0.495 \) as it will be very inefficient to solve problems with higher \( \nu \) using an explicit scheme due to the stability limitation on the time step. For a truly incompressible material, Figure 3 shows the results obtained using \( \nu = 0.5 \). All examples show a smooth pressure distribution throughout the computational domain with absence of volumetric locking or spurious pressure modes.

![Figure 1: Twisting column example, (a) SUPG-SPH (refined); (b) artificial compressibility; (c) SUPG-SPH; (d) JST SPH; (e) PG-FEM; (f) TOUCH; (g) B-bar; and (h) Q2-Q1.](image-url)

6. Conclusion

This paper introduced a second order Updated Lagrangian vertex-centred finite volume algorithm for the numerical simulation of large strain solid dynamics for nearly and truly incompressible materials. A mixed formulation written in the form of a system of first order hyperbolic equations is employed. The linear momentum \( p \), the deformation gradient \( F \) and the pressure \( p \) are regarded as primary conservation
Figure 2: A bending column example, pressure field at $t = 0.5 \text{s}$. (a) Total Lagrangian [4], (b) Updated Lagrangian [3], (c) artificial compressibility.

Figure 3: A bending column example simulated within truly incompressible regime.

variables. For computational efficiency, the artificial compressibility algorithm extensively used in the CFD community is adapted. The algorithm has proved ideal when extending the range of applications to nearly (and truly) incompressibility limit. The overall scheme shows excellent behaviour in bending dominated scenarios and highly nonlinear deformations without spurious pressure oscillations, yielding a second order of convergence for velocities and stresses.

Acknowledgements

The first author gratefully acknowledge the financial support provided by the Erasmus Mundus Program (SEED). The second, third and fifth authors gratefully acknowledge the financial support provided by the Ser Cymru National Research Network for Advanced Engineering and Materials.

References


231
The point collocation method with a local maximum entropy approach

*Lei Fan1, Charles E. Augarde1 and William M. Coombs1

1School of Engineering and Computing Sciences, Durham University, South Road, Durham, DH1 3LE

*lei.fan@durham.ac.uk

ABSTRACT

Point collocation methods (PCMs) are truly meshless, strong form-based methods which present some attractive features as compared to the weak form-based meshless methods. In PCMs, no integration is required and no background mesh is needed which makes these methods straightforward to implement. However, difficulties are experienced in dealing with the imposition of boundary conditions and the calculation of higher derivatives of RKPM shape functions which is complex and time-consuming. In this paper, a new PCM with local maximum entropy (max-ent) shape functions is developed for modelling solid mechanics problems. The proposed max-ent PCM achieves higher accuracy on boundaries than a previous approach. In addition, the calculation of higher derivatives of the shape functions is more computationally efficient.

Key Words: Meshless methods; point collocation method; maximum entropy shape functions.

1. Introduction

Meshless methods have been investigated to approximate solutions for many engineering problems which are described by a set of PDEs. The approximation schemes, including smoothed particle hydrodynamics (SPH) [1], moving least squares (MLS) [2], the reproducing kernel particle method (RKPM) [3] and the element-free Galerkin method (EFGM) [4] overcome difficulties that exist in mesh-based numerical methods and are a promising alternative for solid mechanics problems. However, these weak form methods require a background grid for domain integration. Accurate integration requires the generation of Gauss points and the inversion of a matrix-term in the shape functions [3] which increase substantially computational burdens and complexities. In an attempt to avoid the disadvantages of the weak form meshless methods, strong form PCMs were proposed as truly meshless methods [5]. To date, strong form collocation frameworks have been applied for solving PDEs using shape functions obtained by the RKPM [6]. The classical PCMs are straightforward to implement. However, the numerical results sometimes suffer from instability and accuracy issues. In this work, local max-ent shape functions [7, 8] are combined with the PCM to improve the performance of PCMs.

2. Point collocation methods

In PCMs, a given problem domain and boundaries are defined by collocation points and source points separately. The collocation points are distributed to enforce the governing PDE which is satisfied at each collocation point. The surrounding source points, which fall in the local support domain of each collocation point, are used for the construction of the shape functions and determine the approximation of the solution. The governing PDE and the boundary conditions are described as

\[ L u = f_b \text{ in } \Omega, \quad L_u u = g \text{ on } \Gamma_u, \quad L_t u = h \text{ on } \Gamma_t, \] (1)

where \( L \) is the differential operator in a problem domain \( \Omega \), \( L_u \) and \( L_t \) are the boundary differential operators, respectively. \( u \) is the displacement at source points, \( f_b \) is the body force at collocation points, \( g \) is the prescribed displacement on Dirichlet boundaries \( \Gamma_u \) and \( h \) denotes the known traction on Neumann boundaries \( \Gamma_t \). It is simple to implement, leading to a discrete set of equations based at distinct collocation points. Then the final linear collocation equations are written as

\[ K_{ij} u_i = f_j, \] (2)
in which $i$ is a source point in the support domain $i = 1, 2, \ldots, N_s$ and $j$ is a collocation point $j = 1, 2, \ldots, N_c$.

The least square method is employed to solve the over-determined system obtained as $N_s \leq N_c$.

Here, local max-ent schemes are adopted to construct shape functions which possess several attractive properties such as the Kronecker delta property at the boundaries, non-negativity and satisfaction of reproducing conditions [11]. The local max-ent shape function at the $i$th collocation point is given as

$$
\phi_i(x) = \frac{w_i e^{-\lambda_i |x - x_i|}}{\sum_{i=1}^{N_s} w_i e^{-\lambda_i |x - x_i|}},
$$

where $w_i$ is a weight function to control the locality of the shape functions, $\lambda_i$ is a Lagrange multiplier which can be found by Newton’s method as $\lambda_i(x) = \arg \min \log(w_i e^{-\lambda_i |x - x_i|})$. The first and second derivatives of the max-ent shape functions [10] can be expressed as

$$
\nabla \phi_i = \phi_i \{ (x_i - x)^T [H^{-1} - H^{-1} \sum_{k=1}^{n} \frac{\phi_k}{w_k} (x_k - x) \otimes \nabla w_k] + \frac{\nabla w_i}{w_i} - \sum_{j=1}^{n} \phi_j \frac{\nabla w_j}{w_j} \}
$$

$$
\nabla \nabla \phi_i = \frac{\nabla \phi_i \otimes \nabla \phi_i}{\phi_i} + \phi_i \{ -H^{-1} + (x_i - x) \cdot \nabla H^{-1} + \left[ \sum_{k=1}^{n} \frac{\phi_k}{w_k} (x_k - x) \otimes \nabla w_k \right]^T H^{-1} \}
$$

$$
- \phi_i \{ (x_i - x) \cdot \nabla H^{-1} \left[ \sum_{k=1}^{n} \frac{\phi_k}{w_k} (x_k - x) \otimes \nabla w_k \right] + (x_i - x)^T H^{-1} \cdot \nabla \left[ \sum_{k=1}^{n} \frac{\phi_k}{w_k} (x_k - x) \otimes \nabla w_k \right] \}
$$

$$
+ \phi_i \left\{ \nabla \left( \frac{\nabla w_i}{w_i} \right) - \sum_{j=1}^{n} \frac{\nabla w_j}{w_j} \otimes \nabla \phi_j - \sum_{j=1}^{n} \phi_j \nabla \left( \frac{\nabla w_j}{w_j} \right) \right\}
$$

where $H$ is the Hessian matrix given by

$$
H = \sum_{k=1}^{n} (x_k - x) \otimes (x_k - x) \otimes \phi_k,
$$

and $\otimes$ is the dyadic product of two vectors.

3. Numerical results

For the first example, a 2D Poisson problem with Dirichlet boundary conditions is simulated over a unit square domain using the max-ent PCM and reproducing kernel collocation method (RKCM) to approximate the solution. The governing equation and corresponding Dirichlet boundary conditions are applied on the four edges given as

$$
\nabla u(x, y) = 4, \ \Omega \in (0, 1) \times (0, 1)
$$

and $u_{x=0} = y^2, u_{x=2} = 1 + y^2, u_{y=0} = x^2, u_{y=2} = x^2 + 1$. with the theoretical solution

$$
u(x, y) = x^2 + y^2, \ \Omega \in (0, 1) \times (0, 1).$$
{12 × 12} collocation points and {11 × 11} source points are distributed in the domain and at the boundaries uniformly as shown in Figure 2 and the least square method is employed to solve the linear system. It is worth noting that setting $N_c = N_s$ may lead to less accuracy for the second derivatives of shape functions. The convergence rates using both max-ent PCM and RKCM are demonstrated for different refinements in Figure 3.

![Figure 2: The discretisation of the Poisson problem.](image1)

**Figure 2:** The discretisation of the Poisson problem.

![Figure 3: Convergence rates of the Poisson problem.](image2)

**Figure 3:** Convergence rates of the Poisson problem.

It is clear that the max-ent PCM is more accurate, with a higher rate of convergence as compared to the equivalent RKCM. Here in the RKCM, the $L_2$ norm accounts for the residual of the differential equation in the domain, and at the boundaries, respectively. However, it is unnecessary to consider the $L_2$ norm at the boundaries in the max-ent PCM since the max-ent shape functions satisfy the Kronecker-delta property at the boundaries. As such, the residual is less in the max-ent PCM than RKCM that max-ent PCM presents better performance than RKCM. Table 1 records the CPU time for the two methods.

<table>
<thead>
<tr>
<th>$N_s$</th>
<th>CPU time with max-ent PCM (s)</th>
<th>CPU time with RKCM (s)</th>
<th>Speed up</th>
</tr>
</thead>
<tbody>
<tr>
<td>121</td>
<td>0.058</td>
<td>0.154</td>
<td>3</td>
</tr>
<tr>
<td>441</td>
<td>0.139</td>
<td>0.854</td>
<td>6</td>
</tr>
<tr>
<td>1681</td>
<td>2.398</td>
<td>32.104</td>
<td>13</td>
</tr>
<tr>
<td>2601</td>
<td>9.851</td>
<td>117.594</td>
<td>12</td>
</tr>
</tbody>
</table>

**Table 1:** The CPU time of the max-ent PCM and RKCM.

The second problem is a confined elastic domain subjected to Dirichlet roller boundaries on three sides and an imposed displacement on the fourth (Figure 4).

![Figure 4: Elastic problem model (2).](image3)

**Figure 4:** Elastic problem model (2).

In this model the over-determined linear system is generated by uniformly scattered collocation and source
The $L_2$ norm errors in displacement for different refinements were calculated to demonstrate the convergence rate. It can be seen in Figure 5 that once again the proposed method performs better than the RKCM by comparison of convergence rates. The CPU times of the max-ent PCM and RKCM are shown in Table 2 showing that max-ent PCM is more efficient than RPCM with the same discretization, achieving a lower error for the same number of points and at a lower run time.

<table>
<thead>
<tr>
<th>$N_t$</th>
<th>CPU time with max-ent PCM (s)</th>
<th>CPU time with RKCM (s)</th>
<th>Speed up</th>
</tr>
</thead>
<tbody>
<tr>
<td>121</td>
<td>0.035</td>
<td>1.038</td>
<td>30</td>
</tr>
<tr>
<td>441</td>
<td>0.256</td>
<td>3.916</td>
<td>15</td>
</tr>
<tr>
<td>1681</td>
<td>15.878</td>
<td>53.323</td>
<td>3</td>
</tr>
<tr>
<td>2601</td>
<td>56.613</td>
<td>119.235</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 2: The CPU time of the max-ent PCM and RKCM.

4. Conclusions
A novel PCM using the local max-ent shape functions is proposed to model solid mechanics problems in this paper. The proposed method and previous RKCM are applied on a $2D$ Poisson problem and a simple elasticity problem to validate the efficiency of the max-ent PCM by the comparison of convergence rates and run times.

Acknowledgements
This work has been sponsored by the China Scholarship Council (CSC) and the School of Engineering and Computing Sciences, Durham University.

References
An accelerated black-box Fast Multipole Isogeometric Boundary Element Method for 3D elasticity

*J. Trevelyan¹ and S. Li²

¹School of Engineering and Computing Sciences, Durham University, South Road, DH1 3LE, Durham, UK
²College of Aerospace Science & Engineering, National University of Defence Technology, Changsha, China

jon.trevelyan@durham.ac.uk

ABSTRACT

The isogeometric approach in computational modelling of elasticity makes use of NURBS splines both to describe the geometry and to discretise the displacement field. Because of its boundary-only modelling, with no requirement for a volumetric NURBS definition, the Boundary Element Method is an ideal and natural choice for the isogeometric analysis of solids in 3D. Such analysis has been abbreviated IGABEM. Recently, Simpson and Liu [1] presented an IGABEM scheme accelerated by a black-box Fast Multipole Method (bbFMM) for the solution of the Helmholtz equation. We note that the bbFMM (Fong and Darve [2]) is an approach to the FMM that does not rely on multipole expansions specific to particular kernels, and instead relies upon Chebyshev interpolation to describe the far-field behaviour of any arbitrary kernel.

One computational bottleneck in the bbFMM lies in the description of the so-called multipole-to-local (M2L) operators. This step involves computing the far-field contribution at the Chebyshev nodes for all FMM cells in the interaction list of each cell at each level. In [2] and other bbFMM works, this stage is accelerated by a Singular Value Decomposition (SVD) to compress the low-rank approximation. We present an improvement to the process by replacing the SVD compression by an alternative based on the Proper Generalised Decomposition (PGD) [3]. The accuracy of the final elastostatic solution is not significantly affected by the compression.

Analysis of the computational performance shows the bbFMM to reduce the complexity of IGABEM from $O(n^2)$ to $O(n)$ and the PGD to provide improvements over SVD. For smaller problems, the use of PGD to compress the M2L operation effectively offsets the overheads involved in using FMM.

Key Words: boundary elements, isogeometric, fast multipole, PGD

1. Introduction

Since the seminal paper of Hughes et al [4] researchers have repeatedly demonstrated the benefits of Isogeometric analysis over the use of conventional finite element approaches. The use of Non-Uniform Rational B-splines (NURBS) in preference to piecewise polynomial shape functions simultaneously simplifies the integration of analysis within CAD systems, largely overcomes the difficulties of mesh refinement, and improves the convergence behaviour of the approximations. While the benefits of this approach are amply demonstrated in a finite element context, it can clearly be seen that applying isogeometric concepts to boundary element formulations is a natural development. Since CAD models are likely to be stored as boundary representations, using NURBS surfaces, the use of IGAFEM for the analysis of solids will require a volumetric NURBS representation to be built, and this is far from straightforward. In contrast the boundary-only formulation of the BEM is an ideal complement to the NURBS philosophy since it can proceed with the analysis directly from the boundary representation.

It is well known that the system matrix in the BEM is dense and unsymmetric leading to some computational demands. Some popular techniques have been successfully developed to accelerate BEM schemes, notably the Fast Multipole Method (FMM) [5] and Adaptive Cross Approximation (ACA) [6]. Here we focus on the FMM. Classically the FMM relies on multipole expansions of PDE-specific kernels, but more recently the bbFMM [2] was developed to provide a more general, kernel-independent technique for matrix compression with a fast algorithm based on Chebyshev interpolations.
A major contributor to the cost of the bbFMM scheme is the construction of the so-called M2L operators, which are calculated using a Singular Value Decomposition (SVD). In the current paper, we replace the SVD with a Proper Generalised Decomposition (PGD), reducing the computational effort from $O(mn^2)$ to $O(2mn)$ for an $m \times n$ system.

2. IGABEM formulation

We start with the classical, direct collocation BEM using the boundary integral equation

$$\begin{align*}
C(s)u(s) + \int_{\Gamma} T(s, x)u(x)d\Gamma(x) &= \int_{\Gamma} U(s, x)t(x)d\Gamma(x),
\end{align*}$$

where $s \in \Gamma$ denotes the source point and $x \in \Gamma$ the field point, $u \in \mathbb{R}^3$ the displacement field, $t \in \mathbb{R}^3$ the traction field, $U(s, x) = [U_{ij}]$ the displacement fundamental solutions kernel, $T(s, x) = [T_{ij}]$ the traction fundamental solutions kernel, $C(s) = [C_{ij}]$ the jump term, $\bar{u}_i$ and $\bar{t}_i$ the prescribed displacements and tractions, $i$ and $j$ the indices running from 1 to 3 in three dimensions and $\tilde{f}$ denotes an integral taken in the Cauchy Principal Value (CPV) sense. The problem is solved subject to a combination of Dirichlet and Neumann boundary conditions appropriate for the problem at hand.

We expand the displacement and traction vectors in a set of NURBS basis functions, $R_{ea}(\tilde{\xi})$ and discretise the BIE (1), leading to the form

$$\begin{align*}
C(e) R_{ea_0}(\tilde{\xi}_{ea_0}) \bar{u}_{ea_0} + \sum_{e=1}^{n_e} \int_{\Gamma_e} T(\tilde{\xi}_e, \tilde{\xi}) \sum_{a=1}^{n_a} R_{ea}(\tilde{\xi}) \bar{u}_{ea} J_e(\tilde{\xi}) d\tilde{\xi} &= \sum_{e=1}^{n_e} \int_{\Gamma_e} U(\tilde{\xi}_e, \tilde{\xi}) \sum_{a=1}^{n_a} R_{ea}(\tilde{\xi}) \bar{t}_{ea} J_e(\tilde{\xi}) d\tilde{\xi},
\end{align*}$$

2.1. bbFMM accelerated IGABEM with PGD

No details are given here of the bbFMM algorithm, but it is described by Fong & Darve [2] and has been successfully applied for Helmholtz problems in an IGABEM framework by Simpson [1]. It is important to recognise that the nodes are clustered in cells defined in a hierarchical tree structure, and the $O(n^2)$ problem of finding node-to-node interactions is replaced by a series of Chebyshev approximations of interactions between nodes in cells at different levels. A step of central importance is the Moment-to-Local (M2L) translation in which the interactions between cells at the same level are computed. This is a numerically intensive operation and one we now accelerate using a low rank approximation based on the Proper Generalised Decomposition (PGD).

The PGD [3] is based on a natural phenomenon that any data can be represented by a combination of the information in each direction, i.e. an arbitrary $d$-dimensional function may be written in the form

$$u(x_1, \ldots, x_d) = \sum_{i=1}^{n} f_i^1(x_1)f_i^2(x_2) \cdots f_i^d(x_d).$$

Specifically for the acceleration of the M2L process, we seek the low rank approximation $\tilde{K}(\bar{s}, \bar{x})$ to the kernel matrix $K(\bar{s}, \bar{x})$ that contains the kernels relating a source point $\bar{s}$ and field point $\bar{x}$ in different cells.
Figure 1: CPU time for computation of M2L operators

at the same level. We use an iterative procedure to give progressively improving approximations, the \( k \)th approximation being

\[
\tilde{K}^k(\bar{s}, \bar{x}) = \tilde{K}^{k-1}(\bar{s}, \bar{x}) + S_k(\bar{s}) \circ X_k(\bar{x})
\]

\[= \sum_{i=1}^{k-1} S_i(\bar{s}) \circ X_i(\bar{x}) + S_k(\bar{s}) \circ X_k(\bar{x}), \tag{4}\]

where the operator \( \circ \) denotes a Hadamard product, and the functions \( S_k(\bar{s}) \) and \( X_k(\bar{x}) \) are the only unknowns. In order to solve this non-linear problem, an alternating direction scheme is used. An initial guess can always be made to generate the first approximation, \( \tilde{K}^1(\bar{s}, \bar{x}) \), based on the essential \( 1/r^2 \) and \( 1/r \) behaviour, respectively, of the \( T \) and \( U \) kernels. A suitable stopping criterion is given as:

\[
\tilde{\epsilon}(P) > \frac{||S^{P}_{k}(\bar{s}) \circ X^{P}_{k}(\bar{x}) - S^{P}_{k-1}(\bar{s}) \circ X^{P}_{k-1}(\bar{x})||}{||S^{P}_{k}(\bar{s}) \circ X^{P}_{k}(\bar{x})||}, \tag{5}\]

where the \( ||\cdot|| \) is the \( L^2 \)-norm and \( \tilde{\epsilon}(P) \) is a suitable threshold value. After some enrichment steps, the PGD process will stop once the following criterion is satisfied (with suitable threshold \( \epsilon(k) \)):

\[
\epsilon(k) > \frac{||S_{1}(\bar{s}) \circ X_{1}(\bar{x})||}{||S_{1}(\bar{s}) \circ X_{1}(\bar{x})||}, \tag{6}\]

3. Results

In Figure 1 we display a comparison of the CPU time requirements for the SVD and PGD approaches in constructing the M2L operators. It can be seen that, once a problem size of around 100 DOF is reached, the PGD exhibits \( O(n^2) \) complexity while the SVD exhibits \( O(n^3) \) for the computation of the M2L process. This is a significant improvement that improves the overall run-time, as demonstrated in Figure 2 for a generic elasticity problem. A knot insertion algorithm is used to increase the number of degrees of freedom, and the run-time is shown. All the codes were executed on a 2.80GHz quadcore processor with 8 parallel threads. The figure clearly shows the use of the FMM to give \( O(n) \) complexity, in comparison with \( O(n^2) \) for conventional IGABEM, and also that the PGD acceleration has particular benefits, effectively offsetting the overheads of using the FMM, for smaller models. In this way the \( O(n) \) behaviour applies for the entire range of problem sizes, though it should be noted that for larger problems there may be expected to be some departure from this since the M2L operator requires \( O(n^2) \) operations and the linear solver will require at least this; however, for the problem sizes tested (up to over 100,000 DOF) this departure is not yet apparent.
4. Conclusions

An IGABEM algorithm has been accelerated with the bbFMM for problems of linear elasticity in 3D solids. A low-rank approximation to the Moment-to-Local operators has been produced using Proper Generalised Decomposition in preference to the Singular Value Decomposition. This reduces the complexity of the M2L construction from $O(n^3)$ to $O(n^2)$. The performance of the IGABEM scheme is enhanced across the range of model sizes tested, so that the method becomes a highly promising approach for the efficient and accurate stress analysis of solids.

References


ON THE IMPLEMENTATION OF GRADIENT PLASTICITY WITH THE MATERIAL POINT METHOD

*T.J. Charlton, W.M. Coombs and C.E. Augarde

Mechanics Research Group, School of Engineering and Computing Sciences, Durham University, Durham, DH1 3LE

*t.j.charlton@durham.ac.uk

ABSTRACT

The Material Point Method (MPM) is a computational method which allows solid mechanics problems to be modelled using material points which move through a fixed background grid. State variables are stored at these material points and tracked throughout the simulation. The MPM is ideal for modelling geomechanics problems that require the ability to capture large deformations and non-linear material behaviour. A well documented grid crossing error exists in the MPM which occurs when material points move between grid elements. The Generalised Interpolation Material Point (GIMP) method was proposed to alleviate this problem [2]. An implicit implementation of the GIMP method is used in this work.

Conventional analysis techniques constructed in terms of stress and strain are able to handle large deformations well, however they are unable to deal with structural instabilities such as shear banding. Because there is no measure relating to the microstructure of the analysed material, the width of a shear band is highly mesh dependent. Gradient theories enrich these conventional theories with the addition of higher-order terms to include a length scale. Using gradient methods it is possible to model a shear band with a finite thickness without it being mesh dependent. Although there has been lots of work on gradient theories within the Finite Element Method (FEM) it is an area which has received less attention in the MPM.

In this work an existing gradient elasto-plasticity theory [4], used with the FEM, is applied to the GIMP method. The MPM and GIMP method are first introduced and the key equations that are required to include gradient elasto-plasticity are detailed. The effect of introducing a length scale is then demonstrated in a numerical example.

Key Words: Material Point Method; Gradient Elasto-plasticity; GIMP

1. Introduction to the Material Point Method

The Material Point Method (MPM), first developed by Sulsky et al. [6], is a meshfree method in which calculations take place on a fixed background grid while material properties are carried by a set of material points. Within each loadstep the mesh deforms as in the Finite Element Method (FEM), however variables are then mapped to the material points and the grid is reset so that the material points move through the background grid elements. This allows problems to be modelled where mesh distortions due to large deformations would otherwise not be possible without re-meshing. When particles cross from one background grid element to another, a grid crossing instability occurs which has been well documented in the literature [5]. To remedy this, the Generalised Interpolation Material Point (GIMP) method [2] was introduced.

1.1. Generalised Interpolation Material Point method

In the standard MPM, the material points represent a mass of material but do not have a physical size. Linear shape functions are used for constructing the strain-displacement matrix and for mapping variables to and from the background grid. The GIMP method modifies material points in the MPM to each have an associated influence domain, and the standard FEM shape functions $N$ are replaced by weighting functions $S_{vp}$ where the subscript $v$ refers to vertices or grid nodes and $p$ refers to particles or material
points. These functions are constructed from the FEM shape functions and a particle characteristic function $\chi_p$ specifying the influence of the particle.

$$S_{vp} = \frac{1}{V_p} \int_{\Omega_p \cap \Omega} \chi_p(\xi)N_v(\xi)d\xi,$$

(1)

where $V_p$ is the particle volume (or length in 1D), $N_v$ are the standard linear shape functions, $\Omega$ is the physical domain and $\Omega_p$ is the influence domain of the particle. This results in an increased smoothness of shape functions between elements. To create GIMP shape functions in two or three dimensions, the tensor product of the one dimensional functions is taken. This change has been shown to significantly improve the stress response when compared to the MPM [2]. The GIMP method has been implemented by the author using a fully implicit approach using an updated Lagrangian framework. For brevity, only a short outline is given here.

A domain is discretised into a set of material points, these material points have influence domains which are initially defined in such a way that they cover the whole of the material with no gaps or overlaps. For both the MPM and GIMP method a regular mesh is used which covers not only the physical domain but also extends to where material is expected to move into during a simulation. It is possible to extend the grid during the simulation if the deformed configuration is not known.

When implementing the GIMP method rather than MPM it is important to take into account the fact that material point influence domains can overlap multiple elements. This means that nodes can be affected not only by material points in the same element, but also those in adjacent elements, increasing the connectivity in the global stiffness matrix. At the start of each loadstep the location of each material point with respect to the background grid must be determined, and from this the weighting functions can be computed. A regular background grid is often chosen to make this process less expensive. Grid elements that do not contain material point domains are also determined so that they can be removed from the calculation for the current loadstep. External forces on the material points are then incremented and mapped to the grid nodes. Displacements are calculated by solving in the same way as the FEM, which then allows the calculation of stresses at the material points. At the end of each loadstep, material point positions and domains are updated while the background grid remains unchanged.

2. Gradient elasto-plasticity

Gradient theories extend the classical elasticity equations to account for microstructure of a material in a way that is not considered by conventional analyses. This is done by considering higher order derivatives, usually of displacement or strain. The approach used in this work and described below follows that of de Borst and Muhlhaus [4].

Unlike conventional methods in computational elasto-plasticity, in this approach the plastic consistency parameter $\dot{\gamma}$ is treated as an independent unknown which is solved for at nodes in addition to the nodal displacements. Beginning from the weak form of equilibrium and the Kuhn-Tucker-Karush consistency conditions for plasticity it is possible to develop two equations, (2) and (3), in terms of $\{\Delta \gamma\}$ and $\{\Delta \varepsilon\}$ which can be calculated from nodal values as shown in (4). For a more detailed explanation of this derivation the reader is referred to [3] or [4].


(2)

and

$$-\int_V [h][f_{\sigma_\varepsilon}]^T[D^e][B]dv\{\Delta d\} + \int_V [h][f_{\sigma_\varepsilon}]^T[D^e][f_{\sigma_\varepsilon}][h]^Tdv\{\Delta \Lambda\} = \int_V [h]f(\sigma_n)dv.$$ (3)

where

$$\Delta \gamma = \{h\}^T\{\Delta \Lambda\} \quad \text{and} \quad \{\Delta \varepsilon\} = [B]\{\Delta d\}$$

(4)
where \( \{h\} \) are Hermitian shape functions [1] and \( [B] \) is the strain displacement matrix. This can be re-written as a coupled system

\[
\begin{bmatrix}
[K_{aa}] & [K_{a,1}] \\
[K_{a,1}^T] & [K_{1,1}]
\end{bmatrix}
\begin{bmatrix}
\{\Delta d\} \\
\{\Delta \Lambda\}
\end{bmatrix}
= \begin{bmatrix}
\int_v [N]^T \{\tau\} dv - \int_v [B]^T \{\sigma_n\} dv \\
\int_v \{h\} f(\sigma_n) dv
\end{bmatrix},
\]

where

\[
[K_{aa}] = \int_v [B]^T [D^e] [B] dv, \quad [K_{a,1}] = -\int_v [B]^T [D^e] \{f,\sigma\} [h]^T dv
\]

and

\[
[K_{1,1}] = \int_v \{h\} \{f,\sigma\}^T [D^e] \{f,\sigma\} [h]^T dv.
\]

With this formulation, where the plastic consistency parameter is solved for alongside displacements, it is possible to make the yield strength dependent not only on the plastic strain, but also its Laplacian. To do this, gradient terms must be introduced into the yield function. This means that the yield stress \( \rho_y \) used would be replaced with \( \rho_y - c \frac{d^2 \varepsilon_p}{dx^2} \), for the one dimensional case. \([K_{1,1}]\) terms in \([K]\) are also required to be updated as

\[
[K_{1,1}] = \int_v \{h\} \{f,\sigma\}^T [D^e] \{f,\sigma\} [h]^T - c \{h\} \{p\}^T dv.
\]

where \( \{p\} \) are the laplacians of the Hermitian shape functions and \( c \) is a constant that can be related to the material length scale (see [4] for details).

To apply this to the GIMP method it should be noted that the Hermitian functions used to map the plastic consistency parameter from the nodes to material points should remain the same as in the FEM. The derivatives of shape functions used for mapping the standard strains become the gradient weighting functions, which are derivatives of the GIMP weighting functions given in (1).

### 3. Demonstration in 1D

A 1D bar with a weakened section in the middle subjected to displacement at each end (as shown in Figure 1) was modelled to demonstrate the GIMP method with gradient plasticity. The bar has a Young’s modulus of \( E = 20000 \), a yield strength of \( \rho_y = 2 \) (reduced by 10% in the weakened region) and has a softening(hardening) parameter of \( H = -0.1E \). The bar has an initial length of 100 and is displaced by 0.01 which leads to elasto-plastic behaviour in the weakened section. The problem was modelled over 20 loadsteps using 160 elements, each with two material points. Using the gradient approach the length scale is introduced into the yield function which is defined in this case as

\[
f = \rho_y + H \lambda - c \Delta \lambda
\]

where \( c = -l^2 H \). The results of the simulation are shown in Figure 2 and Figure 3 where it can be seen that the plastic strains throughout the bar and the axial stress in the bar agree well with finite element simulations. In 1D the plastic strain \( \varepsilon^p \) is equivalent to \( \lambda \).

![Figure 1: Bar with weakened central section subject to end displacements.](image-url)
4. Conclusions

This paper has outlined a framework to deal with problems containing strain localisations using gradient elasto-plasticity combined with the GIMP method. A fully implicit GIMP method has been used and the elasto-plastic gradient approach of de Borst [4] has been adopted as it provides a straightforward way to implement gradient effects in MPMs (as well as standard rate-independent plasticity). The plastic consistency parameter is treated as an additional nodal unknown that is mapped to the material points and the yield function at the material points becomes an additional error that must be minimised in the coupled non-linear algorithm. Hermitian shape functions are used for the mappings due to the requirement for higher-order continuity. The approach has been demonstrated in a 1D example in which the results using the GIMP method agree well with the FEM. Work is currently being undertaken to extend this to 2D, where the technique will be used to achieve a finite thickness in shear banding without mesh dependency.

References


ROCKING OF SINGLE AND DUAL RIGID-BLOCK SYSTEMS SUBJECT TO GROUND EXCITATION: EXPERIMENTAL AND COMPUTATIONAL ANALYSIS OF OVERTURNING CONDITIONS

Gordan Jelenić*, Nina Čeh and Nenad Bićanić†

Faculty of Civil Engineering, University of Rijeka, R. Matejčić 3, 51 000 Rijeka, Republic of Croatia
†Deceased
* gordan.jelenic@uniri.hr

ABSTRACT

A prismatic block is analysed for overturning when subject to a constant ground acceleration of prescribed magnitude and duration. The analytical overturning condition and a special numerical procedure are developed and assessed against experiments. Generalisation of the approach to rocking of a dual-block stack is outlined.

Key Words: rocking; rigid block; constant ground acceleration; overturning

1. Introduction

The esteemed member of the United Kingdom Association of Computational Mechanics, and Emeritus Professor at University of Glasgow, Nenad Bićanić, joined the Engineering Mechanics research group at the Faculty of Civil Engineering of University of Rijeka in his native Republic of Croatia upon his retirement from Glasgow in autumn 2010. Following his life-long interests in earthquake engineering and computational dynamics and recognising the need to characterise in more detail dynamic sensitivity of discontinuous systems, from dry walls in ancient and traditional construction to thermal insulation of graphite cores in nuclear power-plant reactors, he set up an experimental dynamics laboratory and started a number of new and exciting research topics in experimental and computational dynamics. Following his untimely demise in October 2016, we present to the Association a part of the research its valued member led so enthusiastically, related to rocking of blocky structures subject to ground motion.

For this occasion, we investigate the conditions under which a single slender prismatic rigid block overturns under influence of constant-acceleration ground motion of various duration analytically, numerically and experimentally. A closed-form solution clearly separating the regions of pure translation, stable rocking, and overturning, is derived. A non-linear numerical time-stepping scheme specifically designed to detect the precise time of contact and preserve the angular momentum balance at the time of contact is also presented and its accuracy assessed against the analytical solution. An experimental test rig is described next involving the set-up designed to eliminate slipping and prescribe various magnitudes of constant acceleration and their duration, and used to validate the analytical and numerical results.

The method may be generalised to the dual-block stack, where a situation in which the ground is set in motion by an impulse through a relatively short time period, left in uniform motion during which the system rocks in a stable fashion, and then subjected to a counter-impulse, is of critical importance. Such acceleration history often makes the upper block overturn and was a subject of Nenad’s special interest, and we conclude this contribution by presenting a test-rig designed by Nenad himself, capable of performing such a counter-impulse in a controlled manner.

2. Single block: analytical, numerical and experimental analysis

A rigid prismatic block of mass $m$, a rectangular base of unit thickness, width $b$ and height $h$ (or the half-diagonal $R$ of its frontal side and the angle of slenderness $\alpha = \tan^{-1} \frac{b}{R}$) lies on a rigid ground platform subject to a constant acceleration $a_0$ during the prescribed time-segment $t \in [0, t_a]$ which drops
to zero for \( t > t_a \). We address the case whereby sliding between the block and the ground is prevented and investigate whether for a prescribed set of input parameters \( R, \alpha, a_0, t_a \) the block will translate with the ground, rock in a stable fashion or overturn. It is assumed that contact between the block and the ground is maintained throughout the motion.

For a relatively small \( a_0 \), the block moves along with the ground without rocking. The block shall tilt around one of its corners when the moment of its weight with respect to that corner becomes equal to an infinitesimal time change of the corresponding angular momentum. In particular, for \( a_0 > g \tan \alpha \) the block ceases to move translationally and starts rotating by \( \theta \) around one of its corners according to

\[
\dot{\theta} + p^2 [\sin(\alpha - \theta) - a \cos(\alpha - \theta)/g] = 0,
\]

where \( p = \frac{1}{2} \sqrt{\frac{2g}{\pi}} \) is the so-called frequency parameter. For small \( \alpha \) and \( \theta \), this equation becomes linear with a constant coefficient of the form \( \dot{\theta} - p^2 \theta = p^2 (a/g - \alpha) \), having the solution \( \theta = (\alpha g/a) (\cosh pt - 1) \) for \( t \leq t_a \) and \( \theta = \alpha (1 - \cosh pt) + \frac{a_0}{g} \left((1 - \cosh pt) \cosh pt + \sinh pt \sinh pt\right) \) for \( t > t_a \). The least critical situation in which the block will overturn takes place when \( \theta = \alpha \) and \( \dot{\theta} > 0 \) (i.e. when \( \theta > \alpha \)) for \( t > t_a \). This gives the following condition for overturning

\[
\frac{\alpha - a_0}{g} (1 - \cosh pt_a) \left< \tanh pt \right. \leq 1 \quad \Rightarrow \quad pt_a > -\ln \left(\frac{\alpha g}{a_0} - 1\right).
\]

The problem may be also analysed numerically. The motion is described via

\[
\begin{align*}
\dot{\theta} + p^2 [\sin(\alpha - \theta) - a \cos(\alpha - \theta)/g] &= 0, \quad \theta \geq 0 \\
\dot{\theta} - p^2 [\sin(\alpha - \theta) + a \cos(\alpha - \theta)/g] &= 0, \quad \theta \leq 0.
\end{align*}
\]

These equations will be numerically solved using Newmark’s trapezoidal time-stepping rule [1] at discrete time instants separated by a time step \( \Delta t \), along with the Newton–Raphson iterative solution procedure. To make the transition from one of the equations of motion to the other without any constraint violation it becomes important to detect the time of contact precisely. We propose a technique in which the rotation at the end of a time step is monitored throughout the analysis for the change of sign. When such change is detected, say at a time \( t_{n+1} \), dynamic equilibrium over the time step is repeated for an unknown time-step length \( \Delta t^* \) under the condition that \( \theta_{n+1} = 0 \). After the impact, the original time-step length is restored and the time-stepping procedure switches to the other equation of motion.

When the exact time of the impact is detected, angular velocity \( \dot{\theta}^+ \) at the start of the first post-impact step needs to be reduced with respect to that at the end of the last pre-impact step \( \dot{\theta}^- \) following the angular-momentum balance via \( \dot{\theta}^+ = (1 - 1.5 \sin^2 \alpha) \dot{\theta}^- [2] \), while angular acceleration \( \ddot{\theta}^+ \) follows from the corresponding post-impact equation of motion, in effect giving \( \ddot{\theta}^+ = -\ddot{\theta}^- \). The detail is given in [3]. To validate the theory and assess the numerical procedure, a test rig is set up and a range of measurements conducted on a near frictionless air track shown in Fig. 1 enabling a constant acceleration of a chosen magnitude to be applied to a slider (blue) for a prescribed duration. The near-absence of friction is obtained by means of an air cushion between the air track and the slider. This is achieved by pumping air, which escapes the air track through a large set of tiny holes drilled on its top surface.

Before the analysis, the block of mass \( m \) is placed on the slider of mass \( M \) and the system is set floating by supplying sufficient air pressure to the air track. The slider–block system is kept in equilibrium through a force in the string attached to the slider and running over a pulley on the right-hand side of the air track and supporting a hanging mass \( \tilde{m} \), which is counter-balanced by the force in the second string securing the slider in a fixed position by connecting it to the left-hand side of the air track.

The contact conditions needed (continuous contact between the block and the slider without slipping) are provided by attaching the block to the slider via adhesive tapes as also shown in Fig. 1 enabling free rotation of the block about both corners without sliding and vertical detachment from the slider.
The slider–block system is set in motion by cutting the left-hand string, thus subjecting the system to a constant acceleration of magnitude \( a_0 = \frac{\ddot{m}g}{M+m+\ddot{m}} \). For the given slider–block system, therefore, the constant acceleration \( a_0 \) is completely defined by the hanging mass \( \ddot{m} \) which may be freely varied.

The exposure \( t_a \) of the system to such acceleration is defined by this mass and the initial distance from the bottom of the hanging mass to the floor \( y \) as \( t_a = \sqrt{\frac{\ddot{m}gM+m+\ddot{m}}{\ddot{m}}^2} \). In other words, for the chosen \( \ddot{m} \) defining \( a_0 \), varying this distance provides different exposures \( t_a \) of the system to such acceleration. When the ground acceleration drops to zero, the slider remains free to move uniformly without any horizontal disturbances thus completely reproducing the problem stated.

We analyse the block with the half-diagonal length \( R = \frac{1}{2}\sqrt{85}\text{cm} \) and angle of slederness \( \alpha \equiv \tan^{-1}(2/9) \) and conduct the time stepping for the range of non-dimensional constant accelerations \( \frac{a_0}{g} \in (0, 3) \) and non-dimensional exposures to such accelerations \( pt_a \in (0, 5) \) using the time-step length \( \Delta t = 0.001 \text{s} \) and the rotation norm in the Newton–Raphson procedure set to \( 10^{-10} \). The results are shown in Fig. 2, from where it is obvious that they agree with the analytical overturning predictions very closely, the difference in the results between the two analyses being completely attributed to the fact that the numerical analyses has been conducted for the non-linear case.

A range of measurements is then made for given mass of the slider \( M = 120 \text{g} \) and the block \( m = 95.5 \text{g} \) and different values of the input data \( (\ddot{m}, y) \leftrightarrow (a_0, t_a) \). The hanging masses are chosen from within the range \( \ddot{m} \in [15 \text{g}, 115 \text{g}] \) and the vertical distances from within the range \( y \in [0.2 \text{cm}, 25.3 \text{cm}] \). The results of the experiment are shown in Fig. 2 and compared to the analytical and the numerical results.

Clearly, the results overall agree quite well and the small differences between the experimental and the numerical results may well be caused by imperfect manual input of the problem parameters.
3. Dual-block stack: problem description, partial overturning and future work

The above analysis may be applied to motion of a non-bouncing dual-block stack subject to ground acceleration \( a \) and in our future work we plan to address this problem in more detail. Such motion can be described by four different motion patterns as shown in Fig. 3.

![Figure 3: Dual-block stack: patterns of rocking motion](image)

For such a problem, the so-called partial overturning (overturning of the upper block) may take place for an alternative acceleration history, in which at a time \( t_b > t_a \) a constant acceleration \( a_1 < 0 \) takes place and lasts until \( t_c > t_b \), after which it again drops to zero.

To analyse this problem experimentally, a bespoke pendulum rig has been designed inspired by the real-size tests conducted at the Roorke University in India [4]. The rig is shown in Fig. 4 and, in contrast to the air track, (i) it sets the slider–block system in motion by providing an input moment impulse via a pendulum arm and (ii) provides a counter-impulse when the slider hits the stopper thus reversing the direction of motion of the slider and potentially causing overturning of the upper block.

![Figure 4: Pendulum test rig](image)

Our future work will address this phenomenon both numerically and experimentally.

Acknowledgements

The results presented in this work have been obtained within the research project Configuration-dependent approximation in non-linear finite-element analysis of structures financially supported by the Croatian Science Foundation under contract No. HRZZ-IP-11-2013-1631.

References


MODELLING MIXED-MODE RATE-DEPENDENT DELAMINATION IN LAYERED STRUCTURES USING GEOMETRICALLY NONLINEAR BEAM FINITE ELEMENTS

*Leo Škec¹, Giulio Alfano¹ and Gordan Jelenić²

¹Department of Mechanical, Aerospace and Civil Engineering, Brunel University London, Kingston Lane, Uxbridge, UB8 3PH
²Faculty of Civil Engineering, University of Rijeka, Radmile Matejčić 3, 51000 Rijeka, Croatia

*leo.skec@brunel.ac.uk

ABSTRACT

Delamination is one of the one most important problems for layered structures, which are widely used in industry (e.g. composite laminates) and also often present in nature (e.g. layered biological tissue). In this work delamination is studied using cohesive-zone models (CZMs) where a discontinuous displacement field and a non-linear traction-separation law on the considered interface are assumed. Authors of the present work have recently shown that beam elements can be used with very good accuracy to model delamination in layered structures both in geometrically linear and non-linear analysis. Beam elements also make use of a smaller number of degrees of freedom, with significant reduction in the overall computational burden. When the fracture process is significantly rate dependent, the traditional fracture-mechanics based approaches can only characterise the phenomenological dependence of the fracture energy on the crack speed. Instead, rate-dependent CZMs, recently developed by the authors, where the different dissipation mechanisms occurring during fracture are separated out, is less phenomenological and better linked to the underlying physics. Combining the highly efficient multi-layer beam model and the novel rate-dependent CZMs is the aim of the project on which the authors of this work are currently collaborating. This work gives a brief overview of authors’ recent work which presents the background for developing a novel multi-layer beam finite element with rate-dependent mixed-mode delamination.

Key Words: multi-layer beam; delamination; finite element analysis; geometrically exact formulation

1. Introduction

This work addresses the problem of how to efficiently model delamination or debonding in layered structures whose layers are efficiently modelled with beam elements and is divided in two main parts. In the first part, recent work by the first and the third author is presented. Their contribution is the development of a computationally efficient and numerically robust multi-layer beam model which accounts for mixed mode delamination. The model uses two- or three-node beam finite elements in conjunction with interface elements with embedded CZM as presented in [1]. In the second part, recent work of the second author on novel rate-dependent CZMs is presented. Building on the principles of thermodynamics, these CZMs are capable of capturing real behaviour of double cantilever beam (DCB) tests across a wide range of loading rates for mode I delamination. In the conclusions, an insight in the current collaboration between the authors is given.

2. Rate-independent geometrically exact multi-layer beam model

A multi-layer beam, composed of \( n \) layers and \( n - 1 \) interconnections is considered. Each layer \( i \) is represented as a beam with a reference axis denoted by \( X_{1,i} \) and since all layers are mutually parallel, \( X_{1,i} = X_1 \) for \( i \in (1, n) \). The principal unknown functions of the problem are the displacements \( (u_i(X_1) \) and \( v_i(X_1) \) and the cross-sectional rotation \( \theta_i(X_1) \) of each layer. Since the problem is highly non-linear in terms of the constitutive law of the interconnection and the kinematic equations of the layers, the solution is obtained numerically using the finite element method. Each layer is discretized in finite number (\( N \)) of
nodes, which results in $3 \times n \times N$ degrees of freedom. Using beam finite elements instead of commonly used 2D plane-strain finite elements significantly reduces the total number of degrees-of-freedom (DOF). If 2-node beam finite elements are used instead of Q4 elements, the reduction in total number of DOF is 25%, while substituting Q8 elements with 3-node beam finite elements can reduce the total number of DOF up to 40%.

Governing equations are derived separately for layers and interconnections (see [6] and [5] for more detail). It is assumed that external loads can be applied only on layers, while the interconnection can produce only internal forces. Kinematic equations for the layers are geometrically exact and non-linear, based on the Reissner’s beam theory, constitutive equations are linear elastic and equilibrium equations are derived from the principle of virtual work. The nodal vector of residual (internal - external) forces for layer $i$ and node $j$ (after the interpolation of the virtual quantities) is written in the following form

$$
\mathbf{g}^{L}_{i,j} - \mathbf{q}^{INT,L}_{i,j} = \int_{0}^{L} (\mathbf{D}_{l}\tilde{\mathbf{P}}_{l,j})^{T} L_{l} \begin{bmatrix} N_{i} \ M_{l} \end{bmatrix} dX_{1} - \int_{0}^{L} \tilde{\mathbf{P}}_{l,j}^{T} \begin{bmatrix} f_{l} \ w_{l} \end{bmatrix} dX_{1} - \mathbf{P}_{l}^{T}(k) \begin{bmatrix} F_{i,k} \ W_{i,k} \end{bmatrix},
$$

where matrix $\mathbf{D}_{l}$ contains the relations between the virtual strains and virtual displacements (mostly derivatives), matrix $\tilde{\mathbf{P}}_{l,j}$ contains the interpolation functions with respect to the global vector of nodal unknowns, matrix $L_{l}$ is basically the rotational matrix, $N_{i}$ is the vector of internal (axial and shear) forces (stress-resultants) and $M_{l}$ is the internal bending moment. Members appearing with the negative sign originate from the virtual work of external forces; distributed external forces and bending moments are denoted by $f_{l}$ and $w_{l}$, while concentrated forces and bending moments at the beam ends ($k = 0$ or $L$) are denoted by $F_{i,k}$ and $W_{i,k}$.

The interconnection is basically attached to the edges of surrounding layers and the relative displacement at the interconnection can be easily defined using displacements, rotations and geometrical properties of surrounding layers. The constitutive law of the interconnection is based on the bi-linear CZM presented in [1] and the equilibrium equations are again derived from the principle of virtual work. The nodal vector of internal forces of the interconnection (after interpolating the virtual quantities) reads

$$
\mathbf{q}^{INT,I}_{\alpha,j} = b_{\alpha} \int_{0}^{L} (\mathbf{Y}_{\alpha}\mathbf{R}_{\alpha,j})^{T} \mathbf{\omega}_{\alpha} dX_{1},
$$

where $b_{\alpha}$ is the constant width of the interconnection, matrix $\mathbf{Y}_{\alpha}$ contains relations between the virtual relative displacements of the interconnection and the virtual displacements and rotations of the surrounding layers, matrix $\mathbf{R}_{\alpha,j}$ contains the interpolation functions with respect to the global vector of nodal unknowns and $\mathbf{\omega}_{\alpha}$ is the vector of contact tractions at the interconnection. Finally, the nodal vector of internal, external and residual forces for all layers and all interconnections may be written as

$$
\mathbf{q}^{INT}_{j} = \sum_{i=1}^{n} \left[ \mathbf{q}^{INT,L}_{i,j} + (1 - \delta_{in})\mathbf{q}^{INT,I}_{\alpha,j} \right], \quad \mathbf{q}^{EXT}_{j} = \sum_{i=1}^{n} \mathbf{q}^{EXT,L}_{i,j} \quad \text{and} \quad \mathbf{g}_{j} = \mathbf{q}^{INT}_{j} - \mathbf{q}^{EXT}_{j} = \mathbf{0},
$$

where $\delta_{in}$ is the Kronecker delta, which equals 1 when $i = n$ (otherwise is zero). By linearizing Eq. (3) nodal tangent stiffness matrix $\mathbf{K}_{j,k}$ can be obtained, where index $k$ refers to the node of interpolation of test functions. Global vector of residual forces (composed of global vector of internal and external forces) and the global tangent stiffness matrix can be assembled using the standard assembly procedures. During the simulation of delamination processes sharp oscillations around the exact solutions may occur unless the FE mesh is very dense. In [5], a novel modified arc-length method taking into account the damage of the system and capable of obtaining convergence for the most critical numerical tests is presented.

Although in many application the use of geometrically exact formulation will not produce results that significantly differ from those produced using the linear theory of small displacement and rotations, in [5] many examples where this differences cannot be neglected are reported. One of the best examples
of that was found for the standard end-notch-specimen for mixed-mode delamination test (see Fig. 1). During the bending of the left-hand side of the upper layer, geometrically exact theory (unlike the linear one) allows the horizontal displacement \(u(0)\) in Fig. 1) which will eventually reduce the arm between the forces \(F_1\) and \(F_2\) and cause a drastic increase of force \(F_1\) after the displacements exceed the limit where the geometrically non-linear effects cannot be neglected.

![Figure 1: Differences between geometrically linear and non-linear formulations in mixed-mode delamination test](image)

3. Rate-dependent cohesive zone model

Authors of the present work currently collaborate on a project aiming to incorporate rate-dependence in the above presented geometrically exact multi-layer beam model which accounts for mixed-mode delamination. The rheological representation of rate-dependent CZMs for mode I delamination presented by Musto and Alfano [3, 4] is given in Fig. 2. The model consists of an elastic and inelastic arm, where a single scalar \(\alpha\) is used as an internal variable. \(\alpha\) denotes the inelastic displacement jump in the viscous unit (Fig. 2(a) as presented in [3]) or visco-elastic unit (Fig. 2(b) as presented in [4]). Energy dissipated during the fracture process is the result of (i) rupture of elastic bonds (decohesion), which is controlled by the damage parameter \(D\), and (ii) viscous flow, which is represented by the viscous or the elasto-viscous part \(\alpha\) of the relative displacement at the interconnection. It is also assumed that decohesion is rate independent, while the rate-dependence is the result of the viscous dissipative mechanism introduced in the model. In the approach presented in [3] the interface response is that of a viscoelastic standard linear solid (SLS) model (see Fig. 2(a)), where the interface stress is the product of a Volterra convolution operator with exponential kernel, and a scaling factor \((1 - D)\) which accounts for interface damage. In [4], a fractional visco-elastic (FSLS) model for the undamaged response is considered. The dashpot in Fig. 2(a) is replaced by a new "Scott Blair element" in Fig. 2(b) in which the stress is proportional to the fractional derivative of order \(\nu\) of the relative displacement of the interconnection \((\nu \in (0, 1))\). The fractional CZM in [4] led to capture with excellent agreement the experimental results for a DCB with rubber interconnection, across entire range of experimentally tested specimens, spanning almost 5 logarithmic decades.

![Figure 2: Rheological representation of the (a) classic (SLS) and (b) fractional Standard Linear Solid (FSLS) model](image)
Both approaches [3, 4] assume that the damage evolution is driven by the energy stored in the elastic arm of either the SLS model or FSLS model. This results in a monotonically increasing total fracture energy $G_c$ with the prescribed relative-displacement speed $v$ resulting with a sigmoidal shape of $G_c - v$ curve. In [2], this assumption is reconsidered by taking into account two additional possibilities, namely, that damage is driven by (i) the energies in the two springs of the elastic and inelastic arms or (ii) the entire free energy including energy stored within the "Scott Blair element" in the FSLS model. Considering either of these assumptions, a non-monotonic $G_c - v$ relationship is obtained, with a bell rather than sigmoidal shape.

4. Conclusions

In this work, an overview of authors’ recent work on which the current research is based, is presented. Combining multi-layered beam model with rate-dependent CZMs shall give a very efficient and robust model for capturing complex rate-dependent behaviour of structures undergoing mixed-mode delamination. The new model will be verified against experimental results for mode I delamination (DCB test) and computationally more expensive models which use plane-strain 2D finite elements with significantly higher number of degrees of freedom.

Acknowledgements

Research presented in the present work is supported by the European Commission under the project H2020-MSCA-IF-2015-EF ”MOLAY-STRUDEL”, project No. 701032. The third author is supported by the Croatian Science Foundation under the project HRZZ-IP-11-2013-1631 ”CANFAS”.

References


Multi-level Monte Carlo methods for large-scale eigenvalue problems

*H. Juliette T. Unwin¹, Nathan Sime¹ and Garth N. Wells¹

¹Department of Engineering, University of Cambridge, Trumpington Street, Cambridge, CB2 1PZ

*hjtu2@cam.ac.uk

ABSTRACT

Monte Carlo simulations can be prohibitively expensive for large stochastic eigenvalue problems. We propose that using Multi-level Monte Carlo methods make it possible to perform stochastic eigenvalue simulations in a feasible time frame. We demonstrate the approach for vibration of a string and for a three-dimensional elastodynamic problem.

Key Words: uncertainty quantification; multi-level Monte Carlo; eigenvalue problem; random vibrations.

Introduction

Small perturbations in engineering structures impact on the natural frequencies of a structure, and avoiding natural frequencies in service may be important. Natural frequencies are computed from eigenvalue problems, therefore it is important to be able to accurately calculate the eigenvalues for systems where randomness has a significant impact on the response.

The Monte Carlo (MC) method is a simple method for quantifying the impact of uncertainties, but is considered too expensive computationally in many practical cases. This is because the error is $O(\sqrt{N})$, where $N$ is the number of samples. However, if Multi-level Monte Carlo (MLMC) [1] methods are employed, it is possible to compute the statistics of eigenvalue problems faster, thereby making Monte Carlo techniques viable.

We briefly introduce MLMC and methods for generating random fields. Then, models for calculating the natural frequencies of a string and a three-dimensional elasticity problem are summarised, and results of applying both MC and MLMC techniques are presented.

Multi-Level Monte Carlo method

Let $Q$ be a quantity of interest, which can be estimated by solving the problem of interest on ‘meshes’ of varying levels of fidelity. We associate each level with an integer index $\ell$, with coarsest mesh denoted by the index 0, through to the finest level denoted by the index $L$. The expectation of $Q$ on level $L$ is given by:

$$\mathbb{E}[Q_L] := Y = \sum_{\ell=0}^{L} Y_\ell,$$

where $Y$ is the multi-level estimator and $Y_\ell$ is the expectation of the estimator at level $\ell$:

$$Y_\ell := \frac{1}{N_\ell} \sum_{i=0}^{N_\ell} (Q_{\ell,i} - Q_{\ell-1,i}),$$

where $Q_{-1} = 0$ and $N_\ell$ is the number of samples on level $\ell$.

To demonstrate why the multi-level approach is cheaper than standard MC, we consider the root mean squared error estimate:

$$\epsilon^2 := (\mathbb{E}[Y - \mathbb{E}[Q]])^2 = \mathbb{V}[Y] + \mathbb{E}[Q_L - Q]^2.$$
This error estimate can be split into two parts: the first, $\mathbb{V}[Y]$, is the statistical error resulting from the variance of the estimator, and the second, $\mathbb{E}[Q_L - Q]^2$, is the discretisation error. To ensure that $\epsilon^2 < TOL$, where $TOL$ is a prescribed error tolerance, it is sufficient to ensure that both terms are smaller than $\epsilon^2/2$. We compare $\mathbb{E}[Q]$ at level $L$ for both MC and MLMC methods, hence the discretisation error is the same for both methods. Therefore this does not impact the computational cost. However with MLMC, the more expensive finer grids can be sampled less often than coarser grids because the variance between the ‘finer’ levels is smaller than the variance between the ‘coarser’ levels. This impacts the statistical error of the estimator and so MLMC can achieve equivalent accuracy to MC methods, but at a much lower cost. To calculate the total variance of the estimator we sum the variance of the estimator at each level:

$$\mathbb{V}[Q_L] = \sum_{\ell=0}^L \mathbb{V}[Y]. \quad (4)$$

We consider uncertainty in our systems from stochastic coefficients in the governing equations. For example, continuous stochastic realisations can be generated using a Karhunen–Loève expansion. However, this method is too expensive for large systems since it requires computing the solution of dense generalised eigenvalue problems, and so is not used in this work. We consider discrete realisations of a random field, and add random point masses (in the form of Dirac delta functions) to the vibration problems. This is similar to commonly used approaches in random vibration research, e.g. [2, 3].

**Vibration of a string**

We are interested in quantifying uncertainty in the linear wave equation and the impact that variations in mass density have on the vibrational natural frequencies. We solve the problem using a standard continuous finite element method (FEM) defined on domain $D$, and let $(\Omega, \mathcal{F}, \mathbb{P})$ be the probability space where $\Omega$ is a sample space, $\mathcal{F}$ is a collection of subsets of $\Omega$ that we can assign probabilities and $\mathbb{P}$ is a probability measure.

Time harmonic mode shapes and corresponding natural frequencies for a string are computed from the eigenpair problem: find $u : D \times \Omega \rightarrow \mathbb{R}$, $u \neq 0$ and the corresponding natural frequencies $f : \Omega \rightarrow \mathbb{R}$, where $f = \frac{1}{2\pi} \sqrt{\lambda}$, such that

$$\tau \frac{\partial^2 u}{\partial x^2} = -\lambda \rho u \quad \text{on } D,$$

where $\omega$ is a realisation of $\Omega$, $\rho(x, \omega) \in L^1(\Omega, \mathcal{F}, L^2(D))$ is the mass density and $\tau(x) \in L^2(D)$ is the tension. We are interested in the impact that random point masses added to the density field has on the natural frequencies.

**Natural frequency comparison**

We compare the expectation and variance of specific natural frequencies to show that the same statistics are found using both MC and MLMC techniques. We choose $\rho = 8000 \text{ kg/m}^3$, $\tau = 200 \text{ N}$ and a unit length domain. We add 30 point masses of random mass (maximum amplitude of $10^{-3} \rho$) at random locations in the domain $D$. Figure 1(a) compares the probability distributions for the 20th to 24th natural frequencies using both MC and MLMC techniques. These natural frequencies were chosen since they can be calculated accurately on relatively coarse meshes. From Figure 1(a), it is clear that there is a very good match between the MC and MLMC results, even though the solutions have only converged with $TOL = 10^{-3}$. The results indicate that the natural frequencies follow a normal distribution.

**Cost comparison**

Figure 1(b) shows a cost comparison between the two models run on an Intel Core i7-5820K processor at 3.30GHz. We see that for a tolerance of $10^{-3}$, MLMC takes approximately 3.5 minutes whereas MC takes 5.8 hours. For a tolerance of $10^{-4}$, MLMC takes 5.7 hours whereas extrapolation predicts that MC would take 17 days.
Vibration in three dimensional elasticity

For the linear elastic wave equation, the time harmonic mode shapes and corresponding natural frequencies are computed using a continuous finite element method. The problem reads: find $u : D \times \Omega \to \mathbb{R}^3$, $u \neq 0$ and the corresponding natural frequencies $f : \Omega \to \mathbb{R}$, such that:

$$-\nabla \cdot \sigma = f^2 \rho u \quad \text{on } D,$$

where $\rho \in L_2(\Omega, \mathcal{T}, L_2(D))$ is the mass density and $\sigma$ is the Cauchy stress tensor,

$$\sigma = C : \varepsilon (u),$$

where $C$ is the stiffness tensor and $\varepsilon (u) = \left( \nabla u + \nabla u^T \right)/2$ is the strain tensor. We consider only isotropic homogeneous media, where the stress is given by:

$$\sigma = 2\mu \varepsilon (u) + \Lambda \text{Tr} (\varepsilon (u)) I,$$

where $I$ is the identity tensor and $\Lambda$ and $\mu$ are Lamé parameters,

$$\Lambda = \frac{E \nu}{(1 + \nu)(1 - 2\nu)}, \quad \mu = \frac{E}{2(1 + \nu)},$$

with $E > 0$ being the Young’s modulus and $\nu \in (0, 1/2)$ the Poisson ratio.

Natural frequency comparison

We compare the probability distributions computed from MLMC and MC simulations for a cube $D = (0, 0.1)^3$, with $\rho = 2700$ kg/m$^3$, $E = 70$ GPa, $\nu = 0.32$. We add 40 point masses with random values (maximum amplitude of $10^{-7} \rho$) at random locations in the domain $D$. Figure 2(a) compares the MLMC and MC distributions for a tolerance of 0.1. Even though Figure 2(a) shows a difference between the MC and MLMC distributions, the mean and variance agree within the error tolerance of 0.1. For MLMC, $\mathbb{E}[Q]$ was also calculated for a tolerance of 0.01. The two MLMC simulations indicate good convergence. MC is too costly for the lower tolerances.
Figure 2: In (a) we compare the MC and MLMC probability density functions for the 6th and 7th natural frequencies of the 3D elasticity equation with 40 randomly located point masses of random amplitude (with maximum magnitude of $10^{-7} \rho$). In (b) we show the time taken to compute the first 20 eigenvalues on one processor.

**Cost comparison**

Since the cost of solving the 3D elasticity system is much greater than for the string, MC soon becomes impractical. Figure 2(b) shows the time taken to find the first 20 eigenvalues of the 3D elasticity FEM system for different sized deterministic problems. The system has 2 Intel Xeon E5-2670 processors at 2.6 GHz. A solve using the finest mesh used in the calculations for Figure 2(a) has 418275 degrees of freedom and so requires approximately 5 minutes on 1 processor. For a tolerance of 0.1, the time required for a MC simulation with 100 solves is approximately 8 hours, whereas MLMC took 6.2 minutes. For a tolerance of 0.01, 10,000 solves are necessary for a MC simulation and the estimated time is 35 days. A MLMC simulation took 11.1 hours.

**Conclusions**

We have shown that the efficiency gains of the multi-level Monte Carlo method can make Monte Carlo methods viable for random vibration problems. The simplicity and flexibility of MLMC enable us to compute quantities of interest when the underlying system have many degrees of freedom without having to make modelling assumptions that may reduce the accuracy of the result.

**Acknowledgements**

HJTU was funded by an EPSRC Doctoral Training Partnership scheme (grant number EP/J500380/1).

**References**


Boundary representation and boundary condition imposition in the material point method

*Yun Bing¹, Michael Cortis¹, Tim Charlton¹, William Coombs¹ and Charles Augarde¹

¹School of Engineering and Computing Sciences, University of Durham, Lower Mountjoy, South Road, Durham, DH1 3LE

*yun.bing@durham.ac.uk

ABSTRACT

Unlike the conventional finite element method (FEM), in which the mesh conforms to the material boundary, the material point method (MPM) [12] does not provide a clear interpretation of the boundary. In the MPM, the problem domain is discretised by a finite number of material points, on which the material properties and history dependent variables are prescribed and carried throughout simulations. The material information is then mapped to a “stationary” background mesh where the equilibrium equations are solved. However, the material boundary and the mesh nodes, in general, do not coincide. This causes difficulties solving boundary-value problems during MPM simulations, in particular, applying traction (Neumann) and non-zero prescribed displacement (inhomogeneous Dirichlet) boundary conditions. However, little attention has been paid to this issue and no literature to date has presented an effective way to model and track boundaries in the MPM. In this paper, a B-spline based boundary approximation method is discussed. A local cubic interpolation technique [10] is employed for boundary representation. Traction are applied through direct integration over the B-spline boundary and displacements are prescribed via a B-spline based implicit boundary method [3, 8, 9].

Key Words: material point method; B-splines; implicit boundary method; boundary conditions

1. Introduction

The material point method (MPM) was developed by Sulsky et al. [12] in 1994 as a solid mechanics extension to the fluid implicit particle method [2] which was an advancement of the particle-in-cell method [6]. The formulation of the MPM is rather similar to the standard finite element method (FEM) as the governing equations are solved on the nodes of the mesh. However, instead of using the mesh elements themselves to describe the problem domain, the MPM discretises the problem domain by a set of material points (MPs). These MPs are similar to the Gauss points in the standard FEM as both methods use these points for stiffness integration except that the MPs follow the deformation of the problem domain whilst the background mesh retains its original shape. In other words, at the end of each MPM load step, the positions of the MPs are updated by the deformed background mesh which is reset for the next load step leaving the MPs at their new positions (see Figure 1). These characteristics of the MPM allow it to model large deformation and fracture problems without going through the expensive processes of re-meshing and re-mapping of state variables.

Figure 1: A simple illustration of the MPM simulation procedure: initialisation (left), deformation (middle) and reset mesh with updated MPs position (right).
Nevertheless, because the problem domain is represented by MPs, boundaries are not clearly defined in the MPM. This makes the application of boundary conditions (BCs) rather inaccurate, especially for Neumann and inhomogeneous Dirichlet BCs. However, this problem is rarely discussed in the literature; many have managed to avoid this issue by aligning the problem boundaries with the background mesh or modelling problems that only involve body forces. Inspired by Kim and Youn [7], in this work a B-spline interpolation method is chosen to represent the boundaries in the MPM. Tractions are enforced by direct integration over the B-spline boundaries and displacements are prescribed by incorporating the B-spline boundaries within implicit boundary method (IBM) [3, 4, 8, 9].

2. B-spline basics and boundary representation

A \( p \)-th degree B-spline curve defined by a set of \( n \) control points, \( \{ P_i \} \), and a knot vector, \( \{ \Xi \} = \{ \xi_0, \xi_1, \ldots, \xi_r \} \) with knots \( \xi_i, i = 0 \ldots r \), being a sequence of nondecreasing real numbers and \( r = n + p + 1 \), can be expressed as

\[
\{ C(\xi) \} = \sum_{i=0}^{n} N_{i,p}(\xi) \{ P_i \},
\]

where \( N_{i,p}(\xi) \) are the \( p \)-th degree B-spline basis functions [10].

A local cubic B-spline interpolation technique has been chosen to represent the boundaries in the MPM. The interpolative nature of this technique allows a greater control on the B-spline represented boundaries and ensures that the key boundary points are included. As a local method, this cubic technique constructs curves in a piecewise fashion. Only local data are used at each step, so a fluctuation in data would only affect the curve locally. Additionally, this method has the ability to deal with sharp corners efficiently [10].

To construct the boundaries of a MPM simulated problem, the outer layer MPs are firstly identified as the sampling points. A cubic Bézier curve [1] is constructed between every two sampling points. Two inner control points are determined by (1). Detailed calculations for the procedures described above can be found in [10].

3. B-spline based Neumann and Dirichlet boundary conditions

Having described a means of boundary representation, the application of traction to a boundary, \( \Gamma \), is straightforward. The equivalent nodal forces due to the applied traction can be determined through

\[
\{ f^t \} = \int_\Gamma \{ M \}^T \{ t \} \, d\Gamma,
\]

where \( \{ M \} \) contains the standard finite element basis functions and \( \{ t \} \) is the prescribed traction.

Numerical integration over a \( p \)-th degree B-spline represented boundary is performed by using \( (p - 1) \)-th order Gauss-Lagrange quadrature [5]. Because the local coordinate of Gauss quadrature has a range of \([-1, 1]\); whereas, the local coordinate of a B-spline curve has positive values only, a two-step mapping between the global coordinates and the B-spline local coordinate \( \xi \) is required, that is

\[
\begin{aligned}
\{ J_B \} &= \left[ \frac{d\{ C \}}{d\xi} \right] = \left[ \frac{d\{ C \}}{d\xi} \right] \left[ \frac{d\xi}{d\xi} \right] \\
\text{with } \frac{d\xi}{d\xi} &= \frac{\xi_{j+1} - \xi_j}{2},
\end{aligned}
\]

where \( \left[ \frac{d\{ C \}}{d\xi} \right] \) is the first derivative of the B-spline approximated boundary [10]. Applying Gauss quadrature to (2), we obtain

\[
\{ f^t \} = \sum_{i=1}^{n_{GP}} \left[ M_i \right]^T \{ t \} \det([J_B]) w_i,
\]

where \( n_{GP} \) is the number of Gauss points and \( w_i \) is the weight associated with Gauss point \( i \).

Dirichlet BCs are imposed by incorporating the B-spline represented boundaries with the IBM which was firstly introduced by Burla and Kumar [3] for FEM problems that use non-conforming meshes. Implementation of fixed Dirichlet BCs with problem boundaries parallel to one of the coordinates has been demonstrated in [3, 8, 9]. This method has later been adopted to the MPM framework and extended to include the imposition of “roller” BCs on
inclined boundaries [4]. The methodology behind the IBM is that essential BCs are enforced by introducing extra penalty stiffness to the system. Dirichlet functions (D-functions) are involved in the solution structure to impose the prescribed displacements directly. In the IBM, the FEM trial solution for an elastostatic problem is expressed as

$$\{u\} = [D][M]\{d^e\} + \{u^e\},$$  \hspace{1cm} (5)

where $\{u\}$ is the displacement within a finite element, $[D]$ contains the D-functions, $\{d^e\}$ are nodal displacements associated with the element and $\{u^e\} = [M]\{u^e\}$ with $\{u^e\}$ being the prescribed nodal displacements. To enforce fully fixed essential BCs, the D-functions are constructed such that they vanish at the degrees of freedoms where non-zero displacements are prescribed and rise to unity when reach the problem domain over a thin band $\delta$. As for roller BCs, the D-functions are assigned to have a value of 1 in the directions that are free to move [4]. Stiffness integration is then performed over $\delta$ and along the B-spline represented boundaries where $[J_B]$ (3) is used for mapping between the global and local coordinates.

4. Numerical example

An example of a 10m $\times$ 2m cantilever beam is shown here to validate the implementations of the B-spline based boundary method. The cantilever beam was modelled under a plane strain assumption and linear elastic material with a Young’s modulus of 1MPa and Poisson’s ratio of 0.25 was used. The left hand side boundary was fixed at the mid height of the beam and with rollers above and below. A constant pressure of 1500Pa was applied along the top boundary, which was maintained perpendicular to the boundary throughout the analysis.

A background mesh with 1.5m by 1.5m elements was used, and the problem domain was discretised by using 896 uniformly distributed MPs. The outer layer of the MPs were identified as the problem boundaries which were approximated by using B-splines. BCs on the left boundary were applied by the B-spline based IBM and the pressure applied through 5 load steps. The initial discretisation and the final deformed cantilever beam are shown in Figure 2a; however, having boundaries represented by B-splines, the boundaries can be tracked after each load step without plotting out all the MPs (see Figure 2b) and the curvature of the deformed shape has been successfully captured by the B-spline approximation.

As there is no analytical solution for this problem, a convergence test on the displacement at the centre of the beam tip (see Figure 2a) was carried out by performing h-refinement on the mesh and increasing the number of MPs. As shown in Figure 3, for all three mesh configurations, the mid-tip displacement converges when more MPs are introduced. Reduction of the change in displacement with mesh refinement indicates that the mid-tip displacement also converges when the mesh size is decreased.

5. Conclusions

This paper has presented a general method of representing boundaries in the MPM by using cubic B-splines and which is also used as a means of enforcing both Neumann and Dirichlet BCs. This B-spline based boundary method not only allows easy visualisation of the deformed problem domain, but has made the MPM capable of modelling problems that were previously not possible. These has been demonstrated through an example of cantilever beam with applied traction. Although this approach of boundary representation and BC impositions has been developed in 2D, the same theory is also applicable to 3D. The formulation of local bicubic B-spline surface interpolation is
straightforward to implement and extending the IBM to 3D is equivalent to introducing penalty stiffness to the 3D MPM.

Figure 3: Convergence of mid-tip displacement.

References


ISOGEOMETRIC BOUNDARY ELEMENT METHOD BASED ON
ADAPTIVE HIERARCHICAL REFINEMENT OF NURBS

*H. Khaki¹, J. Trevelyan²

¹² School of Engineering and Computing Sciences, Durham University, DH1 3LE
*hamed.khaki@durham.ac.uk

ABSTRACT

Potential of isogeometric methods from the promise of cost and run-time saving to more efficient and accurate results, continuity level, convergence and refinement properties attracted numerous computational and numerical researchers in engineering and mathematics to work on different aspects of these methods. The core idea of Isogeometric Analysis (IGA) is to make a shortcut between computer-aided modelling and analysis by describing precise geometries and using them directly in analysis. The direction of this research is to study direct design to analysis by Isogeometric Boundary Element Method (IGABEM) for 3D models by making adaptive refinements to provide reliable solutions even starting from a coarse CAD description. Emphasis will be on the automotive industry. A key aspect of this work is the development of an effective set of algorithms allowing adaptive refinement of Non-Uniform Rational B-Spline (NURBS) surfaces. This work started with IGABEM-NURBS for simple 3D models under simple boundary conditions and the plan is to develop the method for more complex geometries, more boundary conditions, more accurate and fast results by local refinement of NURBS using an adaptive hierarchical scheme.

Keywords: Boundary Element Method, NURBS, Adaptive hierarchical refinement

1. Introduction

Isogeometric Analysis (IGA) was first introduced by Hughes et al in 2005 [1]. The main idea of IGA is to use the same basis functions for representing the geometry in CAD and approximating the solution fields in analysis. Existing CAD models, especially those typically used in industries, are most often NURBS-based. Due to the tensor product structure of NURBS [2] it is difficult to obtain locally refined grids and we aim to develop an adaptive hierarchical scheme in the future.

2. Isogeometric Boundary Element Method (IGABEM)

2.1. Boundary Integral Equations (BIE) for 3D Linear Elastostatic Problem

We solve the problem of elasticity in 3D solids. In absence of body forces, the following boundary integral equation is well known:

\[ C_{ij}(p)u_i(p) + \int_S T_{ij}(p,Q)u_j(Q)dS(Q) = \int_S U_{ij}(p,Q)t_j(Q)dS(Q). \]  

(1)

where \( C_{ij} \) is the jump term that arises from the strongly singular integral, and depends on the geometry of boundaries, \( S \) is the domain boundary \( S=S_u+S_t \), \( T_{ij} \) is the traction kernel, \( U_{ij} \) is the displacement kernel, \( u_i(p) \) is the displacement at a boundary (source) point \( p \), and \( u_j(Q) \) and \( t_j(Q) \) are the displacement and traction components at \( Q \).

2.2. Discretization of BIE 3D

To solve equation (1) numerically, the boundary \( S \) must first be discretized into a series of elements. In this work we use a NURBS description of the solution variables so the discretized BIE becomes:

\[ C_{ij}(p)u_i(p) + \sum_{s=-1}^{+1} \sum_{t=-1}^{+1} \int_{p} T_{ij}(p,Q)R_{s,t}(u,v)J(u,v)du dv A_{s,t} = \sum_{s=-1}^{+1} \sum_{t=-1}^{+1} \int_{p} U_{ij}(p,Q)R_{s,t}(u,v)J(u,v)du dv B_{s,t} \]  

(2)

where \( R_{s,t} \) is the NURBS basis function for the control point \((s,t)\). \( U_{ij} \) and \( T_{ij} \) in equation (2) are functions of \( 1/r \) and \( 1/r^2 \) respectively, rendering them weakly and strongly singular. The weakly singular \( U_{ij} \) kernel does not generally present a problem and can be easily solved by Telles Transformation [3]. However, the \( T_{ij} \) kernel must be integrated in specific method suitable for
IGABEM to cancel the singularity. A regularization method was used in this work. When collocated at a sufficient number of points, $p$, the integral equation (2) yields the matrix form

$$Hu = Gt.$$  

(3)

where $H$ is a square matrix containing a combination of the integrals of the traction kernel and the jump terms, $G$ is a rectangular matrix of displacement kernel integrals, $u$ and $t$ are a mix of unknown values and the values prescribed by boundary conditions. By swapping unknowns and knowns the equation can be rewritten as:

$$Ax = b.$$  

(4)

where $A$ is a fully populated and non-symmetric matrix of coefficients, the vector $x$ holds all unknown displacement and traction components and the vector $b$ arises from known boundary conditions and corresponding boundary integrals. The equation (4) is a linear system which can be simply solved to obtain the coefficients $A_{ij}, B_{st}$, from which values of the unknown displacement and tractions can be recovered.

3. B-Spline, NURBS Curve and NURBS Surface

In order to develop an understanding of B-splines, it is important to start with some key definitions. A knot vector is a non-decreasing set of coordinates, written $\Xi = [\zeta_1, \zeta_2, ..., \zeta_{n+p+1}]$, where $\zeta_i$ is the $i^{th}$ knot, $p$ is the polynomial order, and $n$ is the number of basis functions. The basis function $N_{i,p}$ could be defined using the Cox-de Boor [4] recursion formula:

$$N_{i,0}(u) = \begin{cases} 1 & \text{if } \zeta_i \leq u < \zeta_{i+1} \\ 0 & \text{otherwise} \end{cases},$$  

(5)

$$N_{i,p}(u) = \frac{u-\zeta_i}{\zeta_{i+p}-\zeta_i} N_{i,p-1}(u) + \frac{\zeta_{i+p+1}-u}{\zeta_{i+p+1}-\zeta_{i+1}} N_{i+1,p-1}(u).$$  

(6)

B-splines are combined in a linear approach to generate a curve or surface in following manner:

$$C(u) = \sum_{i=1}^{n} N_{i,p}(u) B_i,$$  

(7)

$$C(u, v) = \sum_{i=1}^{n} \sum_{j=1}^{m} N_{i,p}(u, v) M_{j,q}(u, v) B_{i,j}.$$  

(8)

where $C(u)$ and $C(u, v)$ are the location of the physical curve and surface, $B_i$ and $B_{i,j}$ are control point coordinates in $2D$ and $3D$, $u$ and $v$ are the spatial coordinate in parameter space, $p$ and $q$ are the degree of spline and $n$ and $m$ are the number of control points.

3.1. Rational B-spline Curves and Surfaces

A rational B-Spline is a type of B-spline with weighted control points, and is formulated as:

$$R_{i,p}(u) = \frac{w_i B_{i,p}(u)}{\sum_{i=1}^{n} w_i B_{i,p}(u)},$$  

(9)

$$R_{i,p}(u, v) = \frac{w_i B_{i,p}(u, v) M_{j,q}(u, v)}{\sum_{i=1}^{n} \sum_{j=1}^{m} w_i B_{i,p}(u, v) M_{j,q}(u, v)}.$$  

(10)

where $w_i$ and $w_{ij}$ are the weights of control points. The rational form of B-spline curves and surfaces are as:

$$C(u) = \sum_{i=1}^{n} R_{i,p}(u) B_i,$$  

(11)

$$C(u, v) = \sum_{i=1}^{n} \sum_{j=1}^{m} R_{i,pq}(u, v) B_{i,j}.$$  

(12)

261
4. Location of collocation points

Contrary to the traditional BEM, the control points in IGABEM may lie off the physical problem boundary. This requires us to compute feasible locations for the collocation points. Using the Greville Abscissae method [5] we have:

$$\vec{\xi}_a = \frac{\zeta_{a+1} + \zeta_{a+2} + \ldots + \zeta_{a+p}}{p} \quad a = 1, 2, \ldots, n.$$  \hspace{1cm} (13)

where $n$ is the number of control points, $p$ is the order, $\vec{\xi}_a$ are collocation points and $\zeta_{a+i}$ are knot values. The first and last knots in the knot vector are excluded when applying (13).

5. Numerical Example

A simple example is studied with degree of $p=2$, knot vector [0 0 0 1 1 1] in both the $u$ direction and $v$ direction, and all weights are defined to be 1. Simple geometries like a cube and a quarter cylinder were created by NURBS starting with 3 x 3 control points in each patch and the geometry basis functions were used for analysis under different boundary conditions (Figure 1).

A uniform vertical compression of 1MPa was applied over the top patch of cube and three patches were constrained by roller supports (Figure 2.a). An internal pressure of 1MPa was considered at the inner radius of the quarter cylinder and rollers were again applied as displacement constraints (Figure 2.b). The cube is a unit cube and inner radius of quarter cylinder is 0.4m, outer radius is 1m, height is 1m, and the material for both is of steel with Young Modules of 200GPa and Poisson’s ratio of 0.3.

6. Results
Convergence of the IGABEM algorithm was studied. Knot insertion was used to provide h-refinement, and the effect of the order of Gauss Legendre quadrature also investigated. Figure 3 shows the convergence of the scheme to the analytical displacement of 5E-6 (m) at the top surface.

![Figure 3](image1.png)

**Figure 3**: The trend of IGABEM result for cube by increasing Number of knots and number of Gauss points (a) The trend of Matlab Run-time by increasing number of knots and number of Gauss points(b)

Figure 4 shows the convergence of the IGABEM scheme for the quarter cylinder problem, again in terms of the number of Gauss points and the number of knots.

![Figure 4](image2.png)

**Figure 4**: $\sigma \theta$ calculated by IGABEM and Analytical result for different number of knots and number of Gauss points

7. **Conclusions**

The basic Isogeometric Analysis Boundary Element Method (IGABEM) has been presented, and shown to converge for simple problems in linear elasticity. The aim of this research is to develop an adaptive algorithm through the use of hierarchical B-splines and to test its performance for a range of typical solid components found in the automotive industry.

8. **References**


Implicit MPM with second-order convected particle domain interpolation

*Lei Wang¹, William M. Coombs¹, Charles E. Augarde¹, Michael Brown²

¹School of Engineering and Computing Sciences, University of Durham, DH1 3LE, Durham
²Civil Engineering, University of Dundee, DD1 4HN, Dundee
*lei.wang@durham.ac.uk

ABSTRACT

An implicit material point method (MPM) with the second-order convected particle interpolation (CPDI2) is presented in this paper. In the MPM a body is described by a number of Lagrangian material points, at which state variables are stored and tracked. Calculations are then carried out on a background Eulerian computational mesh. A mapping and re-mapping algorithm is employed, to allow the state variables and other information to be mapped back and forth between the material points and background mesh nodes during an analysis. To reduce the error during these mappings, there are several extensions. The latest extension is termed CPDI2, which uses a quadrilateral particle domain to replace a material point. The CPDI2 extension has been implemented explicitly with using regular grids in published papers. This work develops an implicit CPDI2 method with an elasto-plastic material model. The motivation is that an implicit scheme can reduce the computational cost by allowing a large time step, while enforcing the yield condition accurately and increase stability. Both quadrilateral and triangular particle domains are used. An example shows that the use of a triangular particle domain is more flexible than the quadrilateral particle domain.

Key Words: material point method; convected particle domain interpolation; implicit methods

1. Introduction

The Material Point Method (MPM) is a numerical method used to simulate massive deformation of solids requiring less effort than the FEM and meshless methods. In the MPM a body is described by a number of Lagrangian material points, at which state variables are stored and tracked. Calculations are then carried out on a background Eulerian computational mesh. A mapping and re-mapping algorithm is employed, to allow the state variables and other information to be mapped back and forth between the material points and background mesh nodes during an analysis. However, errors commonly are caused by the numerical noise inherent in the original MPM, that arises when a material point crosses the boundary between elements of the computational mesh [1].

To reduce this problem, some extensions to the MPM have been proposed by replacing a zero-volume material point with a finite-volume particle domain, including the Generalized Interpolation Material Point (GIMP) method [2], Convected Particle Domain Interpolation (CPDI) [3], and Second-order CPDI (CPDI2) [4]. For a 2D problem, the particle domains are tracked as rectangles in the GIMP method, as parallelograms in the CPDI method, and as quadrilaterals in the CPDI2 method. The CPDI2 method can more accurately track particle domains and their deformation than others. The CPDI2 has been implemented explicitly with a regular grid in published papers [4].

This work develops an implicit CPDI2 method with an elasto-plastic material model. An implicit scheme can reduce the computational cost by allowing a large time step, whilst enforcing the yield condition accurately and leading to a general increase in stability [5]. The implicit nature occurs at two stages in the calculations: in the solver of the nonlinear boundary value problem and in the stress integration algorithm. Both quadrilateral and triangular particle domains are used in this study.
2. Method

2.1. Particle domains

In the GIMP method, a particle domain is a fixed axis-aligned rectangle that translates with the particle, so it may result in a gap or overlap between particle domains, e.g. Figure 2(b). In the CPDI method, a particle domain is a parallelogram, without the edge perpendicularity requirement in the GIMP method. In the CPDI2 method, a particle domain is a quadrilateral, with the coordinates of its four corners stored. These particle domains are similar to a finite element mesh constructed using four-node elements. Therefore, they can exactly track the deformation, e.g. Figure 2(c).

2.2. Material models and implicit implementation

The von-Mises elasto-plastic constitutive law is used here. This law consists of a yield function

$$ f(\sigma) = \frac{1}{\rho} \sqrt{2J_2} - 1, \quad (1) $$

where $\rho$ is the yield strength and $J_2$ the second deviatoric stress invariant. The plastic potential $g = f$.

The implicit backward Euler (bE) integration is used for the stress return when the trial stress enters the plastic regime. Given a trial strain $\epsilon_t$, we need to find the elastic strain $\epsilon^e$ and the plastic multiplier $\Delta \gamma$. The returning stress is directly determined by

$$ \sigma^r = [D^e] \epsilon^e, \quad (2) $$

and plastic strain is found from

$$ \epsilon^p = \Delta \gamma \left( \frac{\partial g}{\partial \sigma} \right). \quad (3) $$
CPDI2 with elasto-plasticity and triangular mesh

1. Elasto-plasticity

Figure 1: Cauchy stress against the vertical position from the GIMP code. The solid lines show the analytical solutions. The part with nonzero $\sigma_x$ behaves plastic.

Figure 2: Cauchy stress against the vertical position from the CPDI2 code. The solid lines show the analytical solutions. The numerical results also agree with analytical ones very well. Notably, the two sides of the column are constrained horizontally so that it has the same boundary conditions or assumption in the one-dimensional analytical solutions.

Figure 3: Cauchy stress against the vertical position from the CPDI2 code. The solid lines show the analytical solutions.

Correspondingly, we have two residuals

the yield function \[ f = 0, \]  

balance of strains \[ \epsilon^e - \epsilon_t^e + \Delta \gamma \left( \frac{\partial g}{\partial \sigma} \right) = 0. \]

3. Results

An elasto-plastic column subject to self-weight is modelled. In the first example, shown in Figure 3, a roller boundary condition is applied on the both sides of a column of material, hence this problem is equivalent to the 1D problem for which an analytical solution is available. Good agreement is obtained between the numerical and the analytical results validating the approach for this problem.

In the second example, we use this code to model the deformation of column subject to self-weight without side restraint. The roller boundary condition is applied at the left side and the bottom, while the right side is traction-free. As the loading increases, the distortion of particle domains occurs, see Figure 4(f). Because of a very large deformation, a quadrilateral particle domain is degraded to a triangle. This results in the code failing.

In a third example, we use the triangular particle domain CPDI2. With a low body force, we have the deformed configuration in Figure 5(b). With a large body force, we have the deformed
configuration in Figure 5(c). The performance of the triangular domain CPDI2 is clearly superior to the quadrilateral case, being more robust when particle domains are severely distorted.

4. Conclusions
We have extended the CPDI2 with quadrilateral particle domains to use instead triangular particle domains for modelling very large deformation problems. The elasto-plastic material model has been implicitly implemented in the implicit MPM code. In an example, we have shown that the use of triangular particle domains lead to improved stability.

Acknowledgements
We are grateful for the support by the UK Engineering and Physical Sciences Research Council grant (No. EP/N006054/1).

References


Prediction of Burst Pressure for Steel Pipes with Gouge Defect using Numerical Modelling

Alvan H. Wordu and Kong Fah Tee

Department of Engineering Science, University of Greenwich, Chatham Maritime, Kent ME4 4TB, UK

*Corresponding author: K.F.Tee@gre.ac.uk

ABSTRACT

Burst pipe is a major problem facing the maintenance of pipeline network integrity management. The presence of gouge defect on the surface of these pipes is associated with these burst incidents. Methods for estimating gouge defects on steel pipes have been available, such as NG-18 equation and BS 7910 (or API579). Other methods use a combination of finite element analysis and mathematical expression which has also been proposed in more recent studies. These methods are time-consuming, and known to be cumbersome and complicated. Hence, there is a need for a simple method which adopts an easier procedure to predict burst pressure due to the presence of gouge on the surface of the pipe. To address the issue mentioned above, this study proposes a three-dimensional numerical model by employing finite element method (FEM) based on a stress-based criterion to predict the pipeline failure. Thus, the failure is assumed when the minimum von Mises equivalent stress in the ligament is in equilibrium to the ultimate tensile strength of the pipe material. Results from the proposed method show good agreement with the hydrostatic experimental test. The size of pipe, defect length and wall thickness have the most significant effect on the burst pressure.

Keywords: Burst pressure; Gouge defect; Stress-based criterion; von Mises; Pipeline failure

1. Introduction

Burst pipe incidents hugely restrict the safe movement of hydrocarbons within the pipeline network system. As statistic representation of broken pipes has indicated among the predominant causes of these burst cases are connected with reduced wall thickness due to corrosion and mechanical damages [1–7]. The literature on burst pressure estimation of pipelines with defect has been extensively studied and has led to the provision of various design solutions. The NG-18 Equation and BS 9710 (or API 579) are among predominantly used assessment methods for predicting burst strength of a steel pipe with gouge defect [8]. A good number of these long-standing methods are still accepted and employed in a significant amount of the more recent pipeline applications. However, there has been an increase in the acceptance of more current finite element modelling due to their immense ability to model and predict complex defect and lower conservative solutions.

The current study carried out by Alang [9] and Belachew [10] proposed a method using the combination of numerical modelling and mathematical equation to estimate burst strength of pipes with gouge defect affirming the shortfall in this area of study. This solution type falls short for pipeline engineers, appearing complicated and time-consuming using the combination of numerical modelling and mathematical equation to estimate burst strength of pipes with defect. To resolve this problem, the proposed approach employs only numerical simulation.

2. Numerical Modelling

To simulate burst pressure failure test, a 3-D FE elastoplastic analysis in COMSOL was performed. Incremental pressure load was applied until failure. The mechanical and tensile properties of the pipe material were employed in the model using the provisions in Table 1 and stress-strain data in Figure 1.
Table 1: Mechanical properties of API X42 steel at room temperature

<table>
<thead>
<tr>
<th>Young modulus, $E$ (GPa)</th>
<th>Poisson Ratio, $v$</th>
<th>Yield Strength, $\sigma_y$ (MPa)</th>
<th>Tensile Strength, $\sigma_u$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>207</td>
<td>0.3</td>
<td>284.7</td>
<td>464.4</td>
</tr>
</tbody>
</table>

![Stress-strain data for API X42 steel](image)

**Figure 1**: Stress-strain data for API X42 steel adopted in the FE analysis

2.1 Governing equations

Prediction of burst pressure conducted in this study is governed by these equations:

$$F_v + \nabla \cdot FS = 0$$  \hspace{1cm} (1)

$$F = 1 + \nabla u$$  \hspace{1cm} (2)

$$S = (\sigma_0 + \sigma_{ext} + \sigma_{q}) + C : \varepsilon_{el}$$  \hspace{1cm} (3)

$$\varepsilon_{el} = \varepsilon - \varepsilon_{inel}$$  \hspace{1cm} (4)

$$\varepsilon_{inel} = \varepsilon_0 + \varepsilon_{th} + \varepsilon_{hs} + \varepsilon_{pl} + \varepsilon_{cr}$$  \hspace{1cm} (5)

$$\varepsilon = \frac{1}{2} \left[ (\nabla u)^T + \nabla u + (\nabla u)^T \nabla u \right]$$  \hspace{1cm} (6)

with volume force vector $F_v$, total force $F$, second Piola-Kirchhoff stress $S$, deformation vector $u$, 4th order elastic tensor $C$, double dot tensor product $\cdot$, stress tensor $\sigma$ and strain tensor $\varepsilon$. Subscript ‘0’, ‘ext’, ‘q’, ‘el’, ‘inel’, ‘th’, ‘hs’, ‘pl’ and ‘cr’ denotes initial, external, viscoelastic, elastic, inelastic, thermal, hygroscopic, plastic and critical aspect of stress and strain, respectively.

2.2 Geometry of the studied pipe section

A quarter model is adopted for the numerical simulation to reduce computational time, as shown in Figure 2 and Figure 3. In this study, the gouge depth ($d$), pipe length ($L$) and wall thickness ($t$) are constant with corresponding values of 8.75 mm, 2300 mm and 17.5 mm, respectively. While varying the pipes outer diameter ($D$) and gouge length ($b$), the gouge geometry is assumed to have a 45-degrees V-notch shape and rounded up at the bottom by a groove with a radius of 2 mm. For a full description of model see Alang [9].
2.3 Failure criterion

The von Mises failure criterion used for isotropic materials was adopted. Failure was assumed when the numerical computational algorithm fails to converge. For multi-axial stress states, the von Mises yield criterion expressed in principal stresses as

$$\sigma_{\text{vm}} = \frac{1}{2} \left[ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 \right]^{1/2}$$

(6)

3. Results and Discussions

In this section, the burst test result for X42 steel pipe with gouge defect are presented. Nine test examples were analysed for three different sizes of pipe diameter, and their burst pressures predicted. Table 2 offers a detailed summary of the parametric study performed using the proposed model. The proposed model results show good agreement with relatively small differences from those presented by Alang [9]. Figure 4 shows a plot of burst pressure against pipe thickness in a range of 8.8 – 17.5 mm. Based on the graph the burst pressure declines with thickness reduction.

<table>
<thead>
<tr>
<th>Pipe Diameter, D, mm</th>
<th>508</th>
<th>762</th>
<th>1016</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gouge parameter, mm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Length, ( l )</td>
<td>100</td>
<td>200</td>
<td>300</td>
</tr>
<tr>
<td>Depth, ( d )</td>
<td></td>
<td></td>
<td>8.75</td>
</tr>
<tr>
<td>Burst pressure, MPa</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alang [13]</td>
<td>28.8</td>
<td>25.2</td>
<td>23.6</td>
</tr>
<tr>
<td>Proposed model</td>
<td>32.4</td>
<td>28.2</td>
<td>27.65</td>
</tr>
<tr>
<td>Percentage Deviation</td>
<td>11%</td>
<td>11%</td>
<td>15%</td>
</tr>
</tbody>
</table>

Table 2: Summary of burst test results
4. Conclusions

This study postulates how numerical simulation tool can solely provide burst test results. The methodology adopted demonstrates the ability of FE modelling to predict burst pressure independently such as experimentation. Results from the finite element simulation show good agreement with the finite element approach by Alan [9]. The parametric study suggests the characteristics of the gouge and pipe size and wall thickness have the most influence on the burst pressure of the test pipe.

References

Progressive collapse of braced irregular steel structures located in regions with different seismic activity

Amir Homaioon Ebrahimi1*, Pedro Martinez-Vazquez1, and Charalampos C.Baniotopoulos1

1School of Engineering, University of Birmingham, Edgbaston, Birmingham, B15 2TT, United Kingdom
* Corresponding author: AXH552@bham.ac.uk

ABSTRACT

This paper examines the effect of plan irregularities on the progressive collapse of braced and un-braced steel structures located in regions with different seismic activity and designed in accordance with AISC (2010) and ASCE7 (2010). The collapse patterns of four buildings is examined and compared across seven loading scenarios using non-linear dynamic and static analyses completed as per the GSA (2013) standard. Node displacements above the removed columns and the force increase across adjacent columns, are discussed. Also, the susceptibility of columns to collapse, based on their strength and capacity, is examined and the pushdown curve and yield load factor of the structures, after column removal, is obtained and critically discussed.

Keywords: progressive collapse, irregularity in plans, steel building, non-linear dynamic analysis, non-linear static analysis

1. Introduction

Progressive collapse of buildings is usually caused by abnormal loads induced by ill-construction or design practice, or by accidental actions such as fire or gas explosions (National Institute of Standard and Technology, 2007). The probability associated with such events is however low and therefore buildings are generally not designed against them. The GSA (2013) recommends design solutions and strategies for structural retrofitting underpinned by the Alternative Path Method (APM) which has been widely adopted by researchers in the past. Previous works on progressive collapse have focussed on examining failure mechanisms (Gerasimidis and Baniotopoulos, 2011), structural sensitivity to local damage (Gerasimidis, Bisbos, and Baniotopoulos, 2012, 2013), and on developing strengthening techniques (Gerasimidis, and Baniotopoulos, 2015). Those studies have addressed to some degree the impact of geometrical irregularities on the overall building’s response and the role of individual structural components. The present paper builds on previous research and aims at enhancing our understanding on the effects of plan irregularities with or without braced framing systems on the spread of damage in progressive collapse scenarios, and to illustrate the impact of regional seismicity on such damage.

2. Model structures

Four steel structures (herein named 1, 2, 3 and 4) were selected and designed with the ETABS (2015) and following the AISC (2010) and ASCE (2010) recommendations, hence the elements and connections have high strength and ductility. Steel moment resisting frames form structures 1 and 2 (Fig. 1) and steel moment resisting frames which are concentrically braced form structures 3 and 4 (Fig. 2). Each of the 4 structures has 5 storeys of 3 m height and 6 bays of 4 m wide each. All structures have plan irregularities and are assumed to be located in site class C and E seismic zones. The buildings were loaded with 192 kg/m² and 520 kg/m² dead- and live-load respectively. The location of the columns removed for each of the four structures is shown in Fig. 1 and 2.
Table 2. Detail of sections used in structures

<table>
<thead>
<tr>
<th>Floor</th>
<th>Structure 1 Column (Box)</th>
<th>Beam (PG)</th>
<th>Structure 2 Column (Box)</th>
<th>Beam (PG)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>b</td>
<td>t</td>
<td>b_1</td>
<td>t_1</td>
</tr>
<tr>
<td>First</td>
<td>200</td>
<td>12</td>
<td>150</td>
<td>8</td>
</tr>
</tbody>
</table>

Structure 3

<table>
<thead>
<tr>
<th>Floor</th>
<th>Column (Box)</th>
<th>Beam (PG)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>b</td>
<td>t</td>
</tr>
<tr>
<td>First</td>
<td>200</td>
<td>12</td>
</tr>
</tbody>
</table>

Structure 4

<table>
<thead>
<tr>
<th>Column (Box)</th>
<th>Beam (PG)</th>
</tr>
</thead>
<tbody>
<tr>
<td>b_1</td>
<td>t_1</td>
</tr>
<tr>
<td>200</td>
<td>12</td>
</tr>
</tbody>
</table>

3. Analysis method for progressive collapse

In non-linear dynamic analyses, load configurations of 120% dead loads and 50% live loads were applied to building models with a linear increase and within time frame of five seconds. The load was maintained constant for two seconds and then the relevant column was suddenly removed in the seventh second to examine the response of the structure. In line with the GSA (2013), a dynamic amplification factor of approximately 2 was used to run non-linear static analyses in such a way that the gravity load of the spans that are adjacent to the removed column will be twice as much as that of the other spans. In those (pushdown) static analyses a stepwise increase to vertical loads was applied until the maximum amplified loads were attained - or the structure collapsed. In the non-linear static analyses the imposed load plotted against the node displacement of the removed column indicates the capacity of a structure against progressive collapse. The load value was divided by the normal gravity load so that the vertical axes of the pushdown capacity curve became a load (dimensionless) factor (Eq.1) which establishes a criterion for assessing collapse. Hence, if the load factor associated to yielding displacement is higher than 1 then the structure is resistant to the removal of a column. If not, the structure collapses.

\[
\text{Load Factor} = \frac{\text{Load}}{\text{Nominal gravity load}} \quad (1)
\]

4. Analysis of the results

In all cases the column removed were located at the ground floor as that induced the most critical condition of stability. A range of column-removal scenarios (S1F1PA-S1F1PB in Table 2) assessed through non-linear static analyses led to the pushdown capacity curves shown in (Fig. 3). It can be seen there that the load factor in the structures with steel moment frames (scenario 2) is lower than the load factor in the structures with steel concentrically brace frames. On the other hand, the yield load factor estimated for all the structures and scenarios reveals that structure 4 located in site class E
seismic zone has the highest yield load factor amongst all - as shown in Fig. 4. In addition to that, non-linear dynamic analyses provided the displacement of the top joint of the removed column which is shown in Fig. 5 for scenarios S1F1PA and S1F1PB covering all the structures.

Figure 3: Pushdown capacity curve of all the structures a) Scenario 1 b) Scenario 2

Figure 4: Yield load factors for all the structures and scenarios

Figure 5. Vertical displacement of removal point, a) Scenario 1, b) Scenario 2

Another key parameter to assess the structural performance under progressive collapse is the force taken by columns adjacent to the removed column. In this case, the force acting on the column is plotted vs. time is shown in Fig. 6 in terms of a demand to capacity ratio (D/C). The D/C ratio in the adjacent columns is around 1 in scenario 1 related to structures 3 and 4 which suggests that the adjacent column may not be exposed to total damage and collapse may not be transmitted to the adjacent spans. However, in structures 1 and 2, the required force for both adjacent columns in the progressive collapse analysis is between 1.2 and 1.8 times the column capacity, which indicates that
these columns would have been damaged after the collapse of the target column. This is also shown in Table 2 where all scenarios and node displacements are provided.

Figure 6: The demand force to capacity ratio (D/C) of the adjacent columns in Scenario 1, a) Column 1B

Table 2: Node displacement and maximum D/C ratio of adjacent columns for all the scenarios and structures

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Structure 1</th>
<th>Structure 2</th>
<th>Structure 3</th>
<th>Structure 4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Node Displacement (mm)</td>
<td>D/C</td>
<td>Node Displacement (mm)</td>
<td>D/C</td>
</tr>
<tr>
<td>S1F1PA</td>
<td>Fail</td>
<td>1.77</td>
<td>Fail</td>
<td>1.44</td>
</tr>
<tr>
<td>S1F1PB</td>
<td>Fail</td>
<td>1.29</td>
<td>86</td>
<td>0.92</td>
</tr>
<tr>
<td>S1F1PD</td>
<td>Fail</td>
<td>1.5</td>
<td>Fail</td>
<td>1.23</td>
</tr>
<tr>
<td>S1F4PA</td>
<td>Fail</td>
<td>1.15</td>
<td>84.9</td>
<td>0.87</td>
</tr>
<tr>
<td>S1F4PD</td>
<td>91</td>
<td>1.05</td>
<td>84</td>
<td>0.83</td>
</tr>
<tr>
<td>S1F4PF</td>
<td>Fail</td>
<td>1.31</td>
<td>87.8</td>
<td>0.94</td>
</tr>
<tr>
<td>S1F7PA</td>
<td>Fail</td>
<td>1.67</td>
<td>Fail</td>
<td>1.38</td>
</tr>
</tbody>
</table>

5. Conclusion

Four parameters have been used to assess structural performance against progressive collapse, namely push-down capacity curves, yield load factors, joint displacement of the top joint of removed columns, and demand to capacity ratio (D/C). The analyses showed that those structures located in site class E seismic risk exhibit lower D/C ratio than those located in site class C and it became evident that bracing tends to increase structural resilience hence reducing the potential of progressive collapse of structures.

References

AISC (2010), Manual of Steel Construction, LRFD, AISC, Chicago IL USA •
ASCE 7 (2010), Minimum Design Loads for Buildings and Other Structures, ASCE, Reston, VA USA •
GSA (2013), Alternate Path Analysis and Design Guidelines for Progressive Collapse Resistance, General Services Administration, Washington, DC USA •
Gerasimidis, S., Bisbos, C., & Baniotopoulos, C.C. (2012), Vertical Geometric Irregularity Assessment of Steel Frames on Robustness and Disproportionate Collapse, J. of Constructional Steel Research, 74, 76-89 •
Gerasimidis, S., Bisbos, C., & Baniotopoulos, C.C. (2013), A computational model for full or partial damage of single or multiple adjacent columns in disproportionate collapse analysis via linear programming, Structure and Infrastructure Eng., 10(5), 1-14 •
BLAST SIMULATIONS AND TRANSIENT RESPONSES OF LONG-SPAN GLASS ROOF STRUCTURES: A CASE OF LONDON’S RAILWAY STATION

*Sakdirat Kaewunruen¹, Guido Pompeo² and Gianni Bartoli³

¹School of Engineering, University of Birmingham, Edgbaston, Birmingham, B15 2TT, United Kingdom
²Dipartimento di Ingegneria Civile e Ambientale, University of Florence, S. Marta, 3 - 50139 Firenze, Italy
³Dipartimento di Ingegneria Civile e Ambientale, University of Florence, S. Marta, 3 - 50139 Firenze, Italy

*s.kaewunruen@bham.ac.uk

ABSTRACT

Long-span structures often are slender by nature. Their span/depth ratio often causes excessive responses and high sensitivity to dynamic actions (e.g. wind, Earthquakes, explosion, etc.). The issues are pronounced when thin-walled glass roof structures gain popularity in design and construction. Especially in railway built environment, long-span and glass-roof structures can often be seen at many landmark railway stations such as St Pancras International, King’s Cross, Birmingham Grand Central, etc. Importantly, these railway stations are considered to be at high risk of terrorist threats. However, many railway critical infrastructures were built or designed long before the explosive actions being taken into account. In this study, the blast simulation and transient responses of a long-span glass roof structure are thus highlighted. The focus is placed on Canary Wharf underground station, which is one deemed to be at risk. Nonlinear modelling, validation and transient analyses of the station roofing structure have been carried out using a finite element package, STRAND7. Sensitivity of explosion intensity has been evaluated to quantify structural capacity and vulnerability of the glass roof. The insight into this transient behaviour will help railway and structural engineers to establish strategic retrofitting methods to minimise catastrophic damage to and potential losses of train passengers, the public & rail assets.

Keywords: blast; transient effect; dynamic response; long span; glass roofing; railway station.

1. Introduction

Railway assets are a critical infrastructure that requires active monitoring and protection against man-made hazards (such as terrorist attack, severe vandalism, derailments, and human errors). The loading actions and design criteria are complex in nature with strict considerations for systemic and sub-systemic compatibility [1-3]. With the active engagement in overseas military missions, Europe’s critical infrastructures remain at high risk of terrorist attack. The purpose of this research is to investigate structural effects of blast loads upon glass-roof structure, and to evaluate the capacity and vulnerability of the structure to resist to this kind of action and then propose some informed structural retrofit to the infrastructure [4-8]. This paper highlights a case study considering the canopy (membrane structure) of Canary Wharf underground station. The double curvatures of canopy are formed by the fabricated tapering arches that are connected with circular purlin supporting the glazing panels with stainless steel spider as shown in Figure 1.

2. Finite Element Modelling

The structure is modelled using STRAND7 finite element package [1], the structural model in three-dimensional space has been established using tapered beam elements for the arches and beam elements for the purlins, while using plate elements for the glass roof panels (Figure 2). To define the dimensions of the mesh, model sensitivity has been verified by a response convergence of a glass panel under a uniform load. The convergence has informed the suitability of the meshing. The material properties of the model have been tabulated in Tables 1 and 2. The dynamic properties of the glass roof structure and the structural steel have been applied to the dynamic transient modelling. Moment resisting support (via stainless steel spider) is applied on the transfer edges of glazing panels.
3. Blast Simulations

The explosion is simulated by rapid and abrupt release of energy as shown in Figure 3. The explosion effects are presented in a wave of high intensity pressure that spreads outward from the source to the surrounding air. It is designed to place the blast load close to the escalators because the location can affect most people/structure. In this study, critical fragility and vulnerable component analyses will be presented so that railway and structural engineers can develop risk-based retrofit program against
terrorist attacks for the railway station [2]. To identify the blast load criticality, the document Unified Facilities Criteria (UFC), Structures to Resist the Effects of Accidental Explosions [3] has been reviewed. The explosive has been considered close to the ground. A charge located on or very near the ground surface is considered to be a surface burst. The initial wave of the explosion is reflected and reinforced by the ground surface to produce a reflected wave as shown in Figure 4.

To find the values to draw the blast load, graphical analysis is adopted from [3] using the scaled distance $Z=R/W$, where $R$ is the distance between the point of the detonation and the structure, whereas $W$ is the weight of the charge. To insert the blast load in the software, it has been simplified by calculating a time step of 2 ms [3, 6]. In this study, various blast patterns are formed because the distance can be varied. The resultant critical blast load found at the central escalators of the station is shown in Figure 5. Nonlinear transient dynamic results can be obtained as shown in Figure 6.

Figure 6: Effect of the blast load on structural dynamic responses, triggering the resonances of structural frames

Figure 7: Damage evolution of long span glass roof structure (white contour: glass panels reach its failure stress)
4. Transient Responses and Sensitivity Analysis

To observe the damage evolution and breakage of glass facades, the Von Mises stress has been evaluated. The failure stress has been surpassed for the first time at 8 ms. The damage of the glass roof structure is demonstrated in Fig.7. The insight from this evolution will help crisis management in railway corridor by enabling safer evacuation [8-9]. It can be observed that the first failure of the glass roof occurs at a time of 8 ms in the glass panels closer to the explosion. Immediately, two glass panels break at 8 ms, while at 9 ms eight other panels begin to break. The blast pressure is then relieved but the blast impulse later excites the structural components of the roof. This impulsive excitation can also incur further damages of glass panels associated with the resonant modes of structural vibration.

5. Conclusion

Long-span structures are prone to excessive dynamic responses to blast and explosion. The issues are pronounced when thin-walled glass roof structures are utilized for the built environment. In this study, the blast simulation and transient responses of a long-span glass roof structure are presented. The finite element model of Canary Wharf underground station has been established using a finite element package, STRAND7. The structural capacity and vulnerability of the glass roof have been evaluated. Since the glass used is usually the laminated one-layer. The most convenient improvement to avoid the glass damage is to laminate another layer of thin films or double glasses, to increase its toughness. Another solution is to renovate using a different type of glass. The insight into these blast behaviours will help railway and structural engineers to establish strategic retrofitting methods to minimise catastrophic damage to and potential losses of train passengers, the public and railway assets.

Acknowledgements

The first author wishes to thank Japan Society for the Promotion of Science for Invitation Research Fellowship (Long-term), Grant No. JSPS-L15701, at Railway Technical Research Institute; and the University of Tokyo, Japan. The second author wishes to thank Erasmus+ Program to sponsor his research visit at the University of Birmingham. The authors are also deeply grateful to European Commission for H2020-MSCA-RISE Project No. 631135 ‘RISEN: Rail Infrastructure Systems Engineering Network’, which enable a global network to tackle a global challenge in rail infrastructure resilience and advanced sensing under extreme environments (www.risen2rail.eu).

References

RECOVERY OF STRONG EQUILIBRIUM IN PLATES REVISITED

*E.A.W. Maunder ¹ and J.P. Moitinho de Almeida ²

¹College of Engineering, Mathematics and Physical Sciences, University of Exeter, Exeter, EX4 4QF
²Department of Civil Engineering, Architecture & Georesources, IST, University of Lisbon, 1096 Lisboa Codex, Portugal

*e.a.w.maunder@exeter.ac.uk

ABSTRACT

The development of dual finite element solutions, with one satisfying compatibility, and the other satisfying equilibrium, has long been recognised to provide a sound basis for error estimation of either solution. The authors have proposed methods for recovering either type of solution from the other based on the use of partition of unity (PU) functions defined over star patches. In the present paper, we extend these concepts and apply them to the recovery of equilibrium from conforming finite element models of thin plate bending problems governed by Kirchhoff’s classical plate theory, and using triangular elements. In this case, strictly conforming models require polynomial shape functions of degree greater than four, with for example, nodal degrees of freedom consisting of deflections, rotations and curvatures. Such freedoms complicate an element by element approach which relies on the use of conjugate generalised nodal forces. However the approach based on star patches and the same linear PU functions remains feasible, using appropriate hybrid equilibrium Kirchhoff elements.

Keywords: finite elements; Kirchhoff plate bending; strong equilibrium; conforming elements; partition of unity

1. Introduction

Most commonly used finite elements for modelling solid continua are based on assumptions concerning displacement fields, which are generally compatible with the derived strains that are assumed, and at element boundaries. Equilibrium is then generally only satisfied in a weak sense, and it can be useful to obtain also a dual solution which satisfies equilibrium in a strong sense. In this case, the engineer is then faced with either undertaking a complete re-analysis with a different type of finite element model, or using a procedure that recovers strong equilibrium from the existing weak form.

The latter alternative has been researched and developed for some 40 years [2,3], and the authors have recently proposed alternative procedures for simplicial elements in modelling 2D and 3D continua [4,6]. Essentially these procedures replace the equilibrium re-analysis of the complete model with separate analyses of local star patches of elements. Their solutions are superimposed using the concept of partition of unity. The elements in such patches share a common vertex/node, and by using information from the compatible model, they are loaded in a balanced way so as to present well posed problems.

In this paper we propose similar approaches for obtaining strong forms of equilibrium from conforming displacement based models of thin plate bending problems governed by Kirchhoff’s classical plate theory which neglects shear deformation. In this case a polynomial degree of at least five is required to approximate transverse displacements to ensure full $C^1$ continuity of conforming elements, as proposed in the TUBA family of elements [1].

2. Recapitulation of plate theory

With reference to Figure 1, the rotation vector $\theta = \text{grad} w$, where $w$ is the transverse deflection. Using the notation in Figure 1, the stress and side traction vectors, in the form of moments and shear forces, are denoted by:

$$\sigma = \begin{bmatrix} m_{xx} & m_{xy} \\ m_{xy} & m_{yy} \end{bmatrix}^T, \quad \tilde{t} = \begin{bmatrix} m_{nn} \\ r_n \end{bmatrix}^T \text{ where } r_n = q_n + \frac{\partial m_{ns}}{\partial s}$$

(1)
in terms of the normal and tangential components of moment and shear force, where \( \overline{r}_n \) denotes the equivalent shear force on a boundary. We also have:

\[
\varepsilon = D_K w \text{ where } D_K = \begin{bmatrix}
\frac{\partial^2}{\partial x^2} & 0 \\
\frac{\partial^2}{\partial y^2} & 0 \\
2 \frac{\partial^2}{\partial x \partial y}
\end{bmatrix} = \begin{bmatrix}
\frac{\partial}{\partial x} & 0 \\
0 & \frac{\partial}{\partial y} \\
\frac{\partial}{\partial y} & \frac{\partial}{\partial x}
\end{bmatrix} = -D_2 D_4,
\]

(2)

and \( D_K^T \sigma + p = 0 \) where \( D_K = -D_K^T = \begin{bmatrix}
\frac{\partial^2}{\partial x^2} & \frac{\partial^2}{\partial y^2} & 2 \frac{\partial^2}{\partial x \partial y}
\end{bmatrix} \begin{bmatrix}
D_1^T \\
D_2^T
\end{bmatrix}^T \)

In Equation (2), \( p \) denotes the transverse pressure load.

The strong form of equilibrium can be written in the form of the virtual work Equation (3).

\[
\int_{\Omega} (D_K w)^T \sigma d\Omega = \int_{\Omega} wp d\Omega - \int_{\Gamma} (D_K^T w) e d\Gamma + \int_{\Gamma} \left( -\frac{\partial w}{\partial n} m_{nn} - \frac{\partial w}{\partial s} m_{ns} + w q_n \right) d\Gamma
\]

(3)

for all kinematically admissible deflection fields \( w \). \( e \) denotes a prescribed field of couples. A conforming finite element model only satisfies Equation (3) for \( w = w_h \in U_h \) where space \( U_h \) contains the finite element functions of deflection, and then we term this equation the weak form of equilibrium.

3. Fictitious loads on star patches.

A star patch of elements consists of those connected to one vertex, as illustrated in Figure 1 for vertex \( i \). Over the patch we define a piecewise linear PU function \( \Psi_i = 1 \) at vertex \( i \).

The strong form of equilibrium can be written in the form of the virtual work Equation (3).

\[
\int_{\Omega} (D_K w)^T \sigma d\Omega = \int_{\Omega} wp d\Omega - \int_{\Gamma} (D_K^T w) e d\Gamma + \int_{\Gamma} \left( -\frac{\partial w}{\partial n} m_{nn} - \frac{\partial w}{\partial s} m_{ns} + w q_n \right) d\Gamma
\]

(3)

for all kinematically admissible deflection fields \( w \). \( e \) denotes a prescribed field of couples. A conforming finite element model only satisfies Equation (3) for \( w = w_h \in U_h \) where space \( U_h \) contains the finite element functions of deflection, and then we term this equation the weak form of equilibrium.

3. Fictitious loads on star patches.

A star patch of elements consists of those connected to one vertex, as illustrated in Figure 1 for vertex \( i \). Over the patch we define a piecewise linear PU function \( \Psi_i \) which has unit value at the vertex and zero value on the sides of the patch not connected to the vertex. The prescribed loads on a patch are weighted by \( \Psi_i \) and in general such loads are not balanced.

When we express displacement \( w_h = \Psi_i v \) with scalar field \( v \), the internal generalised strain (curvature) becomes:

\[
D_K w = -D_2 \left( D_1 (\Psi_i v) \right) = -D_2 \left( \Psi_i^T D_1 v + v D_1^T \Psi_i \right) = \Psi_i^T \left( D_K v \right) - \left( D_2 \Psi_i^T \right) D_1 v + v \left( D_K \Psi_i^T \right) - \left( D_2 v \right) D_1 \Psi_i.
\]

281
If \( v \) represents a rigid body displacement, \( D_K v = 0 = D_K \Psi_i \), and since in any case \( (D_2 v) D_i \Psi_i = (D_2 \Psi_i) D_i v \), then:

\[
D_K (\Psi_i v) = -2 (D_2 \Psi_i) D_i v
\]

for all deflections \( v \). Thus since \( \Psi_i v \) is then piecewise quadratic, and the minimum degree of a fully conforming element is 5, it is correct to assume that \( \Psi_i v \in U_h \).

Then Equation (3) can be rearranged to give (5) where \( \sigma^e \) represents the stress-resultants from the conforming solution, and the terms highlighted in red indicate fictitious loads that are necessary to balance the loads on a patch and present a well posed problem for further analysis.

\[
0 = \int_{\Omega_i} v \left( \Psi_i p - \left( D_i^T \Psi_i \right) e \right) d\Omega - \int_{\Omega_i} \left( D_i^T v \right) \left( \Psi_i e - 2 \left[ D_i^T \Psi_i \right] \sigma^e \right) d\Omega \]
\[
- \int_{r_i} \left( v \frac{\partial \Psi_i}{\partial n} m_{nn} + v \frac{\partial \Psi_i}{\partial s} m_{ns} \right) d\Gamma - \int_{r_i} \left( \frac{\partial v}{\partial n} \Psi_i m_{nn} + \frac{\partial v}{\partial s} \Psi_i m_{ns} - v \Psi_i q_n \right) d\Gamma
\]

Hence we see that we obtain a balanced load on a patch provided we include with the partitioned loads on an element:

- a fictitious pressure field on an element: \( \hat{p}_{ie} = - D_i^T \Psi_i e \), and
- a fictitious couple field on an element: \( \hat{c}_{ie} = -2 \left[ D_i^T \Psi_i \right] \sigma^e \).
- fictitious transverse shear forces on the sides: \( \hat{q}_i = - \left( \frac{\partial \Psi_i}{\partial n} m_{nn} + \frac{\partial \Psi_i}{\partial s} m_{ns} \right) \)

It should be noted that a field of couples can be replaced by a statically equivalent pressure and boundary shear forces.

4. Equilibrating solutions from analyses of star patches with hybrid equilibrium elements.

In this section we outline the analyses of star patches with balanced loads derived from the conforming model. Analysis requires each conforming element to be replaced by a hybrid equilibrium element of appropriate degree [5]. For a generic hybrid element \( e \) we assume internal polynomial moment fields \( \sigma_e \) and transverse displacements \( v_m \) of the boundary entities \( m \) of an element, i.e. its sides and vertices, as in Equation (6):

\[
\sigma_e = S_e \hat{s}_e + \sigma_{e0} \quad \text{and} \quad v_m = V_m \hat{v}_m
\]

where (i) \( S_e \) contains the moment basis for an element with each moment field in equilibrium with zero pressure or body forces, and \( \sigma_{e0} \) is a particular moment field that equilibrates with the weighted prescribed and fictitious loads on a patch; and (ii) \( V_m \) contains the displacement basis independently approximated using polynomials for the sides of the same degree as for the moments, and for a vertex, \( V_m \) is just the 1x1 unit matrix.

4.1 Equilibrium

With equilibrium satisfied within an element, it remains to enforce codiffusivity of boundary tractions or equilibrium with weighted prescribed tractions \( \left( \Psi_i T_e \right) \) and fictitious shear forces \( q_i \) on a boundary. For the hybrid elements this requires for entity \( m \) in star patch \( i \):

\[
\sum_e \int_{r_e \Gamma_m} V_m^T \left( \Psi_i T_e \right) d\Gamma = \int_{r_e \Gamma_m} V_m^T \left( \Psi_i T_e \right) + \text{fictitious terms} \right) d\Gamma
\]
4.2 Compatibility
A weak form of compatibility for the hybrid equilibrium model is expressed element-wise:

\[
\int_{\Omega_e} S_e^T \left( f \sigma_e^f \right) d \Omega = \int_{\Omega_e} S_e^T \left( \Psi_i \epsilon \right) d \Omega.
\] (8)

where the generalised strain \( \epsilon = D_K w \) are the total curvatures from the compatible model. Since

\[
D_K (\Psi_i w) = \Psi_i D_K w - 2 (D_2 \Psi_i) (D_i w), \quad \Psi_i \epsilon = \Psi_i D_K w = D_K (\Psi_i w) + 2 (D_2 \Psi_i) (D_i w),
\]

after integration by parts we obtain:

\[
\int_{\Omega_e} S_e^T \left( f \sigma_e^f \right) d \Omega = \int_{\Gamma_i} \left( S_e^T N_{i_1} D_i \right) (\Psi_i w) d \Gamma + \int_{\Gamma_i} \left( N_{i_2}^T D_i^T S_e \right)^T (\Psi_i w) d \Gamma + 2 \int_{\Omega_e} S_e^T (D_2 \Psi_i) (D_i w) d \Omega
\] (9)

where \( N_{i_1}^T \) projects moment fields, and \( N_{i_2}^T \) projects derived shear forces, onto the sides of an element. The boundary integrals on the right hand side are approximated by using the side and vertex displacements of the hybrid model, and the third integral involves

- fictitious initial curvatures: \(-2 (D_2 \Psi_i) (D_i w)\).

If the deflection field of the conforming element is of degree 5, then its moments are of degree 3 and this is the same degree as the fictitious couples. In order that these are equilibrated in a hybrid equilibrium model of a patch, their moment fields must be of degree \( \geq 4 \). Then their side rotations are of the same degree, with side translations of degree \( \geq 3 \). A moment field of degree 4 in the hybrid assumes that prescribed pressures are linear and prescribed couples are quadratic for the conforming model.

The equilibrium and compatibility equations for the elements and boundary entities of each star patch are assembled and solved to obtain \( \sigma_e^f \) [4,5,6]. The total equilibrating stress field is then formed by the summation \( \sigma_e = \sum \sigma_e^f \).

5. Conclusions

This paper has explained how the numerical technique developed for 2D models of membrane problems [4] can be extended to cover bending of thin plates. This technique has the advantage for plates of using fully stable triangular hybrid equilibrium elements which do not suffer from spurious kinematic modes [5]. The process has been validated for the membrane case in [4], and further work is required to demonstrate its effectiveness, or otherwise, for the case of thin plates.

References


Effective high-fidelity nonlinear analysis of metal sandwich panels using partitioned modelling

Alexander N. Nordas ¹, Luis P.F. Santos ¹, *Bassam A. Izzuddin ¹ and Lorenzo Macorini ¹

¹Department of Civil and Environmental Engineering, Imperial College, London SW7 2AZ, UK
*b.izzard@imperial.ac.uk

ABSTRACT

The considerably superior specific strength and stiffness of sandwich panels in relation to conventional structural components makes their employment for structural engineering applications a highly attractive alternative. An accurate description of the associated mechanical response and encountered failure modes requires highly sophisticated detailed finite element models, capable of capturing geometric and material nonlinearity both globally and locally. The associated discretisation level can render extensive static or dynamic nonlinear analysis impractical, or even impossible, in relation to the associated computational demand when conventional modelling and solution procedures are employed. An effective high-fidelity numerical modelling strategy is proposed in this paper, coupled with an advanced partitioned modelling approach. The latter involves the decomposition of a parent structure into several child partitions, where individual partitions are processed in parallel and their compatibility and equilibrium at the partition boundaries are considered at the parent level.

The implementation of the aforementioned approach on a High Performance Computing (HPC) system leads to a massive reduction of the required computing time and resources, thereby rendering extensive detailed nonlinear analysis of large scale metal sandwich panels a practical prospect. The proposed methodology has been employed for the response evaluation of various panel configurations with core topologies commonly employed in industrial applications, under extreme static loading. An advanced mesh generation tool has been developed for this purpose, which further allows for effective domain partitioning. Two numerical examples are presented in the paper to illustrate the effectiveness and accuracy of the proposed methodology.

Keywords: Metal sandwich panels; Nonlinear analysis; Partitioned modelling; High-fidelity models

1. Introduction

Metal sandwich panels can be classified as composite structural components, comprising two thin and stiff plates connected to a structural core of discrete geometric configuration via adhesion or welding. The core provides essential versatility to the composite mechanical response by maintaining a constant distance between the plates and thereby enhancing the flexural stiffness in a similar fashion to the web of an I-beam, while further serving as the principal load transferring and shear resistance mechanism. Due to the discrete configuration of the core, its beneficial action comes at a minimal weight trade-off and therefore sandwich panels attain considerably enhanced stiffness and strength characteristics in comparison to solid components of equivalent weight. The intrinsically high specific strength (strength-to-weight ratio) and stiffness (stiffness-to-weight ratio) of composite sandwich components renders their employment for structural engineering applications a highly attractive alternative, which subsequently calls for an extensive investigation of their ultimate response and the associated global and local failure modes.

Sandwich panels subjected to extreme static or dynamic loading are rendered susceptible to a wide range of failure modes, mainly associated with the manifestation of localised instabilities and buckling of the plated components of the top and bottom plates and the core. An accurate capturing of these calls for an extensive discretisation of the panel domain with geometrically nonlinear finite elements, alongside the employment of detailed nonlinear material constitutive models. The aforementioned requirements often render extensive nonlinear analysis of large-scale sandwich panel systems prohibitively demanding or impossible, due to the physical limitations imposed by computing resources. In the present paper an effective high-fidelity modelling strategy is proposed, which allows for the effects of geometric and material nonlinearity on the panel response to be effectively captured. The proposed methodology is coupled with a partitioned modelling scheme implemented on a HPC environment, which allows for memory bottlenecks to be effectively overcome and significant speedup to be achieved in comparison to the conventional monolithic approach.
2. High-fidelity finite element modelling of large-scale metal sandwich panels

The plates and the core of sandwich panels have been discretised with 9-node quadrilateral or 6-node triangular shell elements [5], formulated in a co-rotational framework which guarantees enhanced accuracy and convergence for large displacement and rotation, but small strain, problems through the exclusion of the rigid body motion influence from the local element response [3]. Furthermore, a sophisticated optimisation methodology, readily embedded in the formulation of the employed co-rotational shell elements, allows for the elimination of the various potentially encountered shear, membrane and distortion locking phenomena, often leading to a significant accuracy deterioration in the evaluated response under large deformations [1], [5]. A triaxial elastoplastic constitutive model for mild steel has been adopted, allowing for the effects of material nonlinearity, strain hardening and strain rate on the panel response to be accurately captured.

The detailed finite element models have been generated using a versatile mesh generation computing tool, developed to allow for the plates and core modelling to any desired level of discretisation detail and enhanced with domain partitioning capabilities. The adopted strategy has been implemented in ADAPTIC, a highly sophisticated general finite element code for nonlinear analysis of structures under extreme static or dynamic loading [2]. A broad spectrum of sandwich panels with core configurations commonly employed in construction and industrial applications have been considered and an extensive comparative evaluation of their ultimate response under extreme static loading has been performed. Honeycomb and prismatic corrugated core topologies have been identified as the most efficient, with rectangular and hexagonal honeycomb core configurations prevailing as the alternatives with the highest potential for employment in structural engineering applications. The finite element mesh for these configurations is illustrated in Figure 1, where the level of the achieved discretisation detail both globally and at the cell level is clearly highlighted.

![Figure 1: High-fidelity detailed finite element modelling of rectangular (top) and hexagonal (bottom) honeycomb core sandwich panels with 9-node and 6-node co-rotational shell elements](image)

3. Partitioned modelling of large-scale metal sandwich panels

In computational structural mechanics problems where finite element procedures are employed for domain discretisation, the computational demand is inextricably related to the numerical solution of the algebraic system of nonlinear equations describing the static or dynamic system equilibrium for a given set of essential and natural boundary conditions. The size of the aforementioned nonlinear system is determined by the amount of nodal degrees of freedom (DOF) employed for the domain discretisation and therefore increases significantly when a very dense or large-scale mesh is required for the problem description, imposing a massive demand on computing resources.

Several procedures to alleviate these inefficiencies have been proposed over the years, with domain decomposition being the most effective and commonly employed methodology. In the current application, a highly efficient partitioned modelling approach has been adopted, involving the
decomposition of the panel structural domain (parent structure) into dual super-elements along the partitioned boundary, each representing a child partition [4]. In turn, each child partition is discretised with geometrically nonlinear finite elements, in accordance with the modelling methodology outlined in Section 2. Dual super-elements allow for the parent and individual child partitions to be analysed in parallel as separate processes, where the compatibility and equilibrium at the partition boundaries are considered at the parent level. A schematic representation of the adopted strategy is given in Figure 2, for a large-scale rectangular honeycomb core sandwich panel model decomposed into 4 partitions.

Figure 2: Partitioned modelling of a rectangular honeycomb core sandwich panel with 4 child partitions

The implementation of the proposed methodology [4] in a High Performance Computing (HPC) environment with process parallelisation capabilities led to a massive reduction of the computing time and resources associated with extensive nonlinear analyses of the panel models under extreme loading, compared to conventional modelling procedures or serial processing of individual partitions.

4. Numerical Examples

The performance efficiency of different partitioned modelling schemes has been assessed based on the results obtained by extensive nonlinear analyses of large-scale metal sandwich panels under extreme static loading. A comparative evaluation has been performed on the basis of the associated computational demand, which is assumed to be reflected by the computing time required for the respective nonlinear analyses, when the same computing resources per analysis are allocated. A square rectangular honeycomb core sandwich panel with welded core strips, 3m global dimensions, 100mm x 100mm cell planar dimensions and an effective height (distance between top and bottom plate mid-planes) of 100mm has been adopted as a base case for the analyses. The panel is simply supported along all 4 edges and is subjected to Uniformly Distributed Loading (UDL) and localised loading applied centrically on the panel, over a 300mm x 300mm patch (PL). For each load case, besides the monolithic model, 4 different domain partitioning schemes have been considered, with 2-by-2, 3-by-3, 4-by-4 and 5-by-5 partitions along the global X and Y axes, respectively.

The implementation of the adopted partitioned modelling methodology results into an outstanding reduction of the wall time, achieving a speedup factor of 2 in comparison to the monolithic model with the use of just 4 partitions. Further speedup is achieved for an increased number of partitions, up to a factor of 4 for 25 partitions, with a decreasing relative efficiency rate between successive schemes, as observed in Figure 3(b). The nonlinear response obtained by the monolithic model is identical with those of the partitioned models and is illustrated in Figure 3(a). The efficiency of a specific scheme can qualitatively be related to the ratio of the number of nodes along the partition boundary to the number of nodes within the partition domain, for each partition. The progressive efficiency deterioration observed for an increased number of partitions can therefore be attributed to the decrease of the aforementioned ratio, which compromises the essence of the method, i.e. accelerating processing by shifting the focus from the nodes within the partition domain to the nodes along the partition boundary. The adopted modelling strategy allowed for both the global failure mode of the panel, involving the progressive formation of yield lines, and the local buckling phenomena at the centre and the 4 corners to be accurately captured, as illustrated in Figure 3(c) for the PL case.
5. Conclusions

This paper presents a high-fidelity methodology for the nonlinear analysis of large-scale metal sandwich panels, coupled with a partitioned modelling scheme which allows for parallel processing of individual partitions in a HPC system. The proposed strategy enables the detailed evaluation of the panel nonlinear response, while achieving a speedup factor of up to 4, resulting from a 75% reduction of the associated wall time. The potential and significance of the method become highly profound in cases where computing resources limitations render nonlinear analyses prohibitively demanding or infeasible.

Acknowledgements

The support of the High Performance Computing (HPC) Services at Imperial College London is gratefully acknowledged by the authors.

References


Design-Oriented Mechanical Models for Local Buckling Assessment of Sandwich Panels with Metal Cores

Luis Santos, Alexander N. Nordas, Bassam A. Izzuddin and Lorenzo Macorini
Department of Civil and Environmental Engineering
Imperial College, London, SW7 2AZ
http://www.imperial.ac.uk/csm

ABSTRACT

Modern design methods for sandwich panels must attempt to maximise the potential of such systems for weight reduction and achieve highly optimised structural components. A successful design method for large-scale sandwich panels requires the consideration of every possible failure mode. An accurate prediction of the various failure modes is not only necessary but it should also be using a simple approach that is suitable for practical application. To fulfil these requirements, a mechanics-based approach is proposed in this paper to assess local buckling phenomena in sandwich panels with metal cores. This approach employs a rotational spring analogy for evaluating the geometric stiffness in plated structures, and it is employed with realistic assumed modes for plate buckling leading to accurate predictions of local buckling. In developing this approach for sandwich panels with metal cores, such as those with a square honeycomb structure, due account is taken of the stiffness of adjacent co-planar and orthogonal plates and its influence on local buckling. In this respect, design-oriented models are proposed for core compressive buckling, core shear buckling and top plate intercellular buckling, considering typical metallic core topologies. Finally, the proposed design-oriented models are verified against detailed nonlinear finite element analysis, highlighting the accuracy of buckling predictions and the implications of the post-buckling response.

Keywords: Metallic Sandwich Panels; Buckling; Plated Structures; Rotational Spring Analogy

1. Introduction

Sandwich systems are recognised for achieving enhanced structural performance at minimal weight, becoming attractive for applications where saving weight is a fundamental objective. Maximising the potential for weight savings requires a relatively accurate design method to be established, and to increase the practical applicability for sandwich panels a design approach based on a simple methodology is required. Achieving an accurate and practical design methodology requires a comprehensive understanding of possible failure modes, with plate buckling constituting an integral part of such a methodology. The plate buckling capacity can be predicted in several ways, ranging from simple analytical expressions based on idealised support conditions to complete geometric and material nonlinear analysis accounting for initial imperfections, thus achieving different degrees of accuracy obtained with methods of different sophistication and computational demand. A mechanics-based approach is proposed here for predicting the local buckling of plates and assessing the buckling performance of rectangular honeycomb sandwich panels. Intercellular buckling, core compressive buckling and core shear buckling are considered, as they are identified as the critical buckling failure modes for metallic sandwich panels.

The critical buckling stress $\sigma_{cr}$ and critical buckling load $N_{cr}$ for plates can be generally written as:

$$\sigma_{cr} = \frac{k \cdot \frac{\pi^2 \cdot E}{12 \cdot (1 - \nu^2)}}{b \cdot t_f} \cdot \left(\frac{t_f}{b}\right)^2; \quad \sigma_{cr} = \frac{N_{cr}}{t_f}; \quad N_{cr} = \frac{k \cdot \pi^2 \cdot D}{b^2}$$

where $D = \frac{E \cdot t_f^2}{12 \cdot (1 - \nu^2)}$ is the plate bending stiffness, $t_f$ is plate thickness, $\nu$ is the Poisson ratio, $b$ is a dimension of the plate and $k$ is the buckling coefficient that is defined by the restraint conditions along the plate boundaries. Throughout the years, the definition of the buckling coefficient, hence the corresponding buckling load, has been mathematically achieved for idealized support conditions and
loadings. Where the support conditions are mixed, the calculation of the buckling coefficient becomes more complex, where a methodology based on the energy method can be advantageous.

The rotational spring analogy (RSA) [2] enables the geometric stiffness to be expressed based on first-order kinematics, allowing buckling phenomena to be described with linear relations between degrees of freedom and the equivalent spring rotations. This analogy provides a simplified approach for the assessment of buckling loads using common notions from linear structural analysis. The establishment of a mechanics-based design approach enables the critical buckling load associated with different failure modes to be evaluated and subsequently implemented in an optimisation algorithm entirely based on analytical expressions.

2. Plate buckling

The detailed response of a rectangular honeycomb (Figure 1-a) sandwich panel under flexural loads is defined by the sandwich effect: the core resists shear loads while stabilising the top and bottom plates which act together to form a stress couple resisting the external bending moment. This implies that the top plate stiffened by the core might buckle under biaxial compressive stress, mentioned as intercellular buckling. The analysis framework for intercellular buckling is presented in Figure 1:

![Figure 1: Simplified analysis framework for intercellular buckling](image)

An accurate estimation of the critical buckling load is often possible using a single approximation mode. For simply supported or clamped conditions, the RSA produces the exact critical load when employing the exact shape function \( w(x,y) \) using the Rayleigh quotient [1]. Table 1 summarises the single modes, available in the literature for each of the critical buckling failure modes:

<table>
<thead>
<tr>
<th>Intercellular Buckling (Biaxial Loading)</th>
<th>Simple supports</th>
</tr>
</thead>
<tbody>
<tr>
<td>( w(x,y) = \sin \left( \frac{m \cdot \pi \cdot x}{a} \right) \sin \left( \frac{n \cdot \pi \cdot y}{b} \right) )</td>
<td>(2)</td>
</tr>
<tr>
<td>Fixed supports</td>
<td></td>
</tr>
<tr>
<td>( w(x,y) = \left[ 1 - \cos \left( \frac{2 \cdot \pi \cdot x}{a} \right) \right] \left[ 1 - \cos \left( \frac{2 \cdot \pi \cdot y}{b} \right) \right] )</td>
<td>(3)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Shear Buckling</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple supports</td>
</tr>
<tr>
<td>( w(x,y) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \sin \left( \frac{m \cdot \pi \cdot x}{a} \right) \sin \left( \frac{n \cdot \pi \cdot y}{b} \right) )</td>
</tr>
<tr>
<td>Fixed supports</td>
</tr>
<tr>
<td>( w(x,y) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \sin \left( \frac{m \cdot \pi \cdot x}{a} \right) \sin \left( \frac{n \cdot \pi \cdot y}{b} \right) )</td>
</tr>
</tbody>
</table>

As in the Rayleigh quotient, the accuracy of the RSA is dependent on the assumed approximation modes. According to Wong [4], the mode in (3) can only be used to accurately predict the buckling load of clamped plates under uniform biaxial compressive stress.

To estimate the intercellular buckling capacity of a sandwich panel, a MDOF system has to be used to account for the rotational stiffness of the core plates. The implementation of the RSA to MDOF problems is formulated similar to Rayleigh-Ritz variational method [1]:

\[
w(x,y) = u_1 \cdot \phi_1(x,y) + u_2 \cdot \phi_2(x,y) + u_3 \cdot \phi_3(x,y) + \ldots + u_n \cdot \phi_n(x,y) = [\Phi] [u]
\]

where \( \Phi \) = matrix of deformations modes, and \( u \) = vector of unknown coefficients.
To assess the influence of a rotational spring along the edge of a plate, the deflected shape is considered as a linear combination of the approximation modes for simply supported (mode (2)) and clamped plates (mode (3)). Based on the RSA, the geometric stiffness matrix is obtained as follows:

$$ K_G = \int T_\theta^T \cdot \text{diag} (k_\theta) \cdot T_\theta \, dx \, dy $$

(7)

where $k_\theta$ represents the stiffness of the equivalent rotational springs distributed over the area of the plate, which is equal to the respective compressive loads, $T_\theta$ expresses the first-order kinematic relationship between rotations and the unknown coefficients.

The contribution to the material stiffness of a uniform rotational spring $K_s$ is obtained from the rotation on the supported edge ($T_s$) on every approximation mode. The plate material stiffness is obtained using the deformation matrix $B$. Assuming linear elastic isotropic material:

$$ K_E = \int B^T \cdot D \cdot B \, dx \, dy + 2 \cdot \int T_{\theta x}^T \cdot K_s \cdot T_{\theta y} \, dx + 2 \cdot \int T_{\theta y}^T \cdot K_s \cdot T_{\theta y} \, dy $$

(8)

$$ u \cdot T_{xx} = \frac{\partial w}{\partial x}; \quad u \cdot T_{xy} = \frac{\partial w}{\partial y}. $$

(9)

The buckling coefficient, corresponding to an interaction between the assumed modes, is postulated as an eigenvalue problem, in which the critical load is obtained for neutral equilibrium conditions.

The predictions of the proposed analytical method are presented in Figure 2 for three different aspect ratios ($a/b$), where a favourable comparison is achieved against the results of finite element analysis for a varying rotational stiffness along the edge (Figure 1-d). Theoretical values for the buckling coefficient are also included for simple supported (SSSS) and fixed supported (FFFF) conditions.

![Figure 2: Buckling coefficient k for variable spring rotational stiffness – biaxial compression](image)

Compressive buckling of the core plates is not presented as it is a special case of the discussed methodology applied for uniaxial compressive stress. A favourable comparison of the results from the analytical model and finite element analysis applied to shear buckling is presented in Figure 3.

![Figure 3: Buckling coefficient k for varying spring rotational stiffness – Shear (modes (4) and (5))](image)

3. **Intercellular buckling**

Finite element models are developed using ADAPTIC [3] to investigate the accuracy of using the RSA to predict the effect of the core plates on the buckling of the top plate. As the side plates are connected to each other to form a cell, the value for the stiffness of the rotational spring can no longer be constant. The assumed variation is based on the deflected shape observed in the finite element analysis (Figure 4-a), and it is approximated by the shape function considering fixed support conditions on the base of the cell (for plates, $K_s = M/\theta = 4D/L$) and between adjacent core plates (variation along the side). The stiffness of the equivalent spring along the edge is computed as follows:
\[ K_s(x) = \frac{4 \cdot D_{\text{side}}}{h} \cdot 2 \left( 1 - \cos \left( \frac{2 \cdot \pi \cdot x}{a} \right) \right); \quad K_s(y) = \frac{4 \cdot D_{\text{side}}}{h} \cdot 2 \left( 1 - \cos \left( \frac{2 \cdot \pi \cdot y}{b} \right) \right); \]

(10)

where \( h \) is the height of the cell, and \( D_{\text{side}} \) is the flexural stiffness of the side plate.

For the design of a rectangular panel, as for the 3x3 model to be presented, half of the stiffness is used for the equivalent spring to reflect the fact that a single plate will support two adjacent cells.

Results for the single cell (Figure 1-c) model are presented in Figure 4-b, including a favourable comparison of buckling coefficients obtained from the analytical model and finite element analysis for a varying thickness of the side plates as well as the theoretical values for simple and fixed supports.

Figure 4: Buckling coefficient \( k \) for varying thickness of the side plates – biaxial compression, single cell model

Results are presented in Figure 5-a for the 3x3 cell model (Figure 1-b), including a favourable comparison of buckling coefficients obtained from the analytical model and finite element analysis for a varying thickness of the core plates, modelled with sympathetic imperfections. Theoretical values for the buckling coefficient are also included for simple and fixed supports. Figures 5-b and 5-c depict the deformed shapes of the model for a core plate with thickness of 0.5 mm and 10 mm, respectively.

Figure 5: Buckling coefficient \( k \) for varying thickness of the core plates – biaxial compression, 3x3 cell model

4. Conclusion

A mechanics-based design methodology is proposed to assess the buckling load of the critical failure modes for rectangular honeycomb sandwich panels. Verification is undertaken against the results of detailed nonlinear finite element analysis, focusing on intercellular buckling. The analytical method, based on the rotational spring analogy, is shown to provide an accurate yet practical approach for buckling assessment of plates in all-metal sandwich panels.

References


291
Realistic Modelling of Irregular Floor Slabs under Extreme Loading

Stanyslav Grosman and Bassam A. Izzuddin

Department of Civil and Environmental Engineering, Imperial College, London, SW7 2AZ

http://www.imperial.ac.uk/csm

ABSTRACT

This paper presents a new triangular flat shell element for composite and reinforced concrete (RC) slabs of complex planar configuration subjected to extreme loading. The element incorporates the effects of geometric as well as material nonlinearities. The element is developed within a co-rotational framework, where the influence of geometric nonlinearity is accounted for via the transformation between local co-rotational and global reference systems. To improve the approximation of the solution and deal with shear locking, additional hierarchic freedoms are introduced within the local system of the element, providing an option to activate additional higher-order quadratic approximation for the element shape functions. The benefits of this approach include an increased efficiency of transformation of stiffness matrix from local to global coordinate system and ensuring that the transverse displacement shape functions are always one order higher than those used for nodal rotations. The element formulation allows for composite action between different layers under the assumption of perfect bond between the slab concrete material, the reinforcement layers and the steel deck for composite slabs. The paper describes briefly the element formulation, which verified using several numerical examples.

Keywords: Concrete structures; Finite elements; Nonlinear analysis; Slabs; Floors

1. Introduction

For quite some time, the tendency of modern day architects to use singular and non-repeatable shapes has been gaining popularity. There are numerous types of such irregularities: different floor shapes over the height of building structures, inclination of a structure, shapes that twist with each floor, etc. These unique features make such buildings aesthetically pleasing and as such financially attractive. To ensure that the described structures are sufficiently safe, detailed numerical modelling under extreme loading, such as due to blast and earthquakes, is typically required. The most complex part of the numerical modelling process is related to the representation of 2-D continuous bodies such as slabs and walls. The most robust way of discretising irregular 2D continuum structures is based on triangular meshes. Towards this end, a new 2-D shell element has been developed to effectively deal with irregularly shaped floor slabs. This element combines the computational efficiency of three nodded elements with modelling accuracy achieved by incorporation of quadratic and cubic terms into the shape functions, taking into account both geometric and material nonlinearities. In contrast with a rectangular shell element for composite slabs developed by Izzuddin et al. [6], the proposed element allows for arbitrary slab shapes and rebar orientations. These properties allow the proposed element to be used in modelling irregular floor slabs under extreme conditions, including those due to fire, blast and earthquake loading. In addition, the element is applicable to the modelling of concrete slabs strengthened with strips of composite material.

The following assumptions are made in developing the new element:

1. The concrete slab depth and the thickness of the composite steel deck are uniform;
2. Up to two layers of orthogonal steel reinforcement are used;
3. The reinforcement responds uniaxially in the direction of the rebar;
4. Perfect bond exists between concrete and both reinforcement and the steel deck;
5. Direct out-of-plane stresses in the concrete are negligible.

The following section describes the formulation of the new shell element, which has been developed within a co-rotational approach that account for geometric nonlinearity via transformations between the local co-rotational and the global reference systems. The element has been implemented within the nonlinear structural analysis program ADAPTIC [3], which is used in this paper to provide verification of the element.
2. Kinematics of composite triangular element

The proposed kinematic description, representing the Reissner–Mindlin hypothesis, is formulated with reference to a local Cartesian coordinates system, with the origin located at the node 1 of the slab and local X-axis passing through node 2, as depicted in Figure 1. In addition area coordinates, are employed for shape function formulation to simplify the derived expressions.

The kinematic dependency that determines the displacement field \((u, v, w)\) in terms of area coordinates \((\lambda_1, \lambda_2, \lambda_3)\) is related to the reference planar displacements \((u_p, v_p, w_p)\) and rotations of the normal \((\theta_x, \theta_y)\) by the following expressions:

\[
egin{align*}
    u(\lambda_1, \lambda_2, \lambda_3) &= u_p(\lambda_1, \lambda_2, \lambda_3) - Z \cdot \theta_y(\lambda_1, \lambda_2, \lambda_3) \\
    v(\lambda_1, \lambda_2, \lambda_3) &= v_p(\lambda_1, \lambda_2, \lambda_3) - Z \cdot \theta_x(\lambda_1, \lambda_2, \lambda_3) \\
    w(\lambda_1, \lambda_2, \lambda_3) &= w_p(\lambda_1, \lambda_2, \lambda_3)
\end{align*}
\]

(1)

where area coordinates are related to local element coordinates by (2), with \(A_2\) standing for double the element area:

\[
\lambda_1 = 1 - \frac{X \cdot y_3 - Y \cdot x_3}{A_2}; \quad \lambda_2 = \frac{X \cdot y_3 - Y \cdot x_3}{A_2}; \quad \lambda_3 = \frac{Y}{y_3}
\]

(2)

Using derivatives of (1) the following relation for element strains can be obtained:

\[
\varepsilon_x = \frac{\partial u_p}{\partial X} - Z \frac{\partial \theta_y}{\partial X}; \quad \varepsilon_y = \frac{\partial v_p}{\partial Y} - Z \frac{\partial \theta_x}{\partial Y}; \quad \gamma_{xy} = \frac{\partial u_p}{\partial Y} + \frac{\partial v_p}{\partial X} - Z \left( \frac{\partial \theta_y}{\partial X} + \frac{\partial \theta_x}{\partial Y} \right); \quad \gamma_{xZ} = -\theta_y; \quad \gamma_{yZ} = -\theta_x
\]

(3)

where derivatives of reference fields \((\psi)\) can be obtained in the local system from:

\[
\frac{\partial \psi}{\partial X} = \sum_{j=1}^{n_\psi} \frac{\partial \psi}{\partial \lambda_j} \frac{\partial \lambda_j}{\partial X}; \quad \frac{\partial \psi}{\partial Y} = \sum_{j=1}^{n_\psi} \frac{\partial \psi}{\partial \lambda_j} \frac{\partial \lambda_j}{\partial Y}
\]

(4)

Strains in the rebar can be obtained as a sum of projections of element planar strains on the rebar orientation \(a\) (see Figure 1):

\[
\varepsilon_a = \varepsilon_x \cdot \cos(\alpha)^2 + \varepsilon_y \cdot \sin(\alpha)^2 + \gamma_{xy} \cdot \sin(\alpha) \cdot \cos(\alpha);
\]

(5)

For the steel deck, strains can be deduced from (4), by taking \(Z\), equal to \(h/2\).

3. Local element response

The kinematic relationships in the previous section are presented as a relationship between the element strains and the planar displacements \((u_p, v_p, w_p)\) and the normal rotations \((\theta_x, \theta_y)\). These fields are
discretised in terms of basic and hierarchic element degrees of freedom (DOF) using polynomial shape functions as described in [6]. The general form for element discretised displacement is as follows:

\[ \psi = \sum_{i=1}^{n} N^L_i \psi_i + \left[ \sum_{i=1}^{n} N^Q_i \psi_i + \sum_{i=1}^{n} N^C_i \psi_i \right]. \]  

(6)

where \( \psi_i \), \( \psi_i \), \( \psi_i \) represent nodal DOF, hierarchic DOF related to quadratic shape functions and hierarchic DOF related to cubic shape functions, respectively. The linear nodal shape functions as well as the quadratic and cubic hierarchic shape functions are defined in the area coordinate system as follows:

\[ N^L_i = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix}; \quad N^Q_i = 4 \cdot \begin{bmatrix} \lambda_1 \cdot \lambda_2 \\ \lambda_2 \cdot \lambda_3 \\ \lambda_3 \cdot \lambda_1 \end{bmatrix}; \quad N^C_i = 6 \cdot \sqrt{3} \begin{bmatrix} \lambda_1 \cdot \lambda_2 \cdot (\lambda_3 - \lambda_1) \\ \lambda_2 \cdot \lambda_3 \cdot (\lambda_1 - \lambda_2) \\ \lambda_3 \cdot \lambda_1 \cdot (\lambda_2 - \lambda_3) \end{bmatrix}. \]  

(7)

One of the benefits of employing hierarchic DOF is that the element can be used in either linear or higher-order form which allows for a more versatile modelling of complex problems. Another benefit of the hierarchic formulation is that inclusion of these additional DOF does not change the way the co-rotational large displacement approach is implemented. As an added benefit, the hierarchic formulation also allows for transverse displacement shape function to be always one order higher than the rotations of the normal, which reduces shear locking effects [2].

The element force vector and tangent stiffness matrix can be assembled as the sum of contributions from individual materials, i.e. concrete, rebar and steel deck, where each contribution can be readily determined by implementing a Gauss quadrature rule [1] for numerical integration.

It is necessary to mention that while the above local formulation accounts for material nonlinearity, it excludes local geometric nonlinearity. However, the incorporation of the element with a co-rotational framework enable the consideration of geometric nonlinearity, where the influence of local geometric nonlinearity becomes less significant with mesh refinement, as is typically required for modelling complex and irregular floor slab configurations.

4. Co-rotational approach

A co-rotational procedure used in the element implementation is based on the procedure described in [5, 6]. The aim of the procedure is to remove influence of the rigid body rotations from the local element response. Towards this end, a local system is established in such a way as to minimise the rotation of the transformed element. Two existing approaches to perform this task are considered for the proposed element: bisector and zero-macrospin [5, 6], which provide the required discrete transformations between local and global element parameters.

The co-rotational transformation is performed at two separate stages. At the first stage, global parameters are transformed to the local system. After the local element response is established, two more transformations are performed to transform local resistance forces and the local tangent stiffness matrix to the global system. At this stage another benefit of formulation employing hierarchic DOF becomes apparent. Since hierarchic DOF are edge based and are only shared between two elements, they can be excluded from costly co-rotational transformations. It is worth noting though that, unlike the hierarchic DOF employed for the rectangular element in [6], local transformation of the hierarchic DOF is required from their edge-based system to the local element system.

5. Verification

A square plate, clamped along two opposite edges and free along the remaining two edges, is considered under a point load \( (P) \) applied at point A (Figure 2 b)). Two regular meshes of 10×10×2 and 20×20×2 elements are employed to test the influence of mesh refinement on the solution, and one irregular mesh with 209 (Figure 2 a)) elements is used to test the influence of element form on the
solution. The out-of-plane displacement response at points (A) and (B), is provided in Figure 2 using the linear and quadratic Reissner–Mindlin local formulations. The predictions of the quadratic element compare favourably against the results of Izzuddin [4] to 1.12% accuracy.

![Figure 2. Mesh and results for verification problem](image)

6. Conclusion

A new triangular shell element for RC and composite floor slabs is formulated in a local reference system based on the Reissner–Mindlin hypothesis. The element is developed in two hierarchic forms, enabling the selective activation of higher-order quadratic approximation. The element formulation is briefly described, including the displacement and strain approximations in different materials of the composite cross-section, and its incorporation within a large displacement co-rotational approach is discussed. The new element has been implemented within ADAPTIC, which is used to provide basic verification of the element for both small and large displacements.

References


DEBONDING OF CELLULAR STRUCTURES UNDER SHEAR DEFORMATION

*Alexander Safar, Hayley Wyatt and L. Angela Mihai

School of Mathematics, Cardiff University, Senghennydd Road, Cardiff, CF24 4AG

*SafarAT@cardiff.ac.uk

ABSTRACT

Many natural materials at millimetre scale are cellular structures, while at micrometre scale, the cell walls are fibrous elastic composites (e.g. plant stems, vegetables, fruit). Cell separation through debonding of the middle lamella in cell walls is key in explaining some important characteristics or behaviour. To model such phenomena, we consider cellular structures with nonlinear hyperelastic cell walls under large shear deformations and incorporate unilateral contact between neighbouring cells. Numerically, we show that, when finite element models of periodic structures with hexagonal cells are sheared, significant cell separation is captured diagonally across the structure. Our analysis further reveals that separation is less likely between cells with high internal cell pressure than between cells where the internal pressure is low.

Key Words: cellular solids; unilateral contact; hyperelastic materials; finite element method; fruit softening.

1. Introduction

Cellular tissues such as apples, pears and potatoes are a collection of fluid filled parenchyma cells (Figure 1a) bound together by inter-cellular cohesion. In a ripe and juicy apple, fluid is released from cells as the cell wall ruptures (cell bursting). In overripe or cold-stored fruit the strength of the inter-cellular cohesion decreases and the cell wall strength increases, such that it takes less energy to separate cells than to burst [1]. The texture of the fruit becomes dry and bitty (known as ‘mealy’) as the cells fall apart in small clumps and little fluid is released [1,2]. The phenomena of cell separation, or debonding, (Figure 1b) is key in explaining the behaviour of fruit and legumes during storage or cooking, and is decisive for the quality of food products [1].

Cell properties determine tissue behaviour and applied external forces change the cell responses as deformation progresses [4,5]. These relations lead to nonlinear mechanical behaviour and the requirement for a multi-scale approach. This study uses numerical models to provide evidence of how the cell wall, cell contents and inter-cellular cohesion contribute to cell debonding in soft fruits and tissues. Particular focus is given to shear deformation as this has been largely neglected in literature.
2. Contact Problems in Finite Elasticity

The finite (large strain) elastic regime is used to capture nonlinear behaviours in large deformations. The cell walls are modelled by a Mooney-Rivlin hyperelastic material, described by the strain energy function $W = C_1 (I_1 - 3)/2 + C_2 (I_2 - 3)/2$ with material constants $C_1 > 0$ and $C_2 > 0$. The walls of neighbouring cells are assumed to be in unilateral (non-penetrative) contact. The problem is to find the displacement field $u(X) \in \mathbb{R}^3$ satisfying [6]:

- The Lagrangian equation of non-linear elastostatic equilibrium in the body $\Omega$ (no body forces):

$$\text{Div} P(X) = 0,$$

where $P(X)$ is the 1st Piola-Kirchhoff stress, representing the force per unit area in the reference configuration.

- The Dirichlet (prescribed displacement) conditions on the boundary $\Gamma_D$:

$$u(X) = u_D.$$  

- The Neumann (prescribed surface pressure) conditions on the boundary $\Gamma_N$:

$$P(X)N = g_N.$$  

where $N$ is the outward unit normal vector to $\Gamma_N$.

- The non-penetrative frictionless contact conditions on the boundary $\Gamma_C$:

$$\eta(X + u(X)) \leq 0, \quad P(X)N \cdot N \leq 0, \quad (\eta(X + u(X))) (P(X)N \cdot N) = 0,$$

where $\eta$ is the relative distance between contacting cell walls and $N$ is the unit normal vector to the contact interface.

3. Successive Deformation Decomposition Procedure

To improve computational efficiency, we implement the successive deformation decomposition procedure (SDDP) proposed in [6]: (i) first, a continuous deformation is computed for the entire the structure, as in a compact elastic solid, where only the external boundary conditions are imposed while the cells remain in mutual contact; (ii) then, from the pre-deformed structure, the unilateral contact between cell walls are taken into account and cells are able to separate (Figure 2). For our computer simulations, the two-step procedure proved significantly faster and more robust than when the external boundary conditions and contact constraints were imposed simultaneously in a single step.

Figure 2: Diagrammatic representation of the successive deformation decomposition procedure.
4. Empty Cells with Unilateral Contact

The SDDP is applied to periodic structures with hexagonal prismatic cells, subject to horizontal shear, modelled using FEBio (Finite Element for Biomechanics) [3]. Results show that, when structures are subject to shear deformation, gaps appear between adjacent cells, causing extensive cell separation diagonally across the structure (Figure 3).

![Reference configuration.
Continuously deformed state.
Current configuration.](image)

Figure 3: SDDP of a 5x7 cellular tissue, subject to shear. Colour indicates X displacement.

5. Intercellular Cohesion

Cohesion on a contact interface is usually modelled by the condition $P(X)N \cdot N \leq g$ on $\Gamma_C$, where $g > 0$ indicates that a tensile force of magnitude $g$ is permissible whilst two bodies are in contact. Computationally, this leads to highly unstable systems, so we consider instead an internal cell pressure which is normal to the cell walls and has the same magnitude for each cell (Figure 4a). This creates a compressive normal force which must be overcome to separate cell walls, analogous to normal contact cohesion. Results show that a higher surface pressure delays the initiation of inter-cellular gap opening (Figure 4b).

![Representative model with surface pressures.
Relationship between separation and pressure.](image)

Figure 4: Cohesive pressure within cellular tissues.

6. Filled Cells

In our study, the influence of the cell inclusions on the inter-cellular contact is addressed by modelling the inclusions as a nearly-incompressible, softer Mooney-Rivlin material (Figure 5a). A primary effect of this is the cell volume constraint. As shown by our results, the rate of increase in the gap-size, occurring at $X$-displacement of $\approx 0.2$ for empty cells, is delayed by the presence of cellular inclusion, and delayed further by increasing the stiffness of the inclusions (Figure 5b).
Alternatively, the presence of cell inclusions could be modelled by imposing uniform normal pressure on the internal cell walls. Formally, this is similar to our model for inter-cellular cohesion, suggesting that higher cell pressure results in an increased inter-cellular cohesion.

7. Conclusion

We model computationally cellular bodies with nonlinear hyperelastic cell walls in mutual non-penetrative contact under large shear deformations, and propose a two-step strategy which we employ to solve the multi-body contact problems more efficiently. Our numerical results are in agreement with physical observations that tissue from overly mature fruit (apple, pear), where cell pressure is low and intercellular cohesion is weak, breaks down into small clumps of undamaged cells, whereas fruit of a lower maturity, with high cell pressure and intercellular cohesion will not debond easily.

Acknowledgements

The support for L.A.M. and A.S. by the EPSRC and Cardiff University is gratefully acknowledged.

References

A Modified Applied Element Method using Adaptive Gaussian Springs for Elasto-plastic Analysis of Structures

*Mai Abdul Latif, Y. T. Feng

Zeinkiwiz Centre for Computational Engineering, Swansea University, Bay Campus, SA1 8EN

*744973@swansea.ac.uk

ABSTRACT

The Applied Element method is developed and coded to significantly improve the accuracy and reduce the computational costs. The first modification of the method is based on the Gaussian Quadrature for springs distribution, while the second modification is based on adapting the number of springs required depending on the elasticity of the material. The scheme works for both linear elastic, and nonlinear cases, including elasto-plastic materials. This paper will focus on elastic and elasto-plastic material behaviour, where the number of springs required for an accurate analysis is tested. All the work is done using MATLAB and the results will be compared to models of structural elements using the finite element method in ANSYS.

Key Words: Applied Element Method, Gaussian Springs, Elasto-plastic.

1. Introduction

The Applied Element Method (AEM) [1] was developed to aid in the analysis of highly nonlinear behaviour of structures, such as crack initiation, crack propagation, separation of structural elements, rigid body motion of failed elements and total collapse of the structure. Current available methods cannot deal with structural collapse accurately; however, AEM can simulate the behavior of a structure from an initial state of no loading until collapse of the structure. Nonlinear dynamic analysis has been widely modelled using the finite element method for analysis of progressive collapse of structures; however, difficulties in the analysis were found at the presence of excessively deformed elements with cracking or crushing, as well as having a high computational cost, and difficulties on choosing the appropriate material models for analysis [1]. In this paper, a modification to the applied element method spring distribution is proposed, for increase in computational cost and decrease in the number of springs required per analysis. The springs are distributed based on an adaptive method, where they depend on the elasticity of each element.

2. AEM Formulation for 2-D element

The elements in AEM are rigid body elements that are connected with sets of normal and shear springs along the edges of the elements. The springs represent the stresses and strains of the element in that region. The material properties are specified through the spring stiffness. For a 2-D element, three degrees of freedom are considered per element, deflection in x, deflection in y and rotation [1]. The stiffness matrix for a pair of elements is a 6x6 matrix. The upper left quadrant of the matrix is displayed in Equation 1 [1]. Each spring location in the elements is represented by a pair of normal and shear springs, with stiffness displayed in Equation 2 [1]. The elements are displayed in Figure 1.

\[ K = \begin{pmatrix} K_{n1} & 0 & -K_{n1}b_{n1} \\ 0 & K_{s1} & K_{s1} \frac{a}{2} \\ -K_{n1}b_{n1} & K_{s1} \frac{a}{2} & (K_{n1}b_{n1}) + (K_{s1} \frac{a}{4}) \end{pmatrix} \]  

(1)

where,

\[ K_{n} = \frac{E}{a}; K_{s} = \frac{G}{a} \]

(2)
3. Gaussian Springs based AEM

Gaussian quadrature is used for finite element applications because of they have less function evaluation for given orders. The weights and evaluation points are determined so that the integration rule is exact to as high an order as possible [2].

\[
\int_{a}^{b} f(x)dx = \frac{b - a}{2} \sum_{i=1}^{n} W_i f(x_i)
\]  

The Gaussian Quadrature formulation is used to determine the gaussian weights and coordinates using the number of springs. The location of the springs is determined by considering \( w \) as the width of the tributary area of each spring (‘d’ in AEM), and \( x \) as the spring location from Equation 3. Table 1 displays the calculated locations of the spring coordinates, along with \( d \), the width of the tributary area of each spring for 5 points. Assuming the width of the section is 5, then \( x_i \) and \( w_i \) are multiplied by \( 5/2 = 2.5 \).

<table>
<thead>
<tr>
<th>Point</th>
<th>( x_i )</th>
<th>( w_i )</th>
<th>2.5( x_i )</th>
<th>2.5( w_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.906</td>
<td>0.237</td>
<td>-1.359</td>
<td>0.355</td>
</tr>
<tr>
<td>2</td>
<td>-0.538</td>
<td>0.479</td>
<td>-0.808</td>
<td>0.718</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0.569</td>
<td>0</td>
<td>0.853</td>
</tr>
<tr>
<td>4</td>
<td>0.538</td>
<td>0.479</td>
<td>0.808</td>
<td>0.718</td>
</tr>
<tr>
<td>5</td>
<td>0.906</td>
<td>0.237</td>
<td>1.359</td>
<td>0.355</td>
</tr>
</tbody>
</table>

Figure 2: Comparison of Gaussian and Equal Springs

Tributary Area.

Table 1: 5 Gaussian Quadature Points.

4. Elasto-plastic Gaussian Springs

The algorithm for one-dimensional plasticity used to calculate wether springs are elastic or elastoplastic is displayed as follows [3]:

1. Evaluate elastic predictor

\[
\epsilon_{n+1} = \epsilon_n + \delta\epsilon_{n+1}
\]  

\[
\sigma_{trial}^{n+1} = E(\epsilon_{n+1} - \epsilon_p)
\]  

Discrete version of Kuhn Tucker conditions:

\[
f_{n+1} = |\sigma_{n+1}^{trial}| - \sigma_y + H\alpha_n
\]  

2. Check yield criterion

\[
f_{n+1}^{trial} \leq 0 \Rightarrow \Delta\lambda = 0
\]  

\[
f_{n+1}^{trial} \geq 0 \Rightarrow \Delta\lambda > 0
\]
3. Plastic step (if $f_{trial}^{n+1} \geq 0$)

$$\Delta \lambda = \frac{f_{n+1}}{E + K}$$

(8)

$$\sigma_{n+1} = \sigma_{trial}^{n+1} \left[ 1 - \frac{\Delta \lambda E}{\sigma_{trial}^{n+1}} \right]$$

(9)

$$\varepsilon_p^{n+1} = \varepsilon_p^n + \Delta \lambda \text{sign} \left[ \sigma_{trial}^{n+1} \right]$$

(10)

$$\alpha_{n+1} = \alpha_n + \Delta \lambda$$

(11)

where the nonlinear stiffness of the springs is:

$$K = \frac{CA}{L}; \quad C = \frac{EH}{E + H}$$

(12)

5. Adaptive Gaussian Springs

Using the gaussian quadrature for the springs distribution, and the plasticity algorithm for calculating the stresses in the springs, an adaptive method can be implemented. The Newton Raphson iteration scheme is used for convergence. In each iteration, the stress in each spring is calculated and determined whether it is plastic or elastic. If all springs between two elements are elastic, then the initial number of springs will be changed to two springs between elements, since only 2 points are required to model the linear behaviour of the elastic region, as displayed in Figure 3.

![Figure 3: Adaptive Elastic Springs](image1)

If plasticity is observed in a section, then the normal stress is split into 3 regions, plastic, elastic, plastic, as displayed in Figure 4. Therefore, 6 springs in total are required for elastoplastic cases.

![Figure 4: Adaptive Elastoplastic Springs](image2)

The beam is analysed for the first Newton Raphson iteration, and the stresses in the springs are calculated. Based on the springs elasticity - whether they were plastic or elastic, the new springs will be placed between calculated transition points. The transition points are the points calculated where the stress changes from elastic to plastic, and vice versa. Figure 5 displays a cantilever beam fixed on the left end, and loaded on the right end. The springs distribution are resolved from the adaptive Gaussian Springs based Applied Element Method proposed.

![Figure 5: Representation of a cantilever beam using adaptive AEM springs](image3)
6. Results

A cantilever beam (fixed on the left side and loaded on the right side) is analysed using the adaptive Gaussian springs based AEM method. Figure 6 displays the deflection and the normal stress obtained from the Matlab code. This is compared to an ANSYS model using FEM, displayed in Figure 7. It can be seen that the results were similar. Figure 8 displays a beam fixed at both ends and load applied at midspan.

![Figure 6: Analysis of Cantilever Beam - MATLAB](image)

![Figure 7: Analysis of Cantilever Beam - ANSYS](image)

![Figure 8: Analysis of Fixed-Ends Beam - MATLAB](image)

Figure 9 is the log(residual) vs the iteration number. Quadratic convergence was obtained, which was expected from the use of the Newton Raphson time stepping iteration scheme. Table 2 displays the deflection in the free end for a low number of elements in a cantilever beam. It is clear that using Gaussian springs can obtain convergence with low number of springs faster than using equal springs.

<table>
<thead>
<tr>
<th>Springs</th>
<th>Gaussian</th>
<th>Equal</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.148</td>
<td>1.528</td>
</tr>
<tr>
<td>5</td>
<td>1.148</td>
<td>1.195</td>
</tr>
<tr>
<td>10</td>
<td>1.148</td>
<td>1.159</td>
</tr>
<tr>
<td>15</td>
<td>1.148</td>
<td>1.153</td>
</tr>
<tr>
<td>30</td>
<td>1.148</td>
<td>1.149</td>
</tr>
</tbody>
</table>

Table 2: Deflection at Free End

References


Wave and Electromagnetics
Evaluation of highly oscillatory integrals in the Partition of Unity BEM for wave simulations in 2D

B.D. Gilvey¹, G.A. Wagner¹, J. Trevelyan¹, M. Seaïd¹ and J. Gao²

¹School of Engineering & Computing Sciences, Durham University, South Road, Durham, DH1 3LE, UK
²School of Mathematics and Statistics, Xian Jiaotong University, Xianning West Road, Xi’an, Shaanxi, 710049, P.R. China

benjamin.gilvey@durham.ac.uk

ABSTRACT

The Partition of Unity Boundary Element Method (PU-BEM) [1] is one of a class of numerical methods involving plane wave enrichment to enhance the accuracy and computational efficiency of simulations involving medium to high frequency wave propagation. An open problem in this field is to find a robust and computationally efficient method of evaluating the highly oscillatory integrals that arise in order to maximise the benefit of enrichment. Numerical steepest descent in [2] enjoys success for some straightforward cases, but as yet is not a practical method of evaluating the entire spectrum of boundary integrals. In the current work we offer the Filon-type method of Iserles and Nørsett [3] as a viable alternative.

Key Words: Partition of Unity Boundary Element Method; Numerical integration; Asymptotic expansion; Filon; Hermite polynomial

Introduction

The PU-BEM is a variant of BEM in which the acoustics solution is sought in a plane wave basis. This gives highly accurate solutions with a small number of degrees of freedom, but brings the requirement to evaluate some highly oscillatory integrals over elements. Numerical integration is therefore an essential component of the PU-BEM, amounting to a substantial portion of the computational expense. Hence, as systems become larger such as in 3D acoustic or electromagnetic scattering problems, the efficiency of the integration scheme requires consideration.

Traditional approaches to numerical integration generally rely on quadrature formulas, subdividing the interval and integrating over interpolating polynomials. The most ubiquitous of this category being Gauss-Legendre quadrature

\[ \int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} w_i f(x_i), \]

which selects optimal locations \( x_i \) and weights \( w_i \) in order to reduce error. For an \( n \) point Gauss scheme an exact result is expected when applied to a polynomial of degree \( 2n - 1 \). The benefit of using Gauss-Legendre is convergence provided a sufficiently large value of \( n \) is selected, however when the integrand becomes highly oscillatory the number of ‘Gauss points’ required will increase linearly with frequency.

There are a number of more exotic methods for integrating highly-oscillatory functions such as the asymptotic method using integration by parts evaluated in [4], the method of stationary phase [5] and numerical steepest descent as in [2]. More recent and more relevant to this paper are the Levin-type in [6] and Filon-type methods, the latter will be elaborated on in the following section.

This paper aims to investigate the efficiency of the Filon method compared with Gauss-Legendre in computing the integral

\[ I_2 = -\frac{ik}{4} \int_{-1}^{1} H_1(kr)N_j(\xi)e^{\frac{i}{2}d\cdot q} \frac{\partial r}{\partial n_d} Jd\xi \] (2)
where \( i = \sqrt{-1}, k \) is the wave number, \( H_1 \) is the Hankel function of the first kind and of order 1, \( r \) is the distance from the collocation point \( p = (x_p, y_p) \) to the field point \( q(\xi) = (x_q, y_q) \). \( N_j \) is the shape function for node \( j, \xi \in (-1, 1) \) is the parametric coordinate of the element, \( d = (d_x, d_y) = (\cos(\phi), \sin(\phi)) \), \( n_q \) is the outward normal at \( q \) and \( J \) is the Jacobian. The Hankel function and the exponential term can be highly oscillatory, hence evaluating (2) using Gauss-Legendre quadrature may require thousands of Gauss points. In this preliminary work we consider cases in the absence of stationary points.

Filon method

In recent years there has been increasing focus on Filon-type methods which extend the ideas of Filon [7] to highly-oscillating integrals of the form

\[
I = \int_a^b f(x)e^{ikg(x)} dx, \tag{3}
\]

in which \( f(x) \) and \( g(x) \) are ‘smooth’ functions. The essence of Filon-type methods is to approximate the slowly varying function \( f(x) \) with an interpolating polynomial thereby allowing the integral to be evaluated analytically by parts.

Within the umbrella of Filon-type methods there are multiple approaches to interpolating the function \( f(x) \), with effort being concentrated on optimal location of nodes. A popular method is the Filon-Clenshaw-Curtis (FCC) rule which is explored in [8], where the function is sampled at classic Chebyshev locations and no derivatives are used. An advantage of using FCC is that as the weights for the polynomial can be precomputed using the Fast Fourier Transform it is readily applicable for a variety of frequencies, simply adjusting the number of nodes to achieve desired accuracy.

In the interest of improving performance, however, the method applied by the authors is that of Iserles [3] in which \( f(x) \) is sampled only at the end points of the interval, using higher derivatives to increase the accuracy in these key regions. A benefit of this approach is that it targets the end points as this is where the majority of information is located due to rapid oscillations largely cancelling each other out in the central region of the element.

In order to evaluate (2) we begin by replacing the Hankel function with its asymptotic expansion from [9] at large \( kr \),

\[
H_s(kr) \approx \left( \frac{2}{\pi kr} \right)^{\frac{1}{4}} e^{ikr - \frac{1}{2} \pi - \frac{1}{4} \pi} \sum_{s=0}^{\infty} \frac{i^s a_s(v)}{(kr)^s}, \tag{4}
\]

with

\[
a_s = \frac{(4v^2 - 1^2)(4v^2 - 3^2)...(4v^2 - (2s - 1)^2)}{s! 8^s}, \quad a_0(v) = 1. \tag{5}
\]

Inserting (4) into the original equation (2) results in the following:

\[
I_2 \approx -\frac{i}{4} \left( \frac{2}{\pi} \right)^{\frac{1}{4}} e^{-\frac{3i\pi}{4}} \sum_{s=0}^{S} \frac{i^s a_s(1)}{k^{s+\frac{3}{2}}} \int_{-1}^{1} f_2(\xi, s)e^{ikg(\xi)} d\xi, \tag{6}
\]

where

\[
f_2(\xi, s) = \frac{N_f(\xi)(y_q - y_p)}{r^{s+\frac{3}{2}}}. \tag{7}
\]

Transforming the coordinate of integration to \( g \), and making use of a Hermite polynomial approximation of degree \( M \) to \( f_2 \), i.e.

\[
H_s(g) = h_{s,0} + h_{s,1}g + h_{s,2}g^2 + ... + h_{s,M}g^M \approx f_s(\xi(g), s) \frac{dg}{dg} =: F_s(g, s), \tag{8}
\]
subject to the following interpolation conditions:

\[ H_s(a) = F_2(a, s) \]
\[ H_s(b) = F_2(b, s) \]
\[ H'_s(a) = F'_2(a, s) \]
\[ H'_s(b) = F'_2(b, s), \]

produces the following

\[ I \approx \sum_{s=0}^{S} \sum_{m=0}^{M} h_{s,m} \int_a^b g^m e^{ikg} dg, \quad a = g(-1), b = g(1). \]  

(9)

The integrals, called Filon moments, can be integrated analytically by parts. Thus the evaluation of (2) reduces to a small number of operations to generate the Hermite polynomial coefficients \( h_{s,m} \) and compute the Filon moments.

**Numerical example**

We consider a numerical example of a flat element lying in \( y = 0 \), and take \( N_j \) to be the quadratic Lagrangian shape function

\[ N(\xi) = -\frac{1}{2}(\xi)(1-\xi). \]  

(10)

Table 1: Solution time of each integration method in seconds.

<table>
<thead>
<tr>
<th>( k )</th>
<th>Filon</th>
<th>Gauss</th>
<th>Trapezium</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>0.039</td>
<td>0.051</td>
<td>0.738</td>
</tr>
<tr>
<td>1000</td>
<td>0.036</td>
<td>0.082</td>
<td>1.431</td>
</tr>
<tr>
<td>2000</td>
<td>0.036</td>
<td>0.141</td>
<td>2.889</td>
</tr>
<tr>
<td>10000</td>
<td>0.037</td>
<td>0.572</td>
<td>14.027</td>
</tr>
</tbody>
</table>

Table 1 compares Gauss-Legendre and trapezium schemes with the Filon method using a single 3rd degree polynomial, interpolated using only 2 sample points. The results provided are for the case \( (x_p = -3, y_p = -3, y_q = 0, \bar{J} = 2, \phi = 60^\circ) \), and show the time required to evaluate the integral to 6-digit accuracy.

**Conclusions and further work**

Initial results, along with its simple implementation, prove the Filon method to be a promising candidate to replace Gauss-Legendre for a large number of applications. When the frequency increases we observe the true benefit as not only is further subdivision not required but the accuracy actually increases, which is contrary to traditional quadrature schemes.

Before moving into three-dimensional space, further refinement is required for cases where stationary points are allowed in the oscillator, i.e. \( g'(x) = 0 \), as they will make up a larger proportion of the integrals requiring evaluation. In order to design a robust method which is fully applicable, another consideration is when \( r \) is small relative to the element length, as when the collocation point \( p \) approaches the field point \( q \), accuracy decreases.

**Acknowledgements**

The authors are grateful for the financial support awarded by the Royal Society and the National Science Foundation of China under their International Exchanges Scheme.
References


Boundary Elements and Mesh Refinements for the Wave Equation

*David Stark¹, Heiko Gimperlein¹

¹Department of Mathematics, Heriot-Watt University, Edinburgh EH14 4AS

*ds221@hw.ac.uk

ABSTRACT

We discuss time domain boundary element methods for singular geometries, in particular graded meshes and adaptive mesh refinements. First, we discuss edge and corner singularities for a Dirichlet problem for the wave equation. Time independent graded meshes lead to efficient approximations, as confirmed by numerical experiments for wave scattering from screens. We briefly discuss adaptive mesh refinement procedures based on a posteriori error estimates. A modified MOT scheme provides an efficient preconditioner (or stand-alone solver) for the space-time systems obtained for the Galerkin discretisations.

Key Words: Wave equation; time-domain boundary element method; adaptive mesh refinements; graded meshes.

1. Introduction

Boundary element methods provide an efficient, extensively studied numerical scheme for time-independent or time-harmonic scattering and emission problems. Unlike finite element discretisations, they reduce the computation from the three dimensional domain to its two dimensional boundary. Recently, boundary elements have been explored for the simulation of transient phenomena, with applications e.g. to environmental noise [2] or electromagnetic scattering [7]. Galerkin time domain boundary element methods prove to be stable and accurate in long–time computations and are competitive with frequency domain methods for realistic problems [3].

In this talk we discuss recent work on adaptive mesh refinements and graded meshes for singular geometries, as motivated by the sound emission on tires [2].

2. Problem description and time domain BEM

We consider the wave equation outside a scatterer $\Omega^-$ in $\mathbb{R}^3$, where $\Omega^-$ is a bounded polygon or a screen with connected complement $\Omega = \mathbb{R}^3 \setminus \overline{\Omega^-}$. The acoustic sound pressure field $u$ due to an incident field or sources on $\Gamma = \partial \Omega$ satisfies the linear wave equation for $(t, x) \in \mathbb{R} \times \Omega$:

$$\partial^2_t u(t, x) - \Delta u(t, x) = 0$$

with Dirichlet boundary conditions $u(t, x) = f(t, x)$ for $x \in \Gamma$, and $u(t, x) = 0$ for $t \leq 0$.

A single-layer ansatz for $u$,

$$u(t, x) = \int_{\Gamma} \frac{\phi(t - |x - y|, y)}{4\pi|x - y|} ds_y,$$  

results in an equivalent weak formulation as an integral equation of the first kind in space-time anisotropic Sobolev spaces [6, 3]:

Find $\phi \in H^1_{\sigma t}(\mathbb{R}^+, \widetilde{H}^{-\frac{1}{2}}(\Gamma))$ such that for all $\psi \in H^1_{\sigma t}(\mathbb{R}^+, \widetilde{H}^{-\frac{1}{2}}(\Gamma))$

$$\int_{0}^{\infty} \int_{\Gamma} (V \phi(t, x)) \partial_t \psi(t, x) ds_x \, d\sigma t = \int_{0}^{\infty} \int_{\Gamma} f(t, x) \partial_t \psi(t, x) ds_x \, d\sigma t,$$  

where $d_{\sigma t} = e^{-2\sigma t} dt$ and

$$V \phi(t, x) = \int_{\Gamma} \frac{\phi(t - |x - y|, y)}{4\pi|x - y|} ds_y.$$  

309
A theoretical analysis requires $\sigma > 0$, but practical computations use $\sigma = 0$.

We study time dependent boundary element methods to solve (2), based on approximations by piecewise polynomial ansatz and test functions from the space $V_{h,\Delta}^{p,q}$ spanned by

$$
\phi_i(t,x) = \tilde{\Lambda}_i(t)\Lambda_i(x). 
$$

Here, $\Lambda_i$ a piecewise polynomial shape function of degree $p$ in space and $\tilde{\Lambda}_i$ a corresponding shape function of degree $q$ in time. For $p \geq 1$, resp. $q \geq 1$, the shape functions are assumed to be continuous.

We obtain a numerical scheme for the weak formulation (2): Find $\phi_{h,\Delta t} \in V_{h,\Delta t}^{p,q}$ such that for all $\psi_{h,\Delta t} \in V_{h,\Delta t}^{p,q}$

$$
\int_0^\infty \int_T (V \phi_{h,\Delta t}(t,x)) \partial_t \psi_{h,\Delta t}(t,x) \, dx \, dt = \int_0^\infty \int_T f(t,x) \partial_t \psi_{h,\Delta t}(t,x) \, dx \, dt. 
$$

From $\phi_{h,\Delta t}$, the sound pressure $u_{h,\Delta t}$ is obtained in $\Omega$ by evaluating the integral in (1) numerically.

3. Error estimate and adaptive mesh refinements

Computable error indicators are a key ingredient to design adaptive mesh refinements. We recall from [3]:

**Theorem:** Let $\phi, \phi_{h,\Delta t} \in H^1([0,T], H^{-\frac{1}{2}}(\Gamma))$ be the solutions to (2) resp. (4). Assume that $R = \hat{f} - V\phi_{h,\Delta t} \in H^0([0,T], H^1(\Gamma))$. Then

$$
\|\phi - \phi_{h,\Delta t}\|_{0,-\frac{1}{2},T}^2 \leq \max\{\Delta t, h\}(\|\partial_t R\|_{L^2([0,T], L^2(\Gamma))} + \|\nabla R\|_{L^2([0,T], L^2(\Gamma))})^2.
$$

The error indicators $\eta(\Delta)$ lead to

**Adaptive Algorithm:**

Input: Mesh $T = T_0$, refinement parameter $\theta \in (0,1)$, tolerance $\epsilon > 0$, data $f$.

1. Solve $V\psi_{h,\Delta t} = \hat{f}$ on $T$.
2. Compute the error indicators $\eta(\Delta)$ in each triangle $\Delta \in T$.
3. Find $\eta_{\text{max}} = \max_\Delta \eta(\Delta)$.
4. Stop if $\sum_\Delta \eta^2(\Delta) < \epsilon^2$.
5. Mark all $\Delta \in T$ with $\eta(\Delta) > \theta \eta_{\text{max}}$.
6. Refine each marked triangle into 4 new triangles to obtain a new mesh $T'$.
7. Go to 1.

Output: Approximation of $\psi$.

4. Graded meshes

The realistic scattering and diffraction of waves in $\mathbb{R}^3$ is crucially affected by geometric singularities of the scatterer, as solutions of the wave equation exhibit well-known singularities at non-smooth boundary points of the domain. For such geometric singularities, graded meshes adapted to the geometry are known to provide optimal convergence rates for time independent problems. We have generalised to time-independent theory to the transient setting [4] and illustrate the improved convergence rates in numerical experiments below.

Our computations are mainly conducted on the square $[-1,1]^2$. To define $\beta$-graded meshes, due to symmetry, it suffices to consider a $\beta$-graded mesh on $[-1,0]$. We define $y_k = x_k = -1 + (k/N)^\beta$ for $i = 1, \ldots, N_0$ and for a constant $\beta \geq 0$. The nodes of the $\beta$-graded mesh are therefore $(x_k, y_l)$, $k,l = 1, \ldots, N_j$. We note that for $\beta = 1$ we would have a uniform mesh.
5. Numerical results

1) If $\Gamma$ is a screen, the density $\phi$ exhibits edge and corner singularities. Motivated by recent work by Müller and Schwab for 2d FEM, in [4] we adapt a classical analysis by von Petersdorff for time-independent problems and obtain the precise singular behaviour of $\phi$ near $\partial \Gamma$: $\phi(t, x) \sim \text{dist}(x, \partial \Gamma)^{-1/2}$ near an edge, $\phi(t, x) \sim \text{dist}(x, \partial \Gamma)^{-0.703}$ near a right-angled corner.

Time-independent graded meshes provide a quasi-optimal approximation of these singularities. The numerical experiment depicted in Figure 2 compares the convergence in energy norm on graded and uniform meshes for $\Gamma = [0, 1]^2 \times \{0\}$ and illustrates the theoretically predicted convergence of order $\text{DOF}^{-1}$, resp. $\sim \text{DOF}^{-1/2}$. We present an application to the singular horn geometry between a vibrating tire and the road.

2) We use provably reliable residual error indicators, as well as heuristic ZZ and hierarchical indicators to steer adaptive mesh refinements. Figure 3 shows that the residual indicators converge at the same rate as the energy error for an example problem with $\Gamma = S^2$. We briefly recall the theoretical results on reliability and (weak) efficiency of the residual error indicators (see [3]) and compare the adaptive methods obtained from the different error indicators.

3) To obtain provably stable methods and a rigorous error analysis, we require conforming Galerkin discretisations. In general, the discretised equation (4) corresponds to a lower Hessenberg linear system in space-time, with one band above the diagonal. Motivated by adaptivity and $C^\infty$ temporal basis functions, there has been much recent interest in works by by Sauter-Veit, Merta et al., Schanz and others in efficient solvers. We present an approximate time-stepping scheme [5], based on extrapolation, which becomes exact for $\Delta t \to 0$. It may be used as either a preconditioner or standalone solver. Table 1
Figure 3: Uniform vs adaptive for plane wave problem on \([0,0.5]^2\) screen.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>DOF</th>
<th>Energy</th>
<th>MOT</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>sphere</td>
<td>320</td>
<td>8.5692</td>
<td>8.5470</td>
<td>.26%</td>
</tr>
<tr>
<td></td>
<td>1280</td>
<td>8.6059</td>
<td>8.6059</td>
<td>\textless{} 1%</td>
</tr>
<tr>
<td>icosahed.</td>
<td>320</td>
<td>20.538</td>
<td>21.480</td>
<td>4.6%</td>
</tr>
<tr>
<td></td>
<td>1280</td>
<td>19.879</td>
<td>20.143</td>
<td>1.3%</td>
</tr>
<tr>
<td>screen</td>
<td>288</td>
<td>0.4233</td>
<td>0.4497</td>
<td>6.2%</td>
</tr>
<tr>
<td></td>
<td>1250</td>
<td>0.4589</td>
<td>0.4716</td>
<td>2.8%</td>
</tr>
</tbody>
</table>

Table 1: relative errors in energy: modified MOT vs. GMRES with residual \(10^{-9}\).

compares one step of this method to the (essentially exact) solution of the space-time system as obtained from GMRES.

Acknowledgements

H. G. acknowledges support by ERC Advanced Grant HARG 268105 and the EPSRC Impact Acceleration Account.

References


Numerical simulations of semi–conductor plasmonic nanolasers

*T. R. Drevon¹, R. Sevilla¹ and A. K. Shore²

¹Swansea University, Zienkiewicz Centre for Computational Engineering, College of Engineering, Swansea, Wales, UK
²Bangor University, School of Electronic Engineering, Bangor, Wales, UK

*840519@swansea.ac.uk

ABSTRACT

We present a method to simulate nano–photonics devices with gain and dispersive plasmonic materials using a high–order accurate discontinuous Galerkin time–domain (DGTD) solver. Special attention is paid to the computation of the dispersion relation and the modal gain of active plasmonic nanowire waveguides. A two–step approach is proposed where a 2D compact formulation is first used to obtain the dispersion relation and mode shapes of the constant energy waveguide. The second step simulates the 3D waveguide including gain and losses to determine the modal gain. The method was validated by comparing with the analytical solutions obtained from a lossy waveguide with perfect electric conducting walls.

Key Words: Discontinuous Galerkin time–domain; Maxwell’s equations; Resonance; Nanowire; Plasmon

1. Introduction

Nanolasers are promising photonic devices for on–chip integrated optoelectronic circuits. Miniaturisation of these devices can be achieved by using plasmonic materials. However, plasmonic materials exhibit optical losses imposing a trade–off between miniaturisation and power consumption. It is thus crucial to determine designs for which optimal performance can be achieved.

To that end, efficient numerical techniques are used to solve Maxwell’s equations. Time–domain solvers are usually preferred because they offer the possibility to study the broadband response of a device. The finite–difference time–domain (FDTD) method is the most commonly used technique in computational electromagnetics but, in its simplest form, suffers from a poor (staircase) geometric representation, limiting its application for nanolasers involving curved boundaries.

In this work, we propose to apply the DGTD method to a plasmonic gain nanowire with a two–step approach. In the first step we compute a range of resonant frequencies and their associated mode shapes [1, 2] for the constant energy waveguide using a 2D compact DGTD formulation. An auxiliary differential equation is introduced to handle dispersive plasmonic materials by employing the Drude model. The second step consists of simulating the same waveguide in 3D adding gain and losses through Joule currents. The 3D simulation is performed by exciting one of the modes found in the first step. The modal gain is finally computed from the spectrum obtained at two different locations along the waveguide.

2. Discontinuous Galerkin time–domain solution of Maxwell’s equations

Maxwell’s curl equations for an isotropic, homogeneous and dispersive medium including gain in dimensionless form can be written as

\[
\begin{align*}
\epsilon \frac{\partial E}{\partial t} &= \nabla \times H - J_D + \sigma_G E \\
-\mu \frac{\partial H}{\partial t} &= \nabla \times E \\
\frac{\partial J_D}{\partial t} &= \omega_D^2 E - \gamma_D J_D,
\end{align*}
\]
where \( \mathbf{E} = (E_1, E_2, E_3) \) and \( \mathbf{H} = (H_1, H_2, H_3) \) are the electric and magnetic field intensity vectors respectively, \( \mathbf{J}_D \) is the Drude polarisation current and \( \epsilon, \mu, \gamma_D, \omega_D \) and \( \sigma_G \) are the permittivity, permeability, collision frequency, plasma frequency and gain conductivity of the medium.

These set of linear hyperbolic equations can be written in conservation form as

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_k(\mathbf{U})}{\partial x_k} = \mathbf{S}(\mathbf{U}),
\]

(2)

where the summation convection is assumed, \( \mathbf{U} = (\epsilon \mathbf{E}, \mu \mathbf{H}, \mathbf{J}_D)^T \) is the vector of conservation variables, \( \mathbf{F}_1 = (0, H_3, -H_2, 0, -E_3, E_2, 0, 0, 0)^T \), \( \mathbf{F}_2 = (-H_3, 0, H_1, E_3, 0, -E_1, 0, 0, 0)^T \) and \( \mathbf{F}_3 = (H_2, -H_1, 0, -E_2, E_1, 0, 0, 0, 0)^T \) are the hyperbolic fluxes and the source term is given by \( \mathbf{S} = (\sigma_G \mathbf{E} - \mathbf{J}_D, 0, 0, 0, \omega_D^2 \mathbf{E} - \gamma_D)^T \).

For the simulation of waveguides, the variation of the fields along the propagation axis is assumed known. By introducing \( \mathbf{U}(x, y, z) = \mathbf{U}(x, y) e^{j\beta z} \) in Equation (2), the so-called 2D compact formulation is obtained.

Discretising the computational domain \( \Omega \) in an unstructured mesh with elements \( \Omega_e \), Equation (2) can be written in weak form on each element as

\[
\int_{\Omega_e} \mathbf{W} \cdot \frac{\partial \mathbf{U}_e}{\partial t} d\Omega + \int_{\Omega_e} \mathbf{W} \cdot \left( \frac{\partial \mathbf{F}_k(\mathbf{U}_e)}{\partial x_k} - \mathbf{S}(\mathbf{U}_e) \right) d\Omega + \int_{\partial \Omega_e} \mathbf{W} \cdot \mathbf{A}_n [\mathbf{U}_e] d\Gamma_e = 0
\]

(3)

where \( \mathbf{W} \) is a test function and \( [\mathbf{U}_e] = \mathbf{U}_e - \mathbf{U}_{\text{out}} \) denotes the jump of the solution across the element boundary \( \partial \Omega_e \). The boundary term \( \mathbf{A}_n [\mathbf{U}_e] \) is derived after introducing a numerical normal flux on the boundary corresponding to a flux splitting technique, see [1] for more details.

By approximating the solution \( \mathbf{U} \) with Lagrange polynomials as basis functions, the weak formulation leads to a system of ordinary differential equations for the vector of nodal values \( \mathbf{U} \), namely

\[
\mathbf{M} \frac{d\mathbf{U}}{dt} = -\mathbf{F}^{DG}(\mathbf{U}),
\]

(4)

where \( \mathbf{M} \) is the block–diagonal mass matrix and \( \mathbf{F}^{DG} \) contains the divergence, source and boundary contributions of Equation (3). This system is advanced in time using a fourth–order explicit Runge–Kutta method.

3. Simulation of a plasmonic gain nanowire waveguide

A nanowire plasmonic waveguide is shown in the left plot of Figure 1. One of the most important quantities of interest is the modal gain of the propagating modes. The modal gain is defined as the rate of growth of the energy of the wave as it propagates along the nanowire axis, as illustrated in the right plot of Figure 1.
The first step of the proposed approach consists of simulating a cross section of the nanowire employing the 2D compact formulation. A computational mesh for the simulation using the proposed DGTD approach is shown in the left plot of Figure 2. The waveguide is assumed with no gain and loss (i.e. \( \sigma_G = \gamma_D = 0 \)). The dispersion relation \( f(\beta) \), shown in the right plot of Figure 2, is obtained by performing a number of time–domain simulations, by changing the value of \( \beta \), and computing the resonant frequencies for each simulation. The insets in the right plot of Figure 2 represent the computed mode shapes at the resonant frequencies. It is worth noting that, even though the mode shapes along the dispersion relation of the \( TE_{01} \) mode are similar, they differ by their level of confinement.

Figure 2: Mesh used for the 2D compact simulations (left), and dispersion relation built by computed the resonant frequencies for different values of parameter \( \beta \) (right).

The second step of the proposed approach involves the simulation of the 3D waveguide including gain and loss. The fields in the waveguide are excited by using the computed mode shapes at the first step (i.e. varying \( \beta \)). More precisely, a broadband excitation of a given mode can be obtained \([3]\) by using

\[
f(x, y, t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} F(x, y, \omega) F(f_0(\tilde{t})) e^{j\omega t} \, d\omega
\]  

(5)

where \( F(x, y, \omega) \) is the selected mode and \( F(f_0(\tilde{t})) \) is the Fourier transform of a time dependent excitation, usually taken as a sinusoidal excitation with Gaussian envelope.

The setup of the 3D simulation is shown in the left plot of Figure 3. The modal gain is obtained from the decay of the spectrum of the guided waves at two different sampling points \( P_1 \) and \( P_2 \) along the propagation axis and is shown in the right plot of Figure 3. The solid line shows the simulated portion. The dark green curves shows the spectrum of the excitation function \( F(f_0(\tilde{t})) \)

Figure 3: Setup for the 3D simulation (left) and modal gain as a function of frequency.

It is worth noting that the mesh requirements for the simulation of the cross section in the first step and the full 3D simulation in the second step can be different.

4. Conclusions and future work

We have proposed a technique to compute the dispersion relation and modal gain in an active plasmonic nanowire waveguide. The proposed approach involves two steps employing a DGTD
method, which enables the computation of a broad range of frequencies in the first step and
the simulation of the broadband response of the 3D structure in the second step. The proposed
method is general and can naturally be adapted to more complex geometries and designs.

In addition to provide a control over the dispersion and dissipation numerical errors, the pro-
posed DGTD approach enables an extremely easy parallel implementation, which allows to
simulate problems that require a high spatial and temporal resolution.

In the simulations, it was assumed that the gain medium conductivity was constant and the
plasmonic material followed the Drude model. More accurate descriptions using generalized
dispersive models [4] for both media are being considered. Additionally, future works would
include non–homogeneous material gain in laser cavity obtained from semi–conductor carriers
models.

The 3D simulation of the waveguide can be extended to the study of nanolasers. By closing the
waveguide with an air interface and computing the reflectivity at this interface, the laser round
trip condition can be found to determine the lasing material gain threshold. Alternatively, the
quality factor of the corresponding 3D cavity can be obtained if the simulation is run for a
large enough final time. The 2D equivalent description of the laser cavity can be used to prove
consistency between both analysis [5].

Acknowledgements

The authors gratefully acknowledge the financial support provided by the Sêr Cymru National
Research Network for Advanced Engineering and Materials, United Kingdom.

References

of a discontinuous Galerkin method for the solution of Maxwell’s equations, Computers &
Structures 137, 2–13.

netic resonant modes in cavities, 24th Conference of the UK Association of Computational
Mechanics, Cardiff (UK).

the Study of 2D waveguide–coupled microring resonators, Journal Of Lightwave Technology,
Vol. 23, No. 11, 2005.

dispersion models coupled to a discontinuous Galerkin time–domain method for Maxwell’s

Author index

Adams, T., 18
Ahangar Asr, A., 179, 199
Ai, W., 130
Al Manthari, M., 155
Al-Ateya, H., 199
Alfano, G., 248
Al-Gahtani, H.J., 98
Aliyu, M.D., 10
Alizadeh Sabet, S., 142
Almuramady, N., 38
AL-SAAD, M.K., 55
Al-Saadi, A., 151
Alzabeebee, S., 183
Arroyo, M., 195
Askes, H., 122
Augarde, C.E., 130, 134, 191, 211, 232, 240, 256, 264
Auricchio, F., 228
Ayşen Lav, M., 207
Baniotopoulos, C., 272
Barboza, B.R. 102, 167
Bartoli, G., 276
Bayly, A., 163
Bicanic, N., 244
Bing, Y., 256
Bird, R., 138
Bonet, J., 34, 228
Bonilla, P., 89
Bordas, S.P.A., 55
Borodich, F.M., 38
Brennan, A., 211
Brown, M., 211, 264
Burns, A., 159
Carson, J.M., 47
Ceh, N., 244
Chapman, D.N., 183
Charlton, T.J., 240, 256
Chen, B., 102
Chen, H.P., 10
Chen, L., 118
Ciantia, M.O., 187, 195
Claus, S., 30
Cleall, P.J., 26
Coombs W.M., 18, 134, 138, 191, 211, 232, 240, 256, 264
Cortis, M., 211, 256
Davies, R., 14
De Almeida, J.P.M., 280
De Borst, R., 118, 122, 126, 142
Dirar, S., 215
Drevon, T.R., 313
Du, X., 77
Ebrahimi, A.H., 272
Estrada-Rodriguez, G., 81
Fan, L., 232
Faramarzi, A., 42, 183, 215
Farhan, A., 159
Featherston, C.A., 110
Feng, Y.T., 6, 300
Freeman, B.L., 26
Gaceša, M., 224
Gadoury, P.A.H., 72
Gao, J., 305
García-Blanco, E., 63
Ghaffari Motlagh, Y., 151, 159, 163, 191
Giani, S., 18, 138
Gil, A.J., 34, 63, 228
Gilvey, B.D., 305
Gimperlein, H., 81, 309
Gitman, I.M., 72
González-Castejón, J., 203
Greto, G., 34
Grosman, S., 292
Hansen-Dörr, A.C., 126
Harireche, O., 215
Harireche, O., 42
Hasan, H.M., 51
Hashim, N.A., 134
Hassan, O.I., 228
Hassanpour, A., 151, 159, 163
Hattori, G., 106, 134
Hewitt, S., 174
Izzuddin, B.A., 284, 288, 292
Javadi, A.A., 22, 146
Jefferson, I., 42
Jefferson, T.D., 14, 26
Jelenic, G., 224, 244, 248
Kaczmarczyk, L., 59, 67, 85, 93
Kaewunruen, S., 276
Kakouris, E.G., 114
Kästner, M., 126
Kawashita, L.F., 110
Kerfriden, P., 30, 77, 89
Khaki, K., 260
Kolo, I., 122
Kulasegaram, S., 34, 55
Kundu, A., 77, 89
Latif, M.A., 300
Lee, C.H., 34, 63, 228
Lewandowski, K., 59, 67
Lewis, M.J., 47
Li, C., 102, 167
Li, S., 236
Liang, R., 6
Ma, X., 170
Macorini, L., 284, 288
Mahdavian, D., 146
Mahmud, T., 151
Margetts, L., 174
Marshall, J.F., 59
Martinez-Vazquez, P., 272
Maunder, E.A.W., 280
Mehrvavar, M., 215
Meng, X., 93
Mihai, L.A., 296
Mukhtar, F.M., 98
Mukwiri, R.A., 191
Nassr, A., 22
Nguyen, H.X., 220
Nithiarasu, P., 51, 155
Nordas, A.N., 284, 288
Ortigosa, R., 63
Pearce, C.J., 59, 67, 85
Pompeo, G., 276
Rassi, D., 47
Reboud, J., 93
Revell, A., 174
Robinson, S., 211
S.M. Al-Azzawi, A.S.M., 110
Safar, A., 296
Salmeron-Sanchez, M., 67
Samin, M., 42
Santos, L.P.F., 284, 288
Saqr, K.M., 170
Sauffisseau, R., 179
Seaid, M., 305
Sevilla, R., 313
Shehadeh, M.F., 170
Shire, T., 187
Shore, A.K., 313
Sime, N., 252
Škec, L., 248
Smith, C., 203
Stark, D., 309
Swadener, G., 170
Tatlıoğlu, E., 207
Tee, K.F., 268
Trevelyan, J., 106, 236, 260, 305
Triantafyllou, S.P., 114
Ülker, M.B.C., 207
Ullah, Z., 85
Unwin, H.J.T., 252
Van Loon, R., 47
Vo, T.P., 220
Wagner, A.B., 305
Wang, L., 264
Wang, Y., 6
Wells, G.N., 252
Wordu, A.H., 268
Wyatt, H., 296
Yang, Z., 2
Zhang, C., 2
Zhang, N., 195
Zheng, Hui, 2
Zidane, I.F., 170