Apply for PhD, live in Scotland and develop MoFEM

MOFEM

http://mofem.eng.gla.ac.uk/mofem/html/research_opportunities.html

University of Glasgow

GCEC
Glasgow Computational Engineering Centre

MOFEM
mofem.eng.gla.ac.uk

Mixed finite element formulation for solid mechanics problems

Łukasz Kaczmarczyk, Callum J. Runcie,
Ananya Bijaya, Adriana Kulikova, Ross Williams,
Andrei G. Shvarts, Chris J. Pearce

James Watt School of Engineering,
Glasgow Computational Engineering Centre

DOI 10.5281/zenodo.15175739

WORLD CHANGING GLASGOW

A WORLD TOP 100 UNIVERSITY

MOFEM
mofem.eng.gla.ac.uk

Exponential of stretch: Neohookean

Classical Neo-Hookean potential expression:

$$\Psi(I_C, J) = \frac{\mu}{2}(I_C - 3) - \mu \ln J + \frac{\lambda}{2}(\ln J)^2$$

$$\delta\Psi = \mathbf{P} : \delta\mathbf{F}$$

$$= \{\mu(\mathbf{F} - \mathbf{F}^{-T}) + \lambda \ln J J \mathbf{F}^{-T}\} : \delta\mathbf{F}$$

Matrix inversion, Logarithm of Jacobian, affect robustness

New formulation exploiting logarithmic strain:

$$\Psi(I_C, J) = \mu(\exp(\mathbf{H}) - \exp(-\mathbf{H})) : \exp_{\mathbf{H}}(\delta\mathbf{H}) + \lambda\mathbf{H} : \delta\mathbf{H}$$

$$\mathbf{H} = \frac{1}{2}\left[\ln(\mathbf{F}^{\mathrm{T}} : \mathbf{F})\right], \quad \lambda^H \in \mathbb{R}$$

No matrix inversion necessary
→ numerical stability

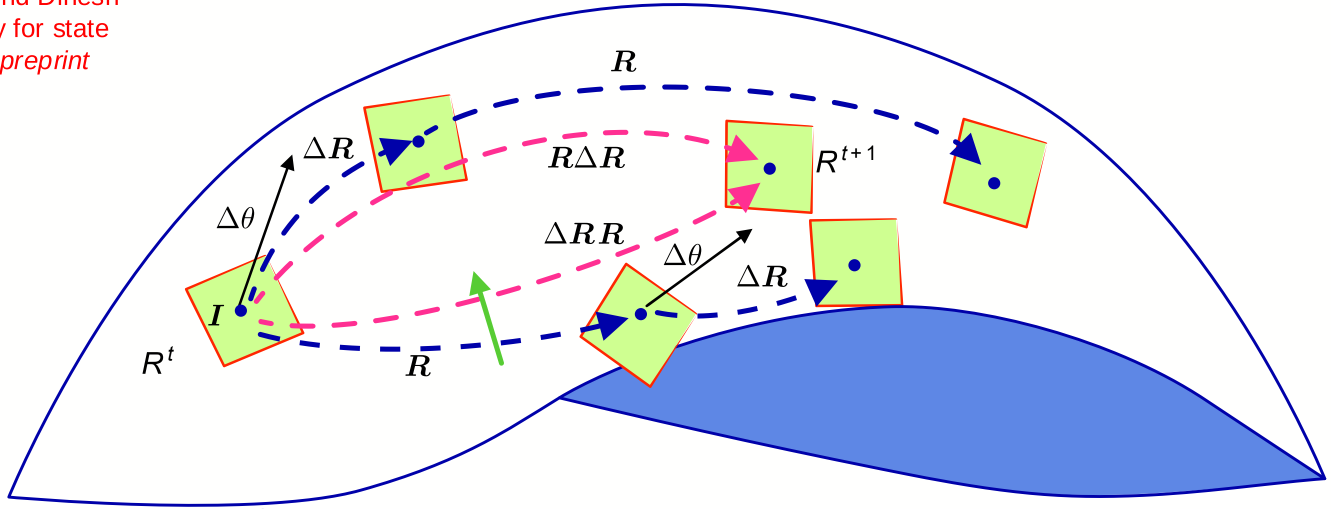
Bonet, Javier, Antonio J. Gil, and Richard D. Wood. *Nonlinear solid mechanics for finite element analysis: dynamics*. Cambridge University Press, 2021.

Poya, Roman, et al. "Generalised tangent stabilised nonlinear elasticity: An automated framework for controlling material and geometric instabilities." *Computer Methods in Applied Mechanics and Engineering* 436 (2025): 117701.

Exponential of axis of rotation: Symmetric Incremental Rotations

Sola, Joan, Jeremie Deray, and Dinesh Atchuthan. "A micro lie theory for state estimation in robotics." *arXiv preprint arXiv:1812.01537* (2018).

SO3 (Rotations in 3D)



$$(\mathbf{R}^{t+1})^T\mathbf{R}^{t+1} \approx \frac{1}{2}(\mathbf{R}\Delta\mathbf{R}+\Delta\mathbf{R}\mathbf{R})^T \cdot (\mathbf{R}\Delta\mathbf{R}+\Delta\mathbf{R}\mathbf{R}) = \mathbf{I}+\mathbf{O}^2(\Delta\boldsymbol{\theta})$$

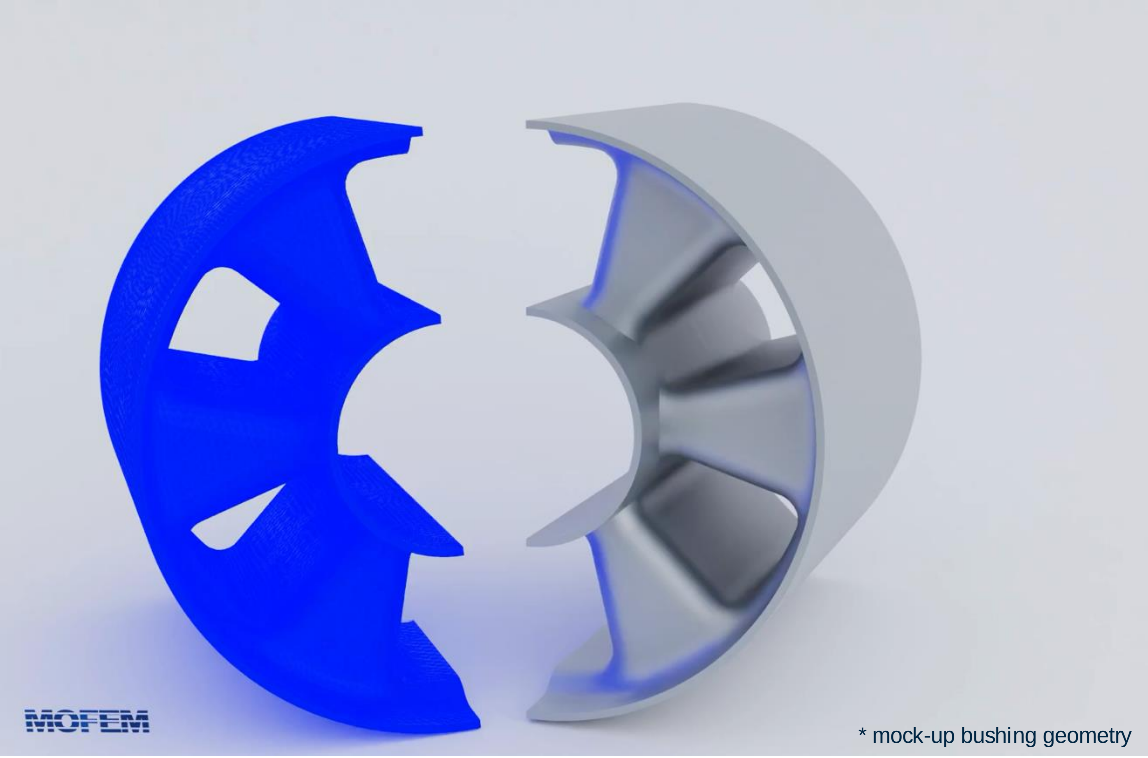
$$\Delta\mathbf{R} = \exp[\Delta\boldsymbol{\theta}]$$

Rodrigues' Rotation Formula. Rotation can be expressed with finite sum series.

$$\mathbf{F}^{t+1} = \mathbf{R}^{t+1}\exp\mathbf{H}^{t+1}$$

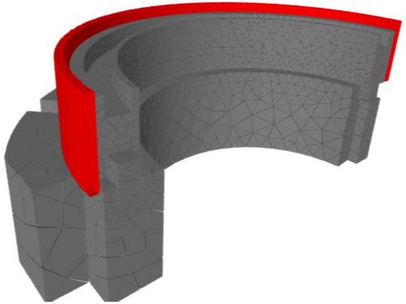
Polar decomposition (material)

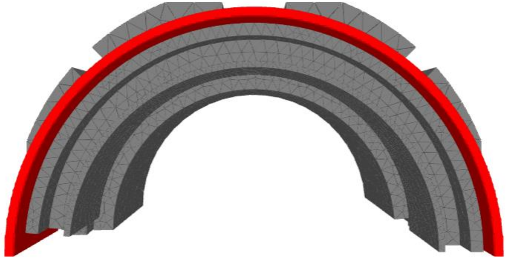
Example application: Bushing

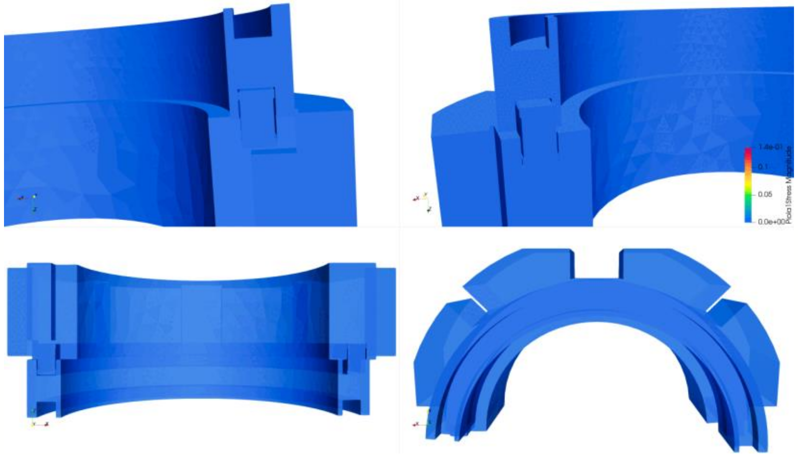


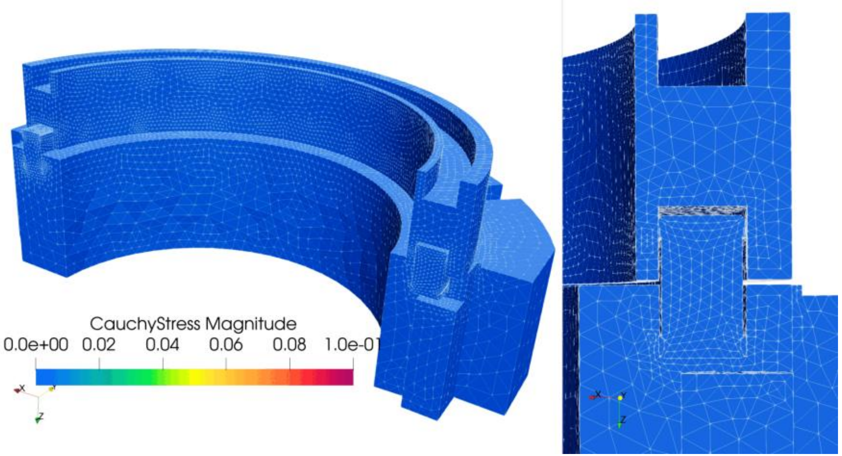
MOFEM
mofem.eng.gla.ac.uk

Example application: Structural integrity problems



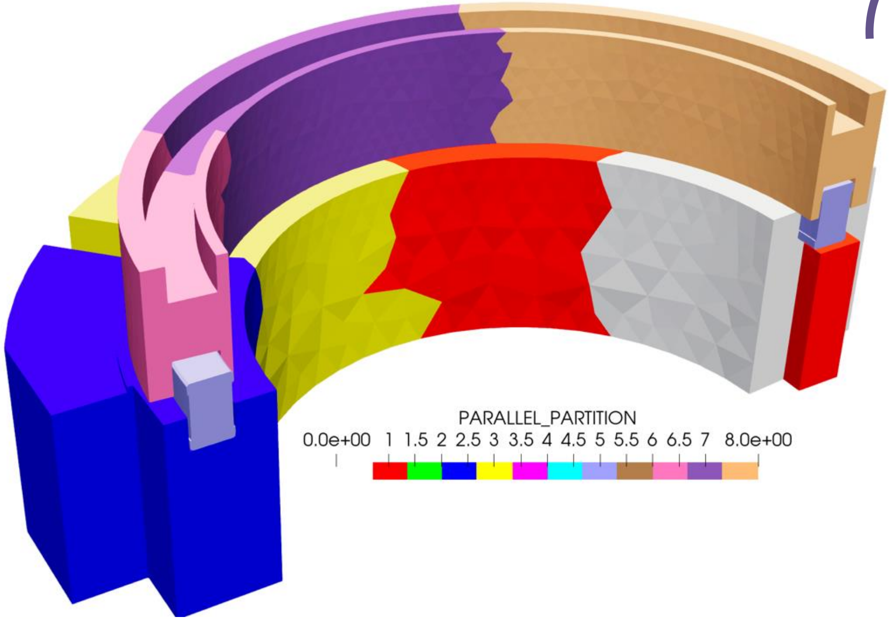


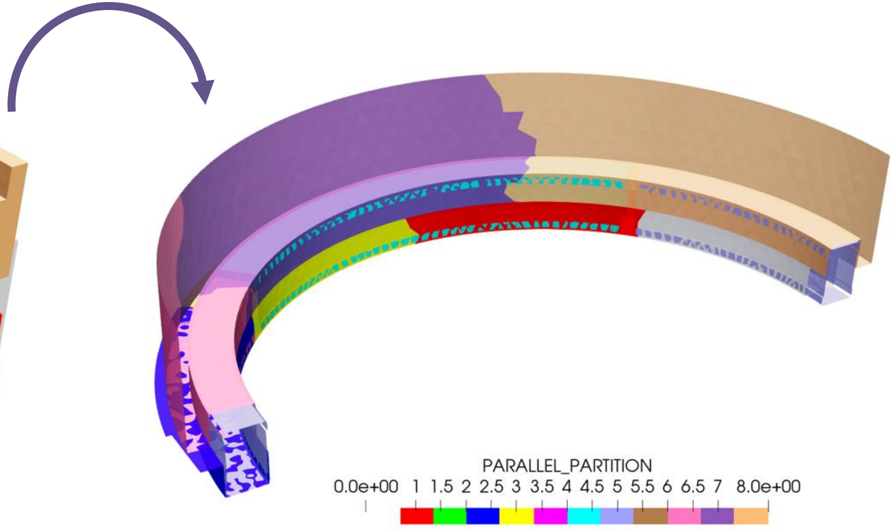




mofem.eng.gla.ac.uk

Messy issue of contact (robustness trumps efficiency in framework design)

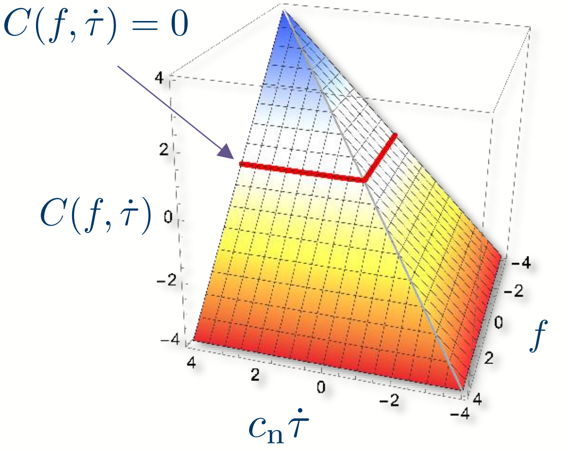




- On exchange surfaces, we share: current positions, tractions
- The kd-tree is built on contact surfaces
- Aircraft's shadow projection method
- Contact surface mesh is arbitrarily refined (take into account HO-approximation)

mofem.eng.gla.ac.uk

Plasticity, contact, damage & fracture

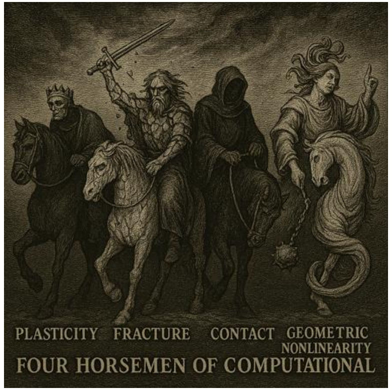


- Structural integrity problems are difficult to scale – heterogeneous materials and complex geometry with many components.

- In structural integrity problems, the devil is in the unilateral constraints, plasticity at integration points, contact on surfaces, or the crack front.

- Strongly nonlinear problems: constitutive equations, history, geometrical nonlinearities, topology evolution & boundary conditions.

- Unavoidable approximation and integration error. Plastic/Contact fronts, Cracks, Wrinkling, Creases, and Cusps, etc



Mechanics

MOFEM
mofem.eng.gla.ac.uk

First commit June 2013

University of Glasgow

Scientific Management
- Łukasz Kaczmarczyk
- Chris Pearce
- Andrei Shvarts
- Andrew McBride
- Vihar Georgiev

Core Developers
- Karol Lewandowski
- Adriana Kuliková
- Callum Runcie
- Ross Williams

Users Modules Contributors
- Richard Olley
- Joshua Gorham
- MD Tanzib Ehsan Sanglap
- Yingjia (Leo) Gao
- Ananya Bijaya
- Lily Sierra Fisher
- Oliver Duncan
- Bohdan Shevchenko

14 Past Contributors

ROYAL ACADEMY OF ENGINEERING

UKRI Engineering and Physical Sciences Research Council

Deep Nano

GCCC

EDF ENERGY

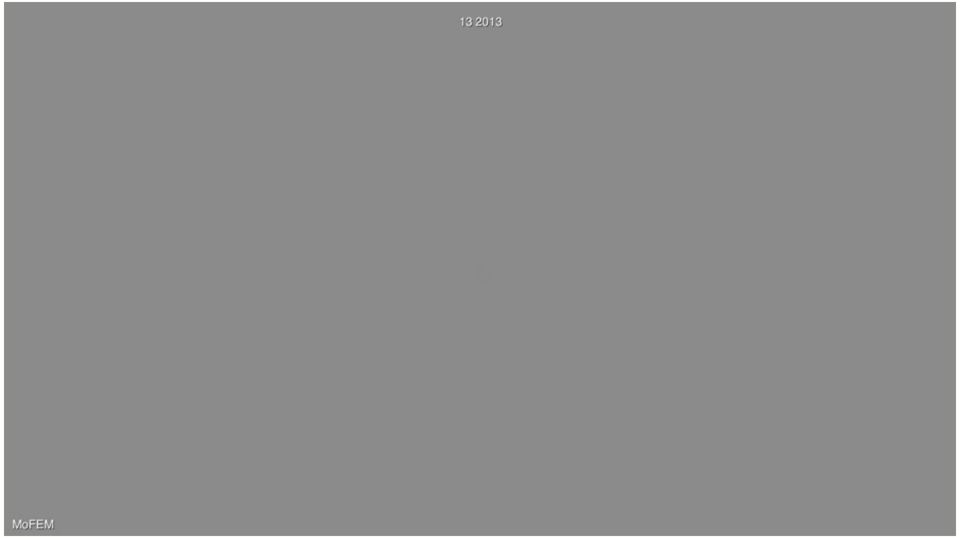
ROLLS ROYCE

MesH-Oriented Solutions

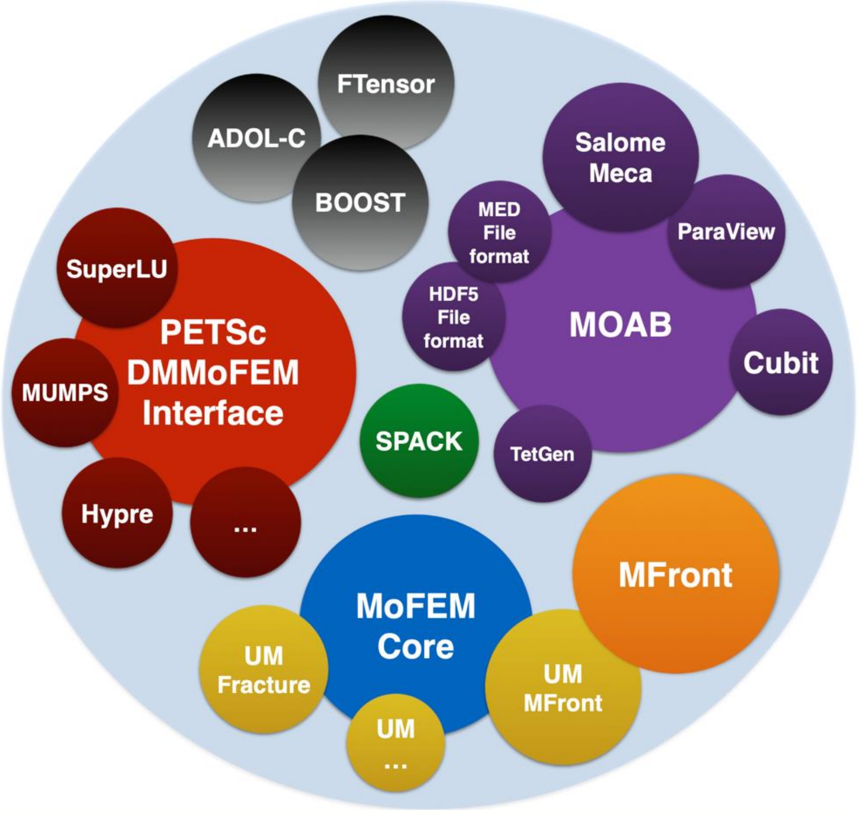
FREUDENBERG INNOVATING TOGETHER

In a nutshell

- Core library has ~270,000 lines of code
- Code made by ~50 contributors
- It would take ~70 years of work of a single programmer to write that code (according to COCOMO model - OpenHub)
- It is mostly written in C++
- Open repository and MIT license



MoFEM ecosystem

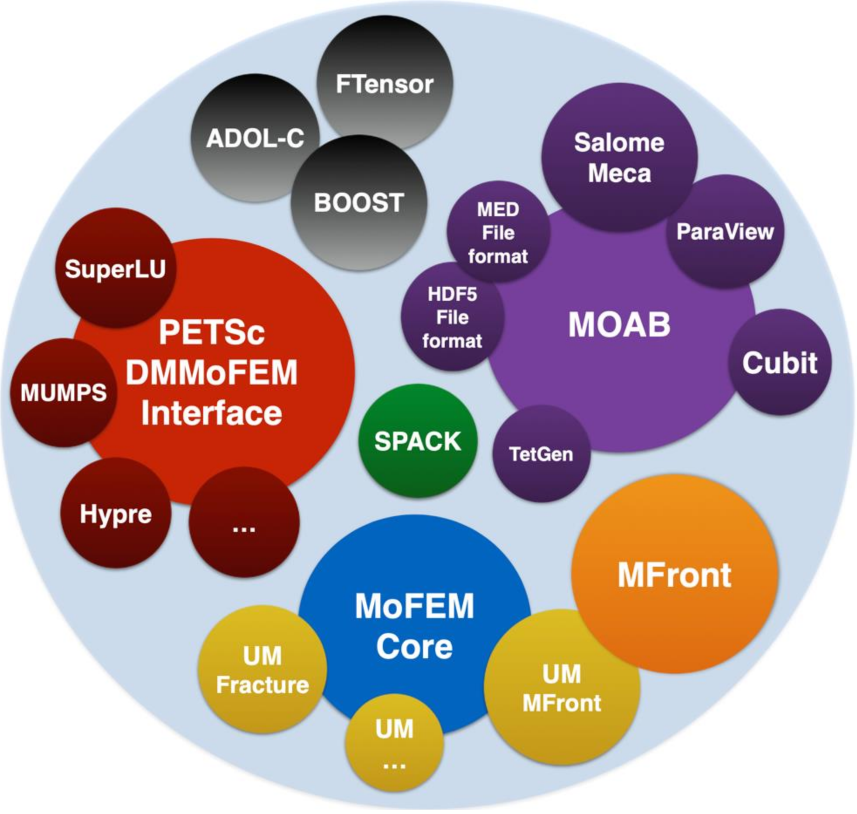


MOFEM
mofem.eng.gla.ac.uk

MoFEM ecosystem

Matrices, vectors
and many solvers

Argonne NATIONAL LABORATORY

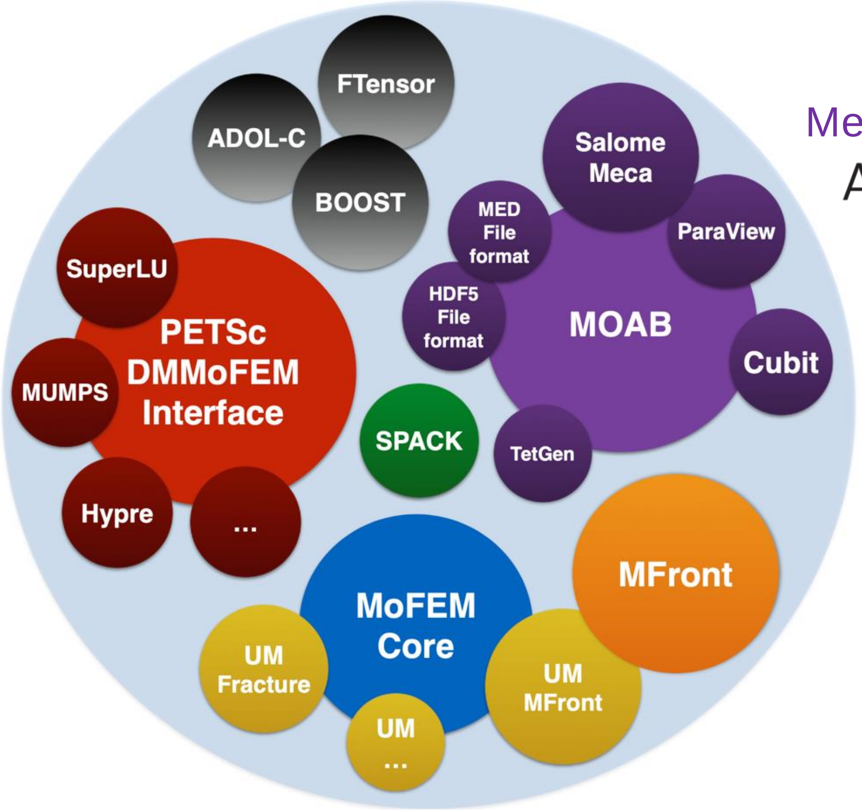


MOFEM
mofem.eng.gla.ac.uk

MoFEM ecosystem

Mesh and data

Argonne NATIONAL LABORATORY



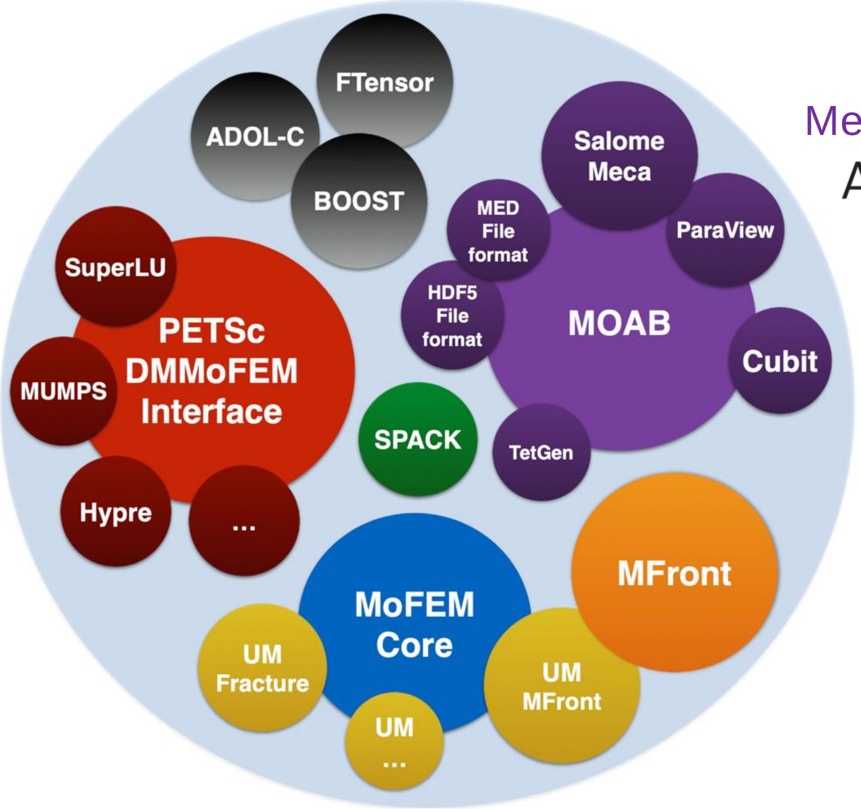
Matrices, vectors and many solvers

Argonne NATIONAL LABORATORY

MoFEM ecosystem

Mesh and data

Matrices, vectors and many solvers



Material behaviour models

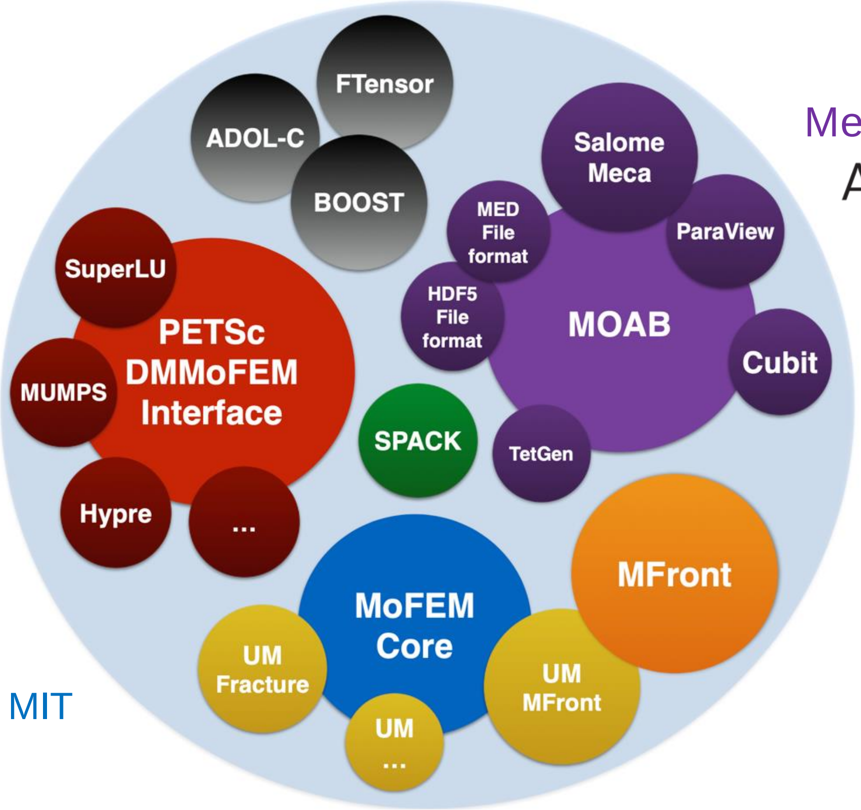
MoFEM ecosystem

mofem.eng.gla.ac.uk

Matrices, vectors and many solvers

Argonne NATIONAL LABORATORY

Open-source MIT license



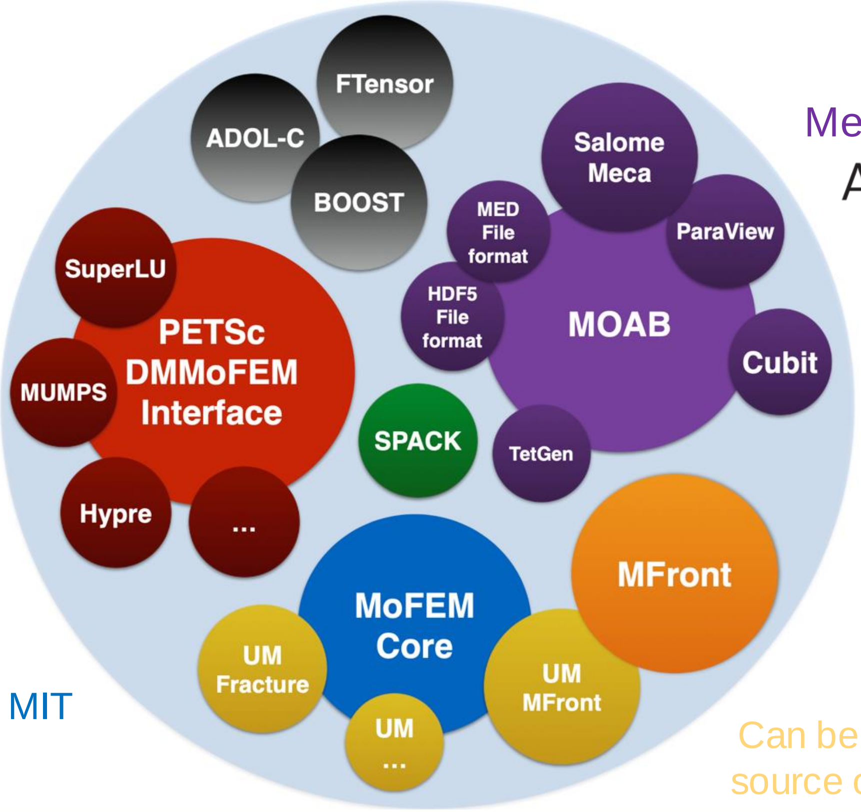
Mesh and data

Argonne NATIONAL LABORATORY

Material behaviour models

MoFEM ecosystem

mofem.eng.gla.ac.uk



Mesh and data

Matrices, vectors and many solvers

Material behaviour models

Open-source MIT license

Can be either open-source or proprietary

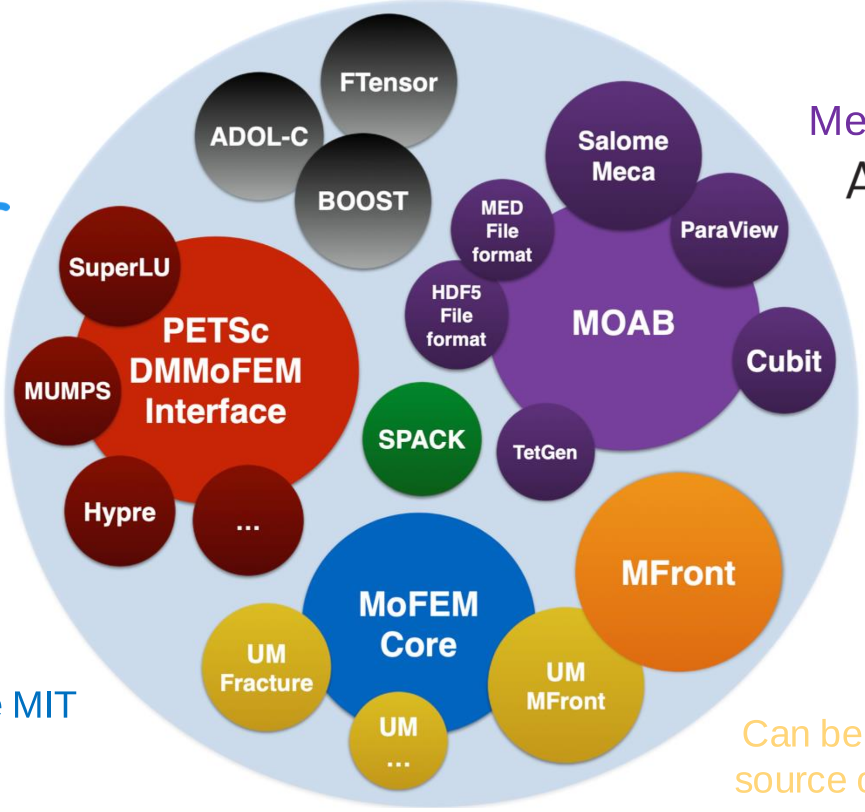
mofem.eng.gla.ac.uk

MoFEM ecosystem

All can be shipped in a Docker container

Matrices, vectors and many solvers

Open-source MIT license



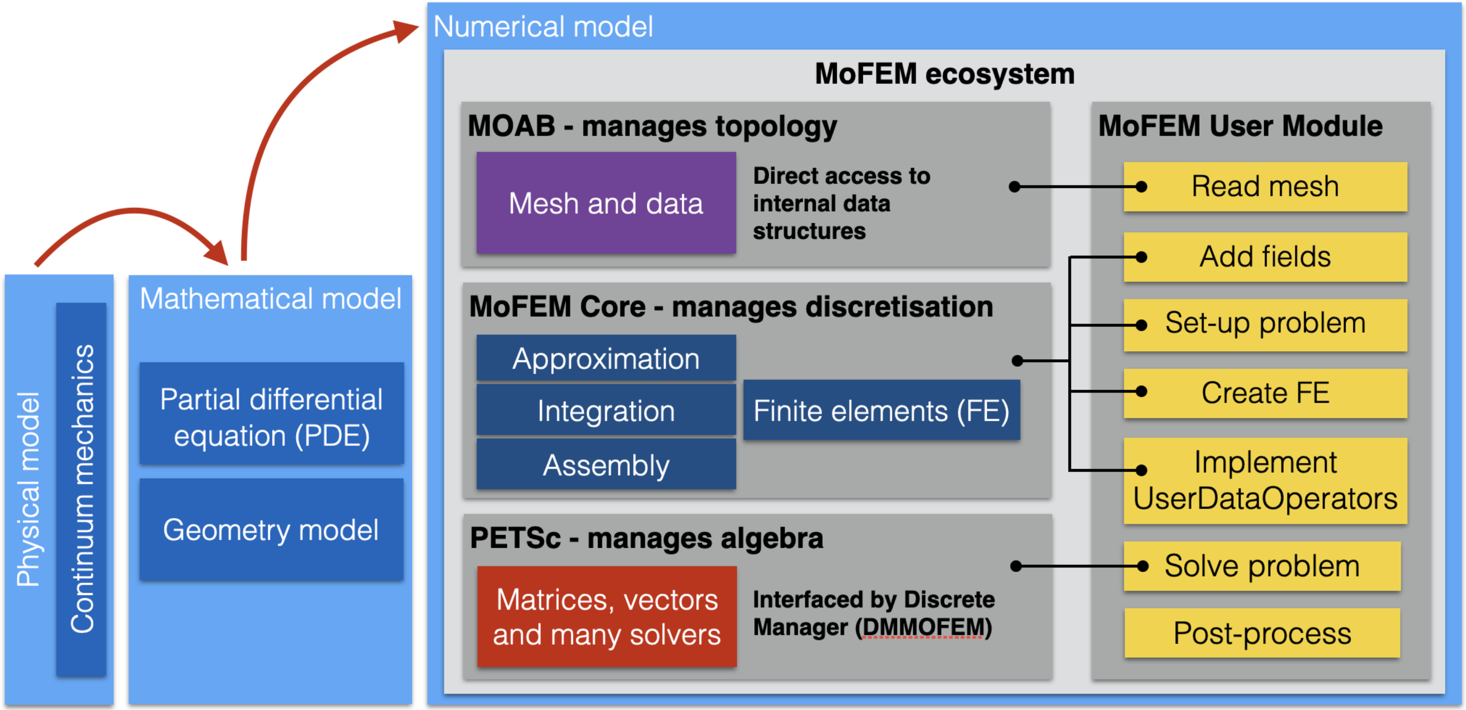
Mesh and data

Material behaviour models

Can be either open-source or proprietary

MOFEM
mofem.eng.gla.ac.uk

High Level Design

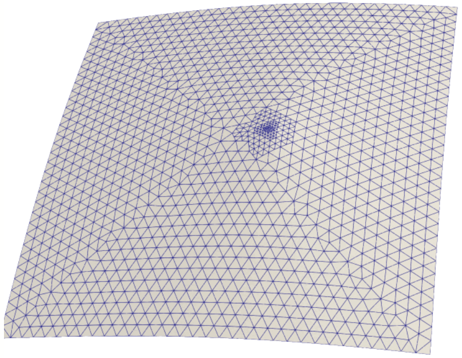


mofem.eng.gla.ac.uk

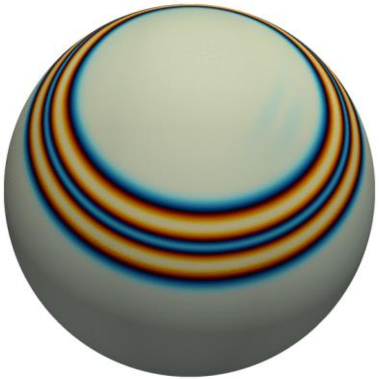
MoFEM Features

- We aim at the whole de Rham complex: L2, H-div, H-curl, and H1.
- L2/DG, H1/DG, and other energetic spaces are also included.
- Hierarchical approximation bases.
- Scalar, vectorial and tensorial bases.
- Hierarchical (p-adaptivity) and Beristain-Bezier base

DG-upwind advection of level set: Tutorial ADV-3.



Shallow-Wave equation on generic curved surfaces



MoFEM Design – Industry First Approach

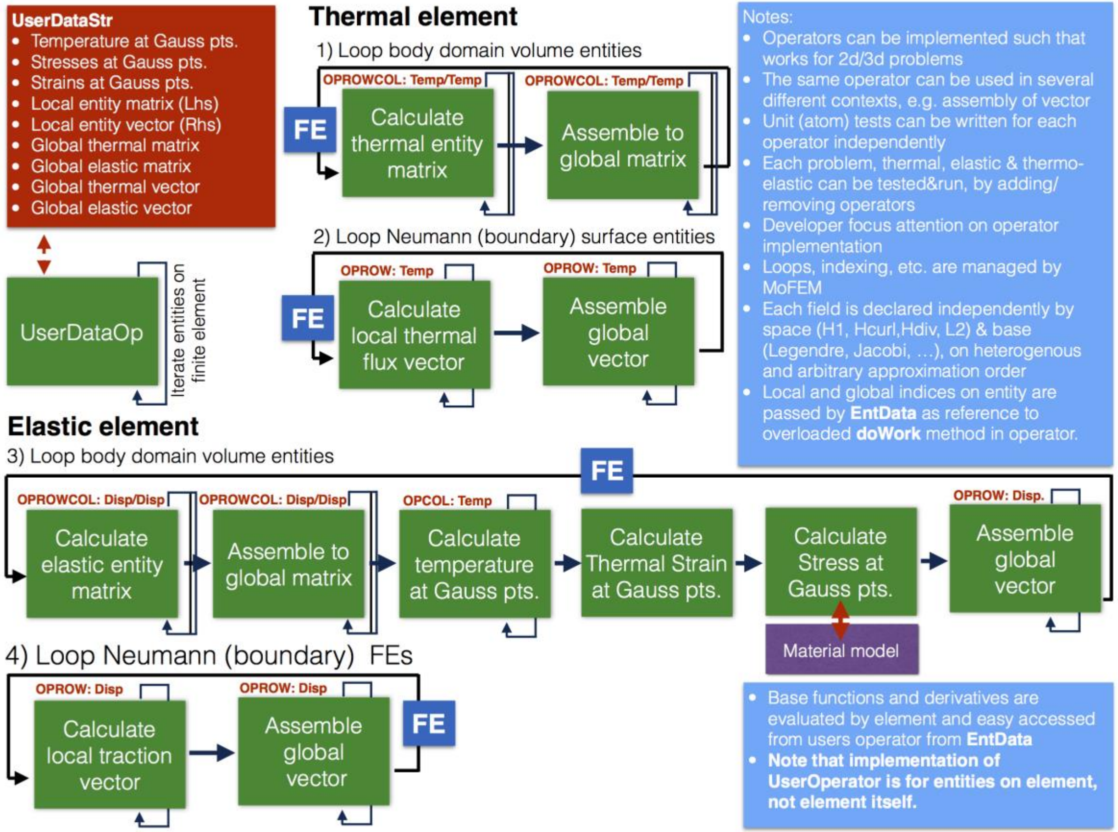
mofem.eng.gla.ac.uk

- Core library (abstraction levels) and modules with physics implementation – two different repositories, licensing, copyright when needed.
- Hollywood model (you do not call us, we call you) – development patterns - high code coverage - research code short pathway to application.

```
MoFEM::Core core(moab);
MoFEM::Interface& m_field = core;
// define fields
CHKERR m_field.add_field("DISP",H1,AINSWORTH_LEGENDRE_BASE,3);
CHKERR m_field.add_field("FLUX",HDIV,DEMKOWICZ_JACOBI_BASE,1);
// meshset consisting all entities in mesh
EntityHandle root_set = moab.get_root_set();
// add entities to field
CHKERR m_field.add_ents_to_field_by_TETs(root_set,"DISP");
CHKERR m_field.add_ents_to_field_by_TETs(root_set,"FLUX");
// set app. order (that is boring same order to all)
int order = 5;
CHKERR m_field.set_field_order(root_set,MBTET,"DISP",order);
CHKERR m_field.set_field_order(root_set,MBTET,"FLUX",order);
// build
CHKERR m_field.build_fields();
```

MOFEM
mofem.eng.gla.ac.uk

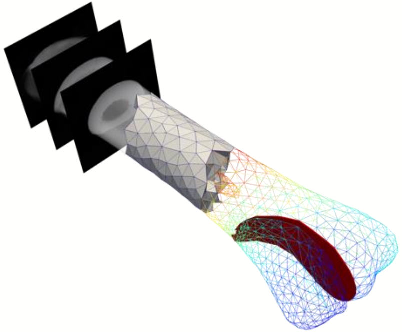
Finite Element is a pipeline of operators



mofem.eng.gla.ac.uk

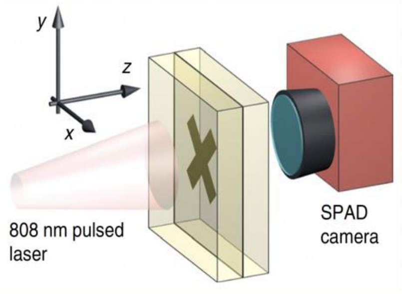
Leverage testing through science applications

Bone remodelling & fracture

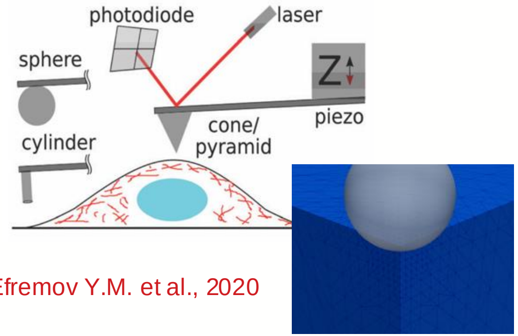


Lewandowski K., et al., 2021

Photon diffusion through turbid media

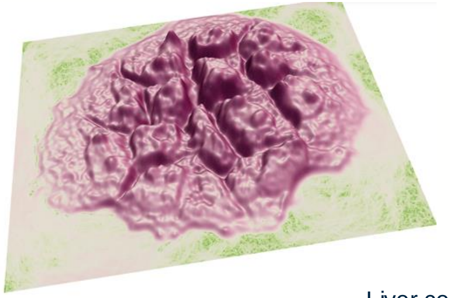


Simulation of nanoindentation for AFM of cells



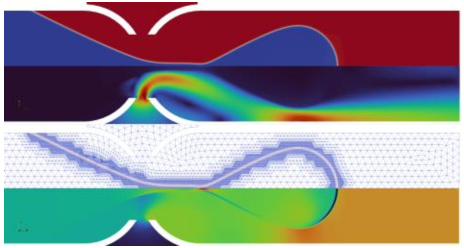
Efremov Y.M. et al., 2020

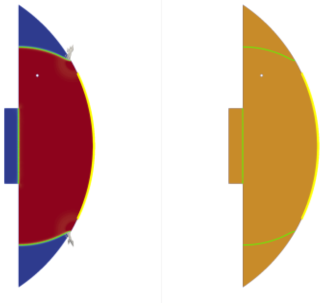
Cell surface reconstruction using ToI



Liver cell

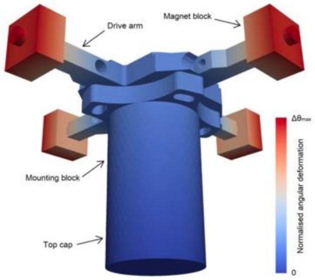
Microfluidics





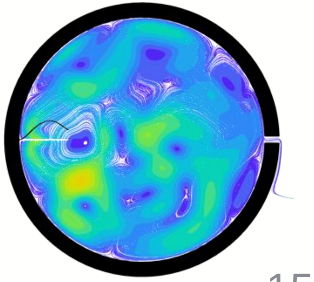
D. Lockington, et al. 2022

Geotechnics



Rieman L., et al. 2023

Fluid-structure interaction



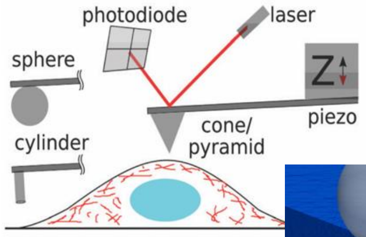
MOFEM
mofem.eng.gla.ac.uk

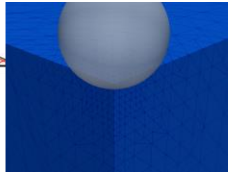
Leverage testing through science applications

Bone remodelling & fracture

Lewandowski K., et al., 2021

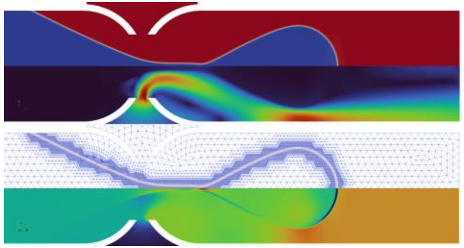
Simulation of nanoindentation for AFM of cells



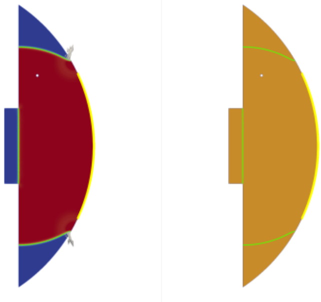


Efremov Y.M. et al., 2020

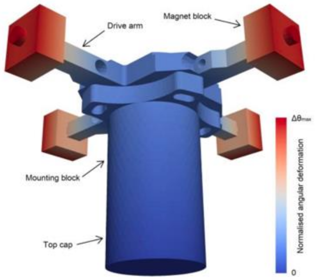
Microfluidics



D. Lockington, et al. 2022

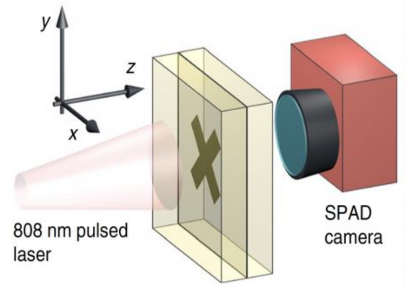


Geotechnics

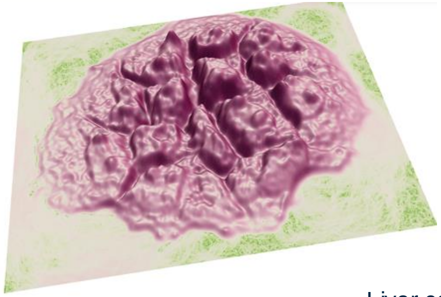


Rieman L., et al. 2023

Photon diffusion through turbid media

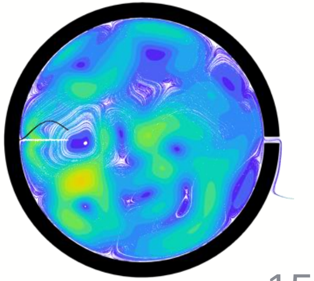


Cell surface reconstruction using ToI



Liver cell

Fluid-structure interaction



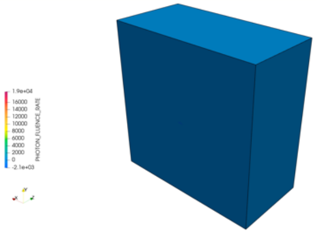
MOFEM
mofem.eng.gla.ac.uk

Leverage testing through science applications

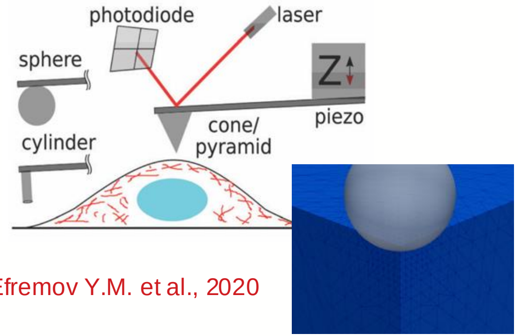
Bone remodelling & fracture

Lewandowski K., et al., 2021

Photon diffusion through turbid media

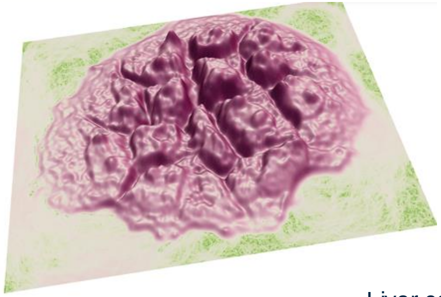


Simulation of nanoindentation for AFM of cells



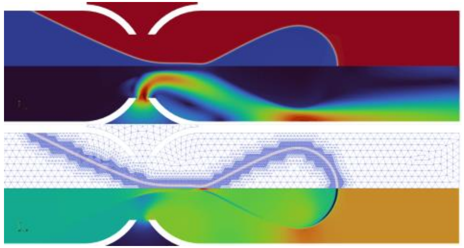
Efremov Y.M. et al., 2020

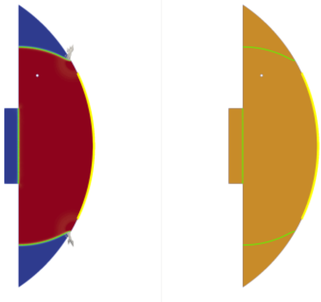
Cell surface reconstruction using ToI



Liver cell

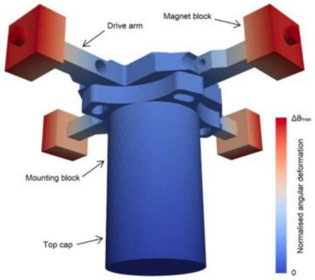
Microfluidics





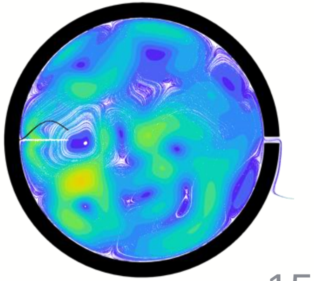
D. Lockington, et al. 2022

Geotechnics



Rieman L., et al. 2023

Fluid-structure interaction

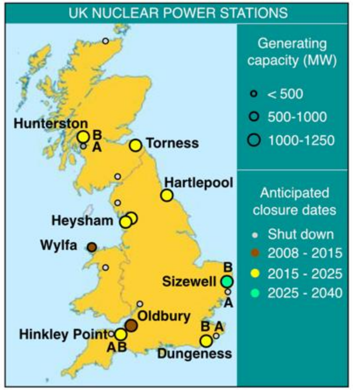


Nuclear power in the UK

Advanced gas-cooled reactors (AGR)

Nuclear power in the UK

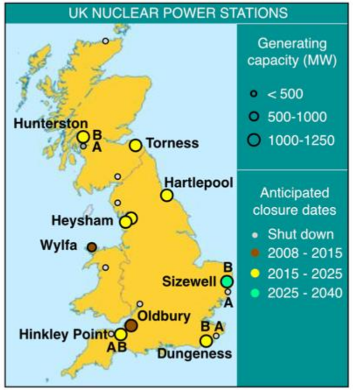
Advanced gas-cooled reactors (AGR)

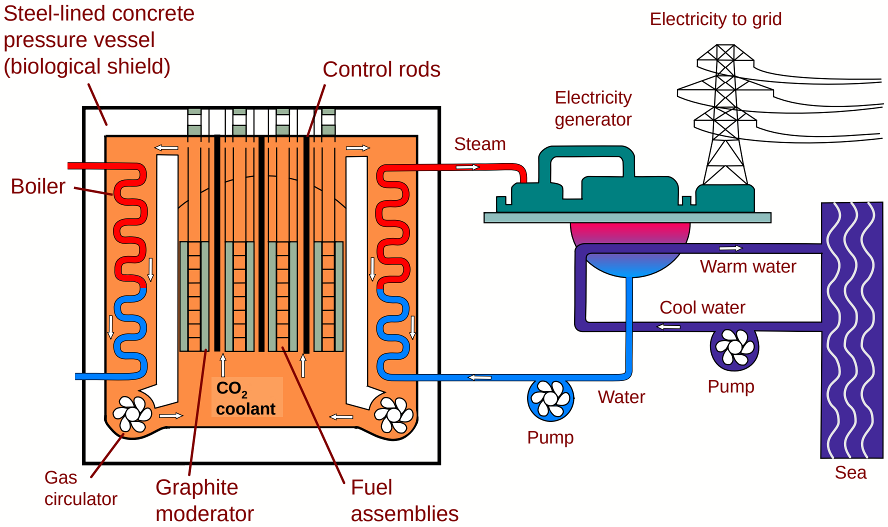


≈20% of energy from nuclear power

Nuclear power in the UK

Advanced gas-cooled reactors (AGR)





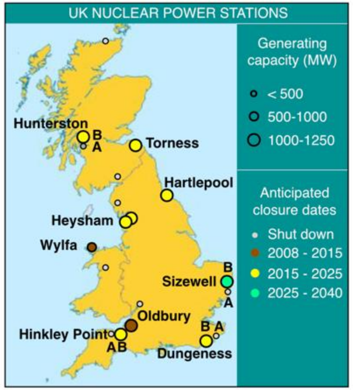
≈20% of energy from nuclear power

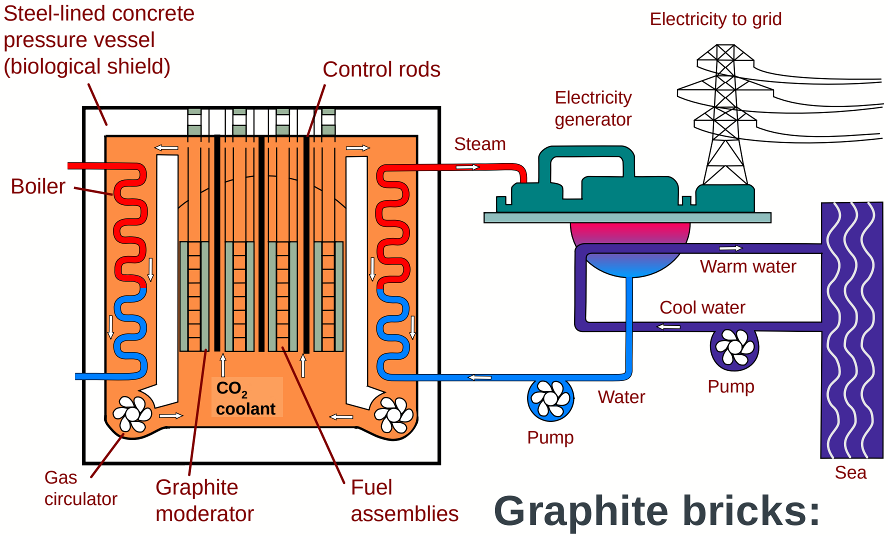
Nuclear power in the UK

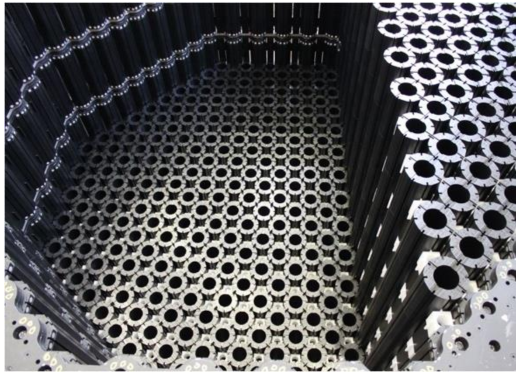
mofem.eng.gla.ac.uk

EDF ENERGY

Advanced gas-cooled reactors (AGR)





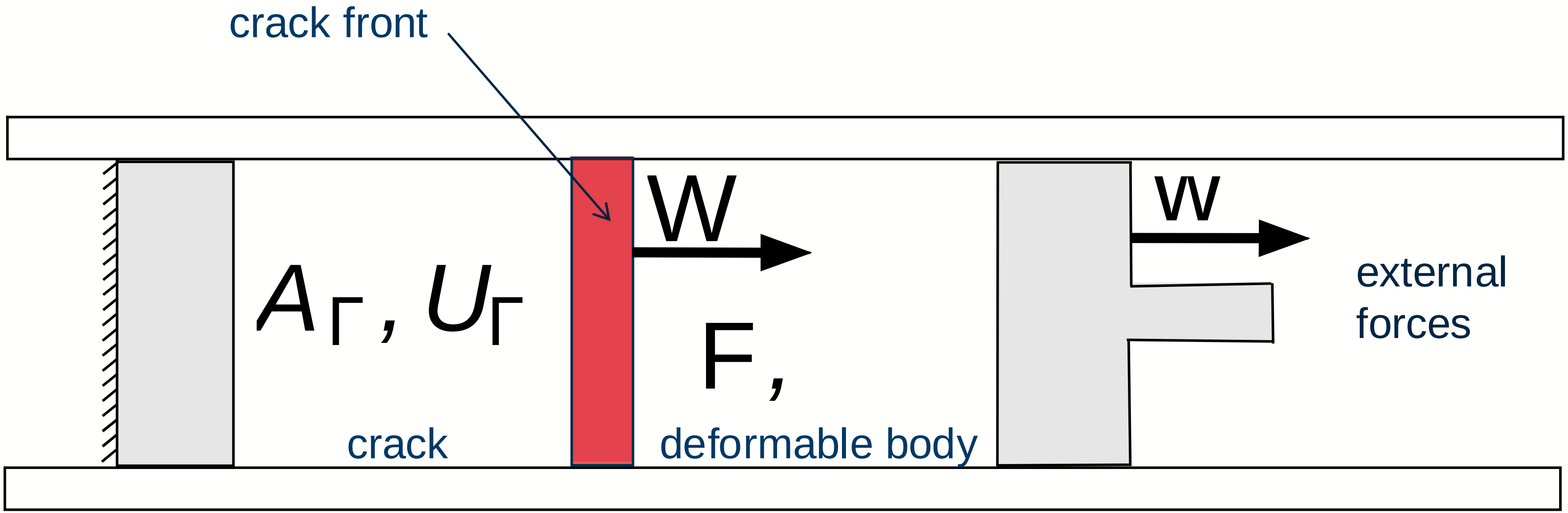


≈20% of energy
from nuclear power

Graphite bricks:
- neutron moderator
- mechanical stability
- thermal inertia

Thermomechanical model

First Law

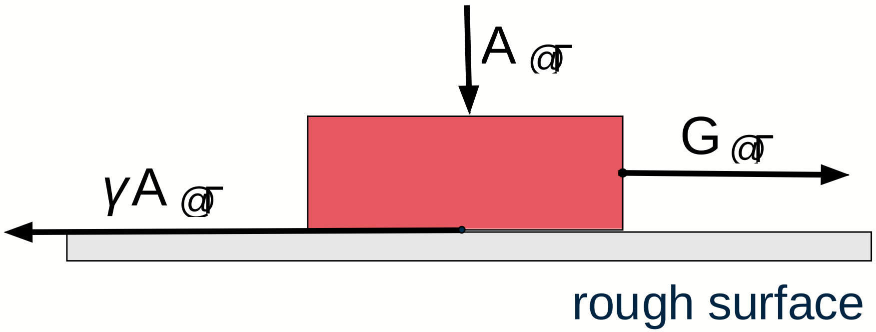


Fracture process

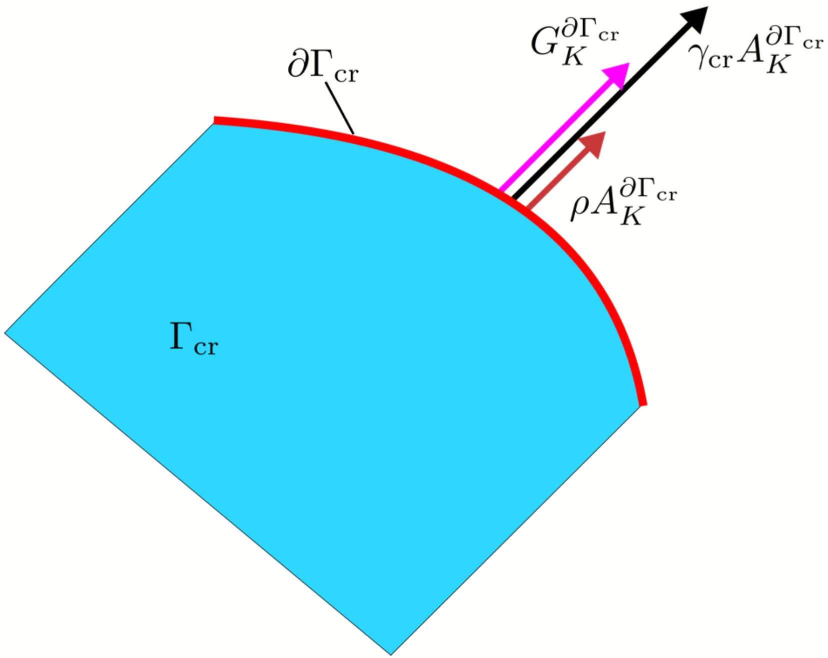
Second Law

Entropy (nothing) is never like it was before

$$D := \gamma \dot{W} \cdot A_{\partial\Gamma} \geq 0$$



Force balance at the crack front



Balance:

$$G_K^{\partial\Gamma_{\rm cr}} - (g_{\rm cr}/2 - \rho) A_K^{\partial\Gamma_{\rm cr}} = 0$$

3 cases:

(i) body is not loaded $\Leftrightarrow G_K^{\partial\Gamma_{\rm cr}} = 0 \Leftrightarrow \rho = g_{\rm cr}/2$

(ii) crack propagates $\Leftrightarrow \rho = 0$

(iii) intermediate state $\Leftrightarrow \rho > 0$ and $G_K^{\partial\Gamma_{\rm cr}} \neq 0$

KKT for crack propagation:

$$A_K^{\partial\Gamma_{\rm cr}} \dot{W}_K \geq 0, \qquad \rho \geq 0, \qquad \rho A_K^{\partial\Gamma_{\rm cr}} \dot{W}_K = 0$$

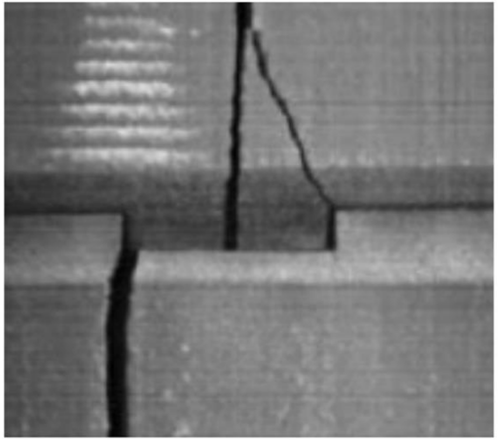
Complementarity function:

$$C_{\rm cr}(\rho, \dot{W}_K) := \rho - \max\left(0, \rho - c_{\rm cr} A_K^{\partial\Gamma_{\rm cr}} \dot{W}_K\right)$$

Fracture of irradiated graphite bricks

Fracture of irradiated graphite bricks

Fracture of irradiated graphite bricks

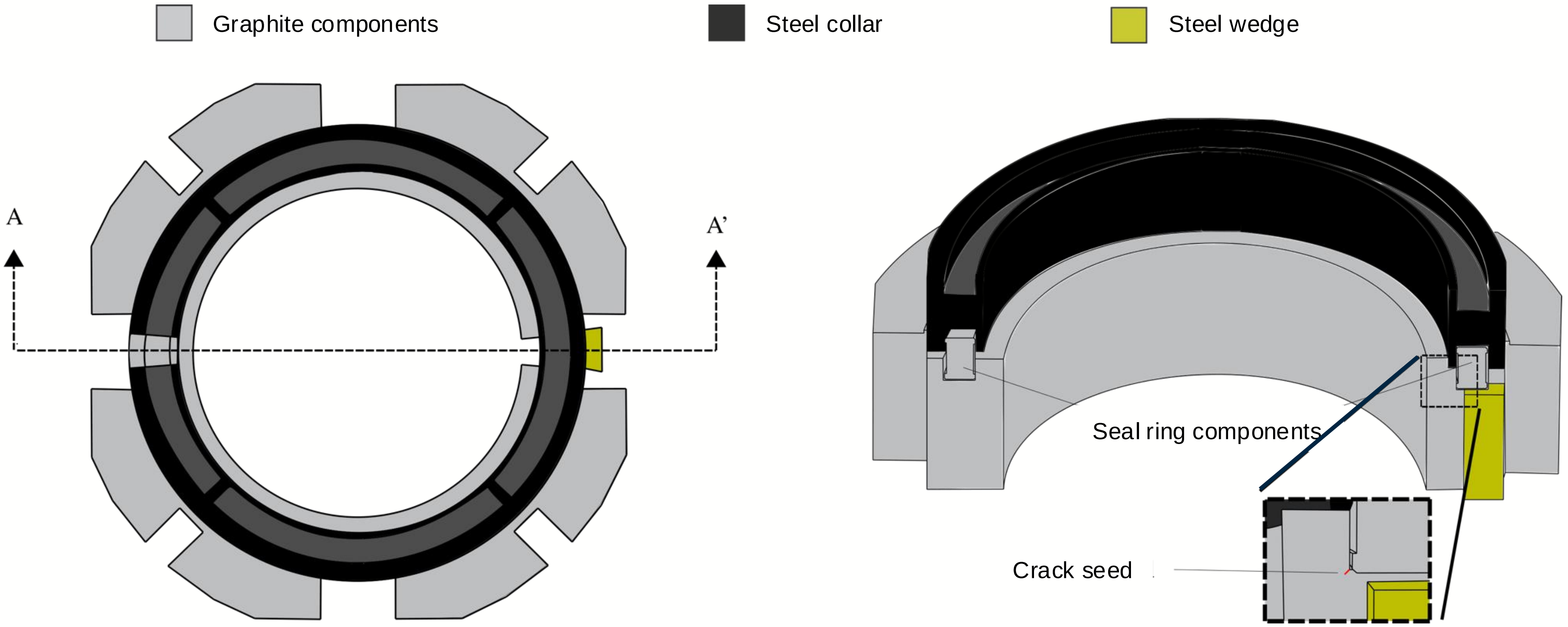


EDF ENERGY

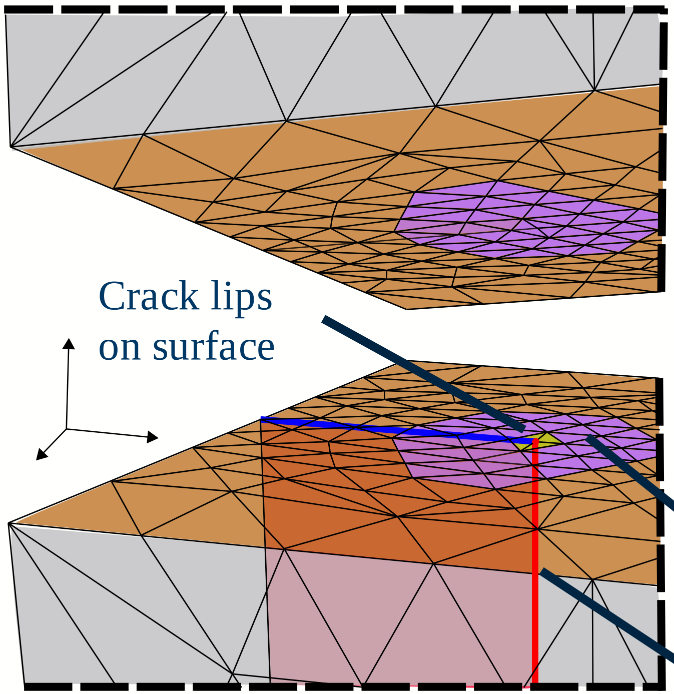
Athanasiadis, I., Shvarts, A.G. et al. *CMAME* (2023)

Scan to access paper

Analysis geometry

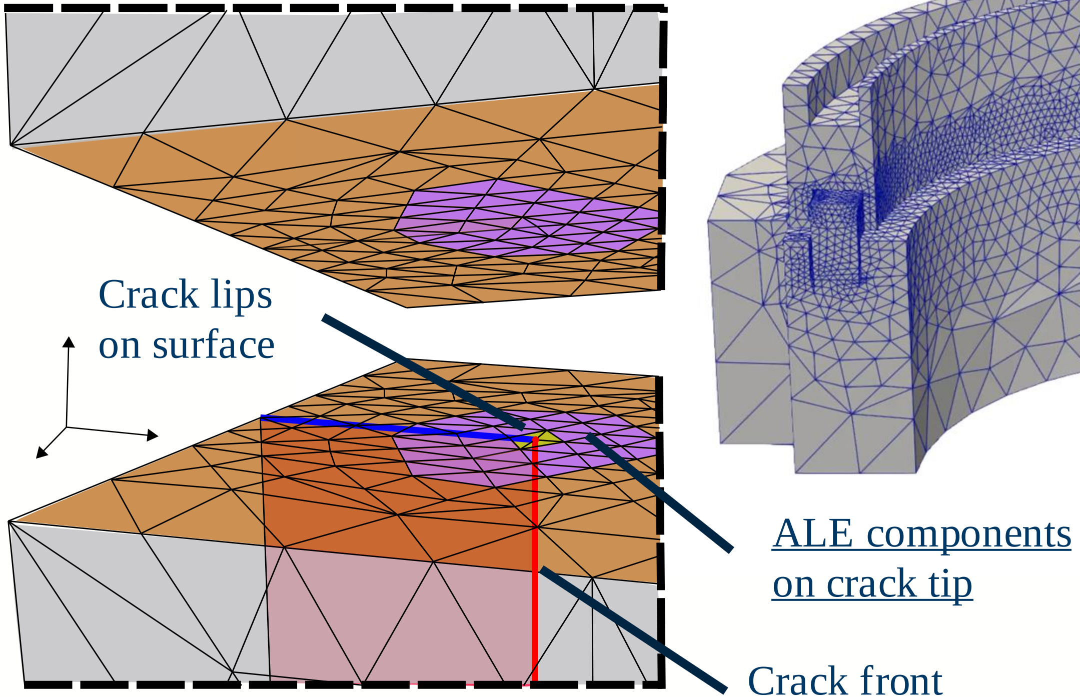


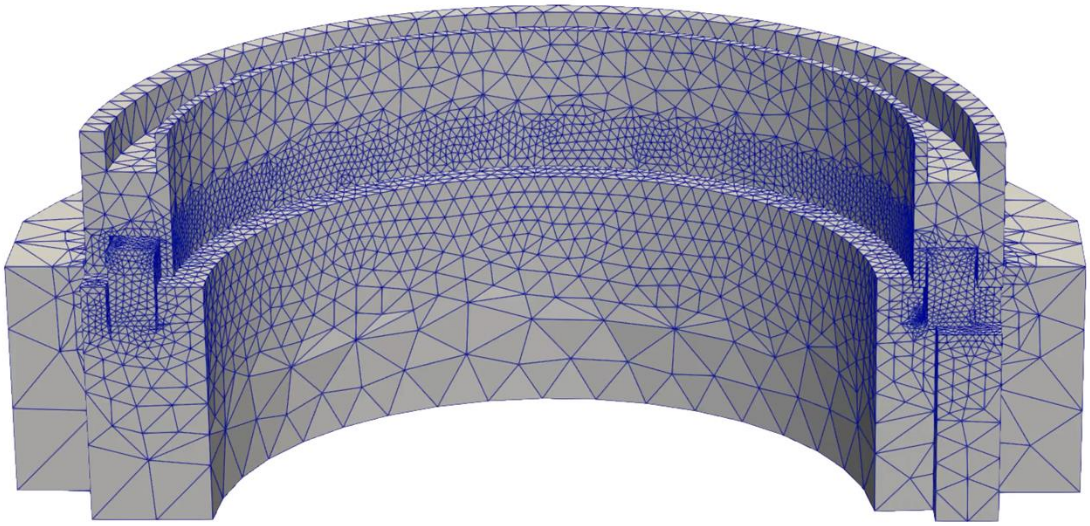
Simulation


Crack lips
on surface
ALE components
on crack tip
Crack front

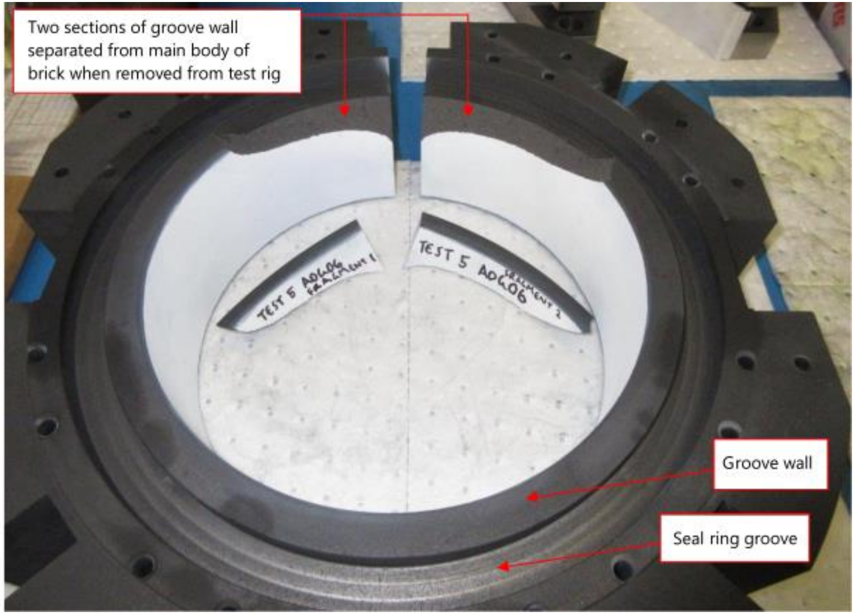
MOFEM mofem.eng.gla.ac.uk

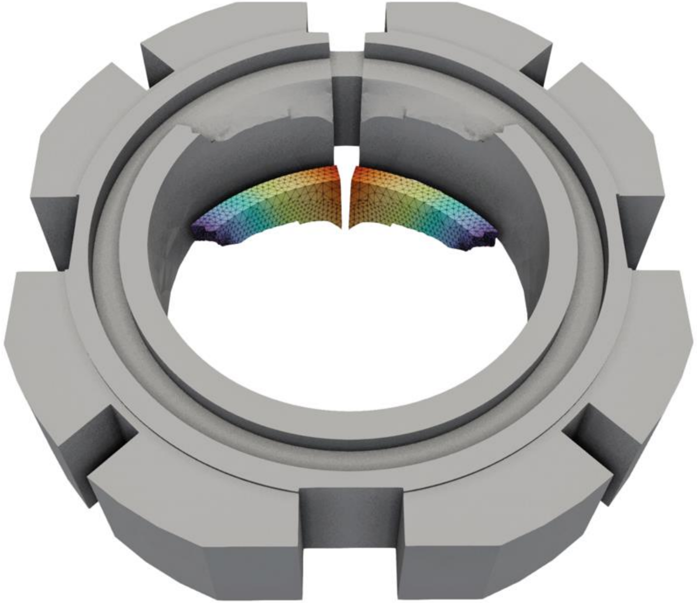
Simulation





Comparison with the experiment





Jacobs

Mixed Elasticity Formulation

mofem.eng.gla.ac.uk

Generalised Hu-Washizu functional $\mathbf{U} = \ln(\mathbf{H})$

$$\Pi = W(\boldsymbol{U}) + \int_{\Omega_0} \left(\frac{\partial x_i}{\partial X_J} - R_{iK} U_{KJ} \right) P_{iJ} \mathrm{d}V - \int_{\Omega_0} u_i f_i \mathrm{d}V - \int_{\gamma_0} \bar{u}_i t_i \mathrm{d}S$$

Consistency equation:

$$\frac{\partial \Pi}{\partial P_{iJ}} \delta P_{iJ} = \int_{\Omega_0} \frac{\partial x_i}{\partial X_J} \delta P_{iJ} \mathrm{d}V - \int_{\Omega_0} R_{iK} U_{KJ} \delta P_{iJ} \mathrm{d}V$$

Physical equation:

$$\frac{\partial \Pi}{\partial U_{KL}} \delta U_{KL} = \frac{\partial W}{\partial U_{MN}} \partial U_{MN} - \int_{\Omega_0} R_{iK} U_{KL,MN} \delta U_{MN} P_{iL} \mathrm{d}V$$

Conservation of angular momentum:

$$\frac{\partial \Pi}{\partial \theta_\alpha} \delta\theta_\alpha = -\frac{1}{2} \int_{\Omega_0} \left(\delta\theta_\alpha \varepsilon_{ij\alpha} R_{jK} + R_{iN} \varepsilon_{NK\alpha} \delta\theta_\alpha \right) U_{KL} P_{iL} \mathrm{d}V$$

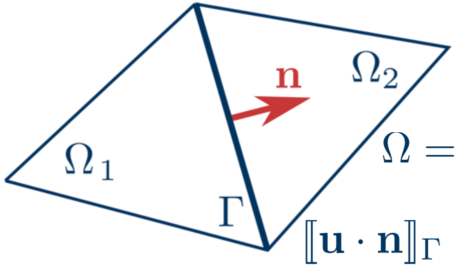
Conservation of linear momentum:

$$\frac{\partial \Pi}{\partial u_i} \delta u_i = \int_{\Omega_0} P_{iJ} \frac{\partial \delta u_i}{\partial X_J} \mathrm{d}V - \int_{\Omega_0} \delta u_i f_i \mathrm{d}V$$

H(div) main properties

$$H(\mathrm{div};\Omega) := \left\{\mathbf{u} \in \left[L^2(\Omega)\right]^2 \mid \mathrm{div}\,\mathbf{u} \in L^2(\Omega)\right\}$$

Normal component of H(div) function is continuous across any inner boundary:



$$\Omega = \Omega_1 \cup \Omega_2$$

$$[\![\mathbf{u} \cdot \mathbf{n}]\!]_\Gamma = 0$$

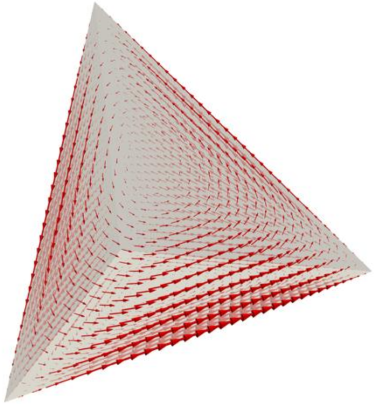
Natural space for flow/diffusion problems

(Classic example: *Raviart-Thomas* FE space)

[1] Boffi D, Brezzi F, Fortin M. Mixed finite element methods and applications (2013)

Spaces

$$\delta\mathbf{P} \in U_0^h \subset H_0^{\mathrm{div}}(\Omega_0^h) := \{\delta\mathbf{P} \in H^{\mathrm{div}}(\Omega_0^h) : N_j \delta P_{ij} = 0 \text{ on } \partial\Omega_0^{h,u}\}$$
$$\tilde{\mathbf{P}} + \mathbf{P} \in U^h := \{\tilde{\mathbf{P}} + \mathbf{P} : \mathbf{P} \in H_0^{\mathrm{div}}(\Omega_0^h)\}$$
$$\mathbf{u}, \boldsymbol{\omega}, \delta\mathbf{u}, \delta\boldsymbol{\omega} \in C^h \subset L^2(\Omega_0^h)$$
$$\mathbf{H}, \delta\mathbf{H} \in S^h \subset S := \{H_{ij} \in L^2(\Omega_0^h) : H_{ij} = H_{ij}^T\}$$



Riviart-Thomas (RT) ← Demkowicz recipe

$$H^{\mathrm{div}}(\mathcal{B}_0^h) = \mathcal{RT}^k(\mathcal{K}) + \mathrm{curl}((\mathrm{curl}\tilde{\mathbf{A}}^k(\mathcal{K}))\mathbf{b}_{\mathrm{K}})$$

Antisymmetric matrix homogenous polynomial

matrix bubble

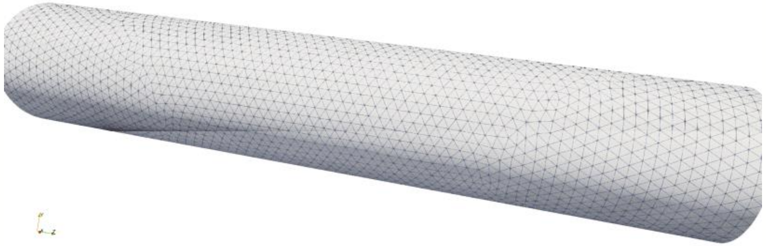
$$b_{\mathrm{K}ij} = \sum_{l=0}^{2} \lambda_{l-3}\lambda_{l-2}\lambda_{l-3}\lambda_{l,i}\lambda_{l,j}$$

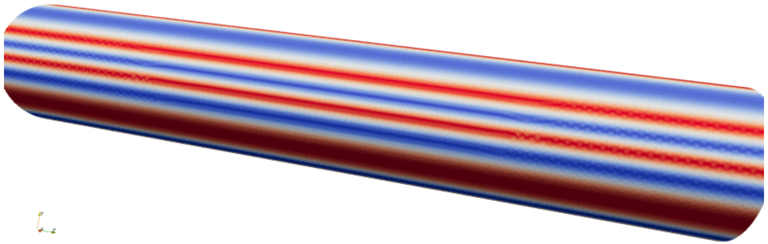
Gopalakrishnan, Jayadeep, and Johnny Guzmn. "A second elasticity element using the matrix bubble." IMA Journal of Numerical Analysis 32.1 (2012): 352-372.

MOFEM
mofem.eng.gla.ac.uk

Why mixed formulation with stress approximation

- ✓ Separation of non-linearities as different equations
- ✓ Conservation equations (momentum flux continuity) is satisfied a priori
- ✓ Trades floating point operations to local and temporal memory access
- ✓ Weaker (ultra weak formulation) suitable for unilateral constraints emerging from contact, fracture, plasticity and geometric instabilities
- ✓ Sparse Dense Block Structure
- ✓ Future hardware ready (GPUs)





Updated Lagrangian formulation

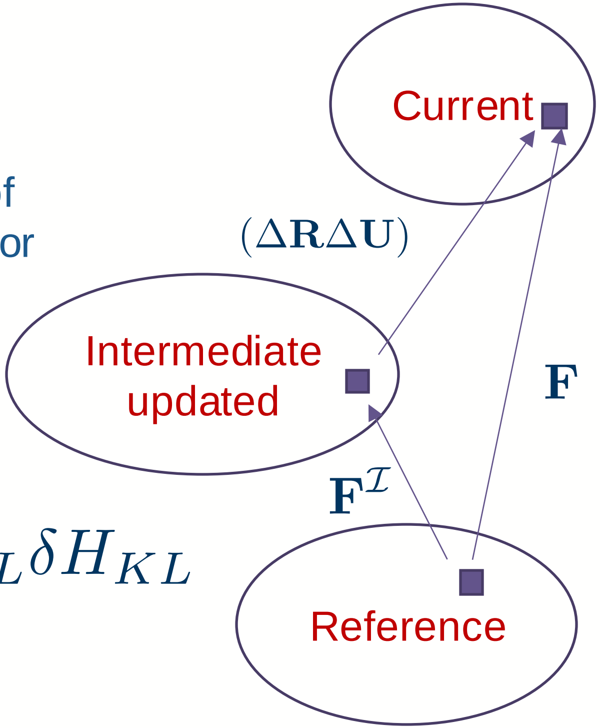
$$F_{iJ} = R_{iK}U_{KJ} = R_{iK}[\mathrm{Exp}(\mathbf{H})]_{KJ}$$

Deformation gradient

Orthonormal rotation tensor

Symmetric stretch tensor

Logarithm of stretch tensor



Physical values of stretches are larger than 1, while logarithm of stretch can take any finite value.

$$U_{IJ} = \mathrm{Exp}(\mathbf{H})_{IJ}$$

Variation: $$\delta U_{IJ} = \mathrm{Exp}(\mathbf{H})_{IJ,KL}\delta H_{KL}$$

Mathematical formulations for small strains:

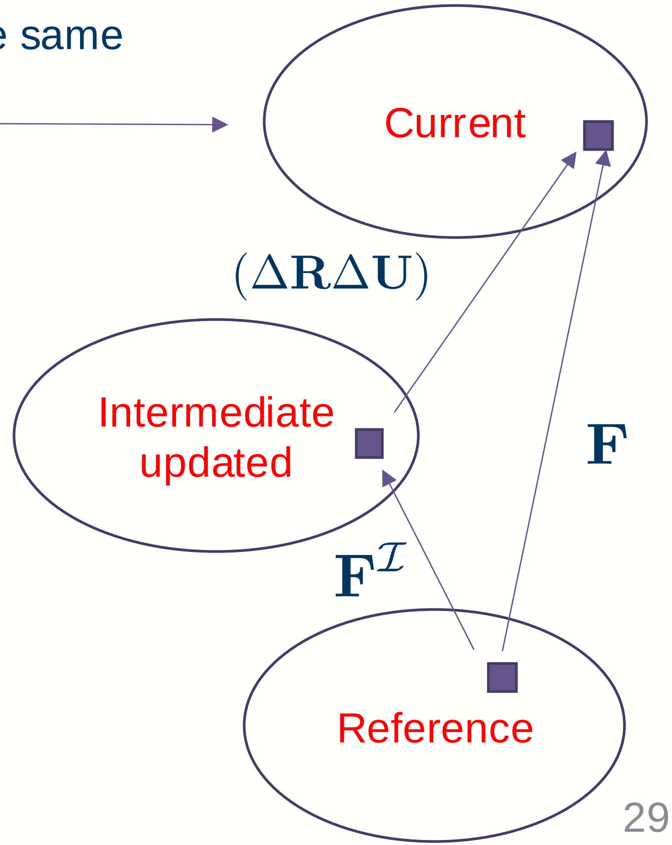
Gopalakrishnan, J., & Guzmán, J. (2012). A second elasticity element using the matrix bubble. *IMA Journal of Numerical Analysis*, *32*(1), 352-372.

mofem.eng.gla.ac.uk

Total vs update Lagrangian formulation

Objectivity: Lagrangian and Total formulations have to yield the same result. Not exactly the case for mixed formulation. ???

$$\|\mathbf{u} - \mathbf{u}^{h,k}\|_{L^2(\Omega)} \leq Ch^{k+1}|\mathbf{u}|_{H^{k+1}(\Omega)}$$

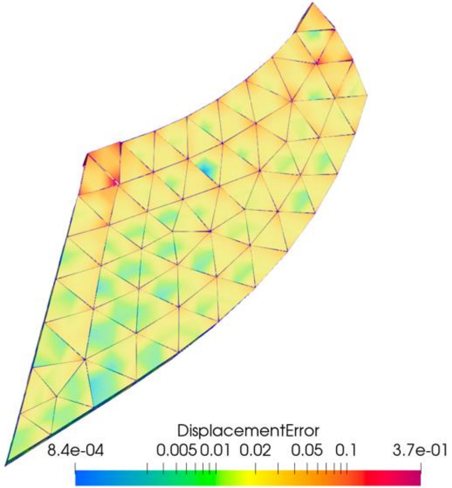


Stenberg, R. (1988). A family of mixed finite elements for the elasticity problem. Numerische Mathematik, 53, 513-538.

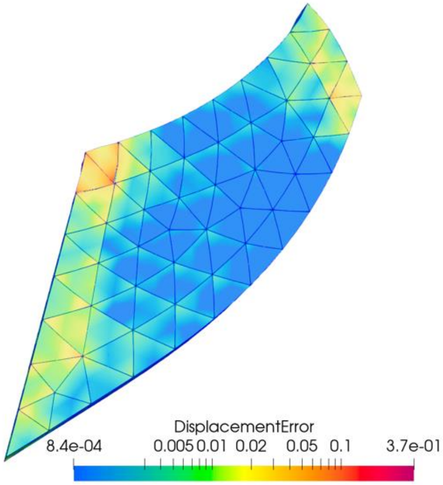
MOFEM
mofem.eng.gla.ac.uk

Cook beam (p-refinement)

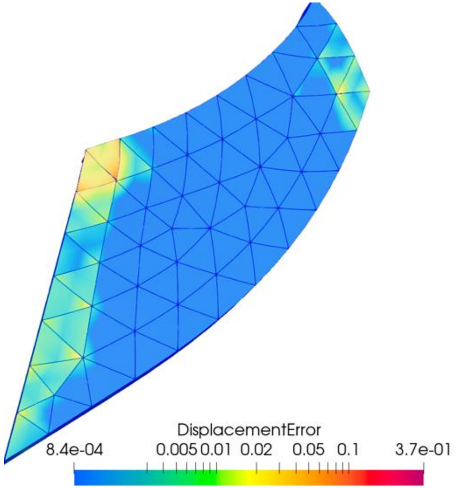
Displacement order 1



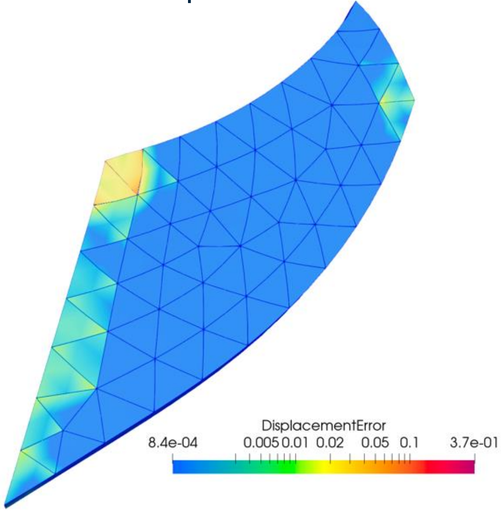
Displacement order 2



Displacement order 3



Displacement order 4



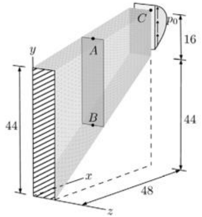
$$W_q(\mathbf{h}, \mathbf{h}, j) = \alpha_q(\mathbf{h} : \mathbf{h})^2 + \beta_q(\mathbf{y} : \mathbf{y})^2 + f_q(j)$$

$$f_q(j) = -24\beta \ln(j) - 12\varepsilon \ln(j) + \frac{\lambda}{2\varepsilon^2}(j^{\varepsilon} + j^{-\varepsilon})$$

$$\alpha_q = 21\ \text{kPa}, \quad \beta_q = 42\ \text{kPa}, \quad \lambda_q = 8000\ \text{kPa}, \quad \varepsilon_q = 20.$$

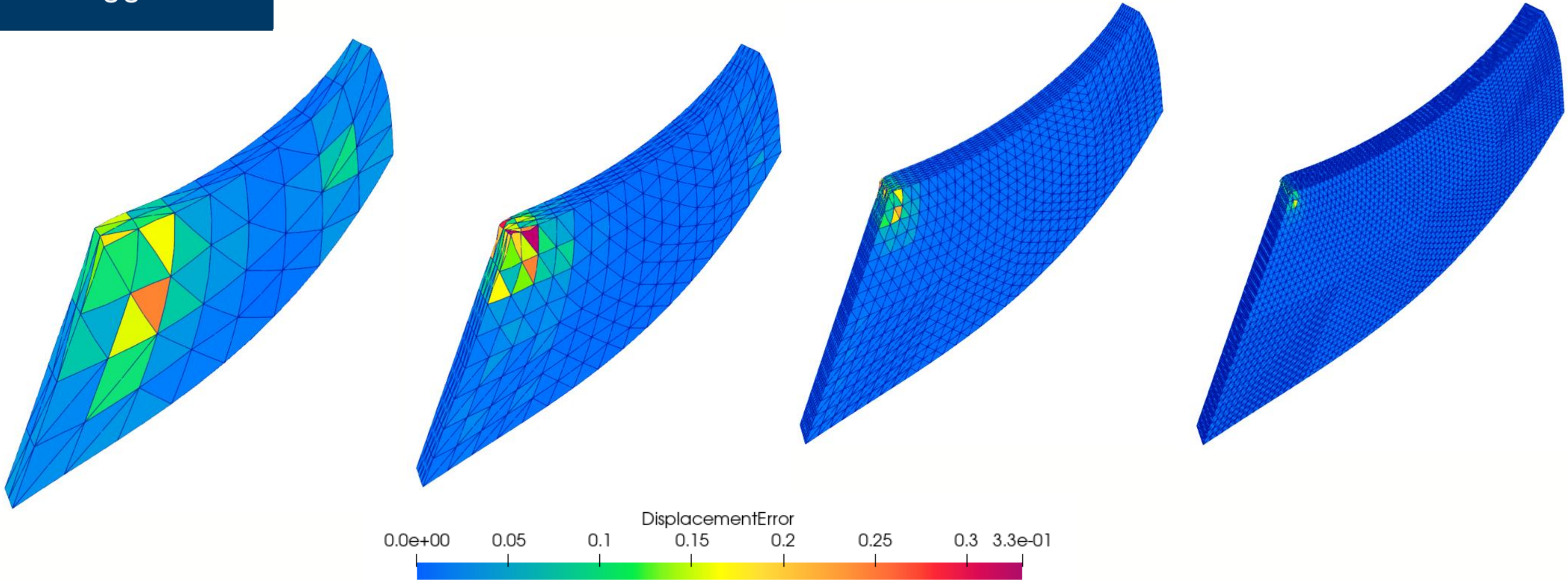
Based on a test by Bonet et al., A computational framework for polyconvex large strain elasticity. Comput. Methods Appl. Mech. Eng. 283 (2015)

Schröder, J., Wriggers, P., & Balzani, D. (2011). A new mixed finite element based on different approximations of the minors of deformation tensors. *Computer Methods in Applied Mechanics and Engineering*, *200*(49-52), 3583-3600.



MOFEM
mofem.eng.gla.ac.uk

Cook beam (h-refinement)

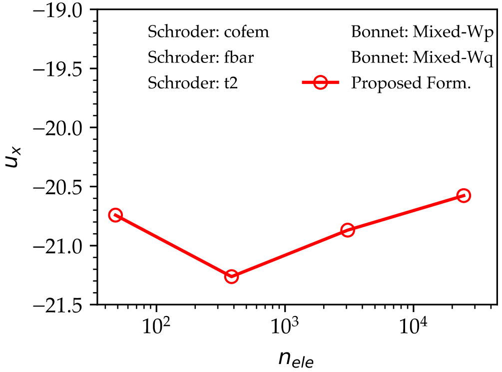


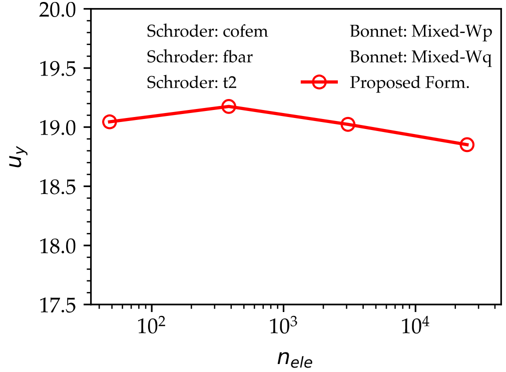
$$W_q(\mathbf{h}, \mathbf{h}, j) = \alpha_q(\mathbf{h} : \mathbf{h})^2 + \beta_q(\mathbf{y} : \mathbf{y})^2 + f_q(j)$$

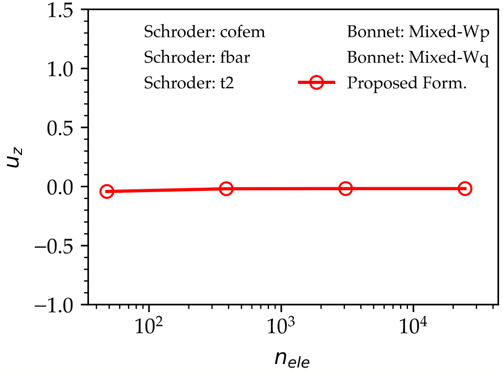
$$f_q(j) = -24\beta \ln(j) - 12↵\ln(j) + \frac{\lambda}{2''^2}(j^{''} + j^{-''})$$

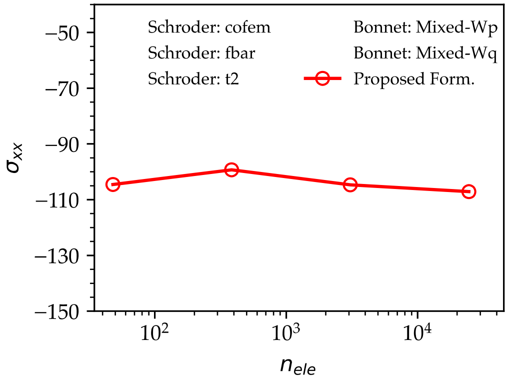
$$\alpha_q = 21\ \text{kPa}, \quad \beta_q = 42\ \text{kPa}, \quad \lambda_q = 8000\ \text{kPa}, \quad \varepsilon_q = 20.$$

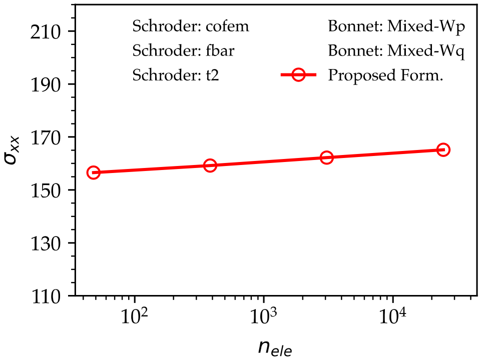
Cook beam: uniform mesh refinement study







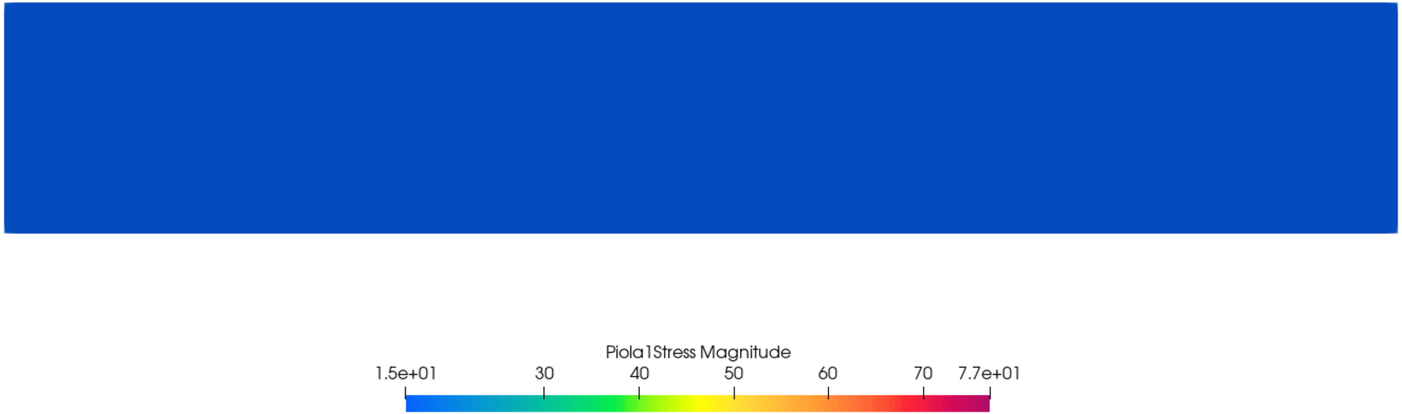




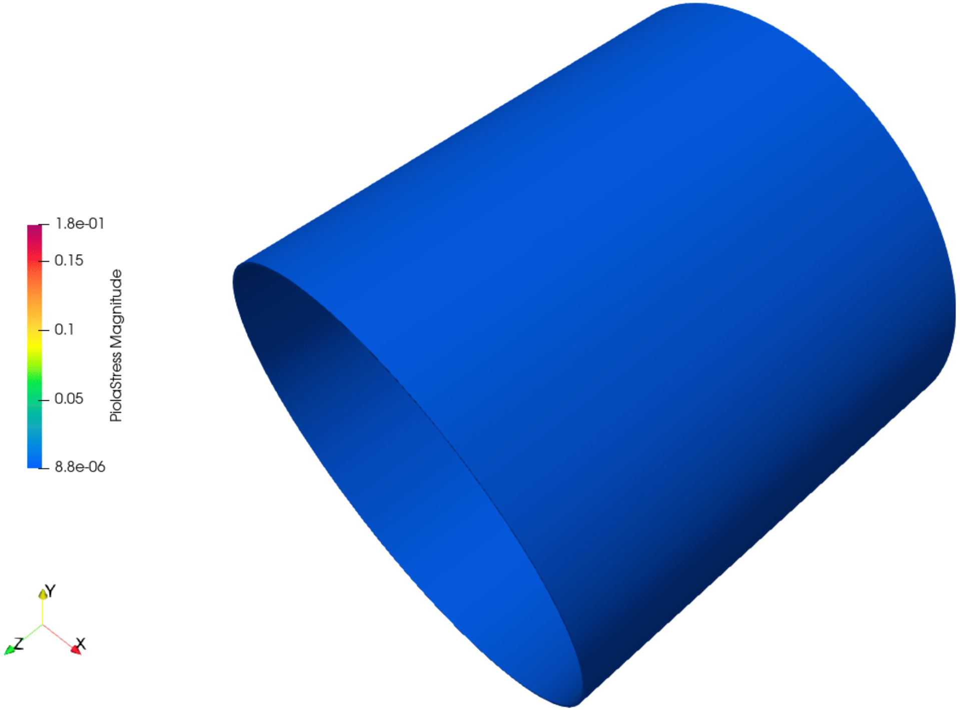
Jörg Schröder, Peter Wriggers, and Daniel Balzani, "A New Mixed Finite Element Based on Different Approximations of the Minors of Deformation Tensors," *Computer Methods in Applied Mechanics and Engineering*
Javier Bonet, Antonio J. Gil, and Rogelio Ortigosa, "A Computational Framework for Polyconvex Large Strain Elasticity," *Computer Methods in Applied Mechanics and Engineering*

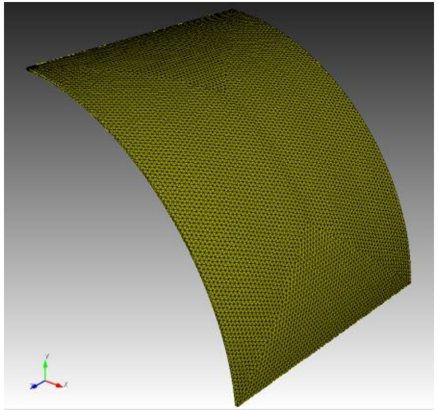
Twisting cantilever beam

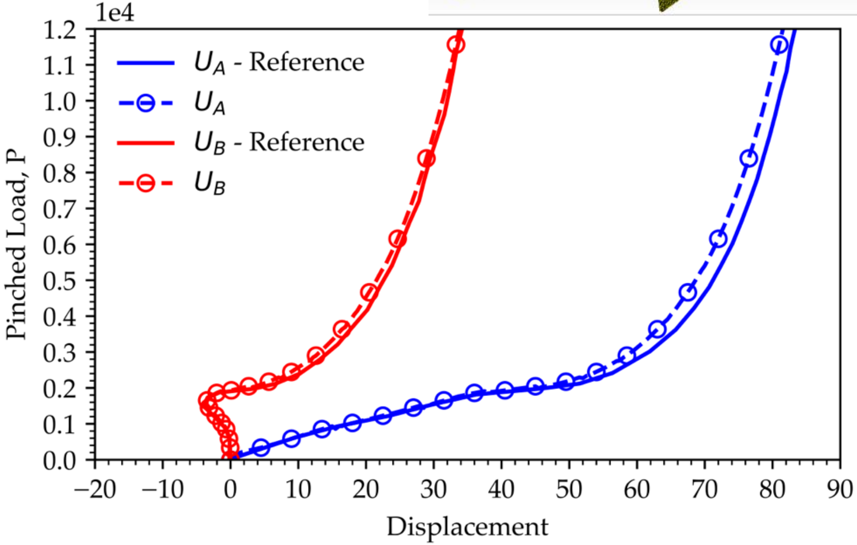
- Large rotations
- Neo-Hookean material–using new formulation.



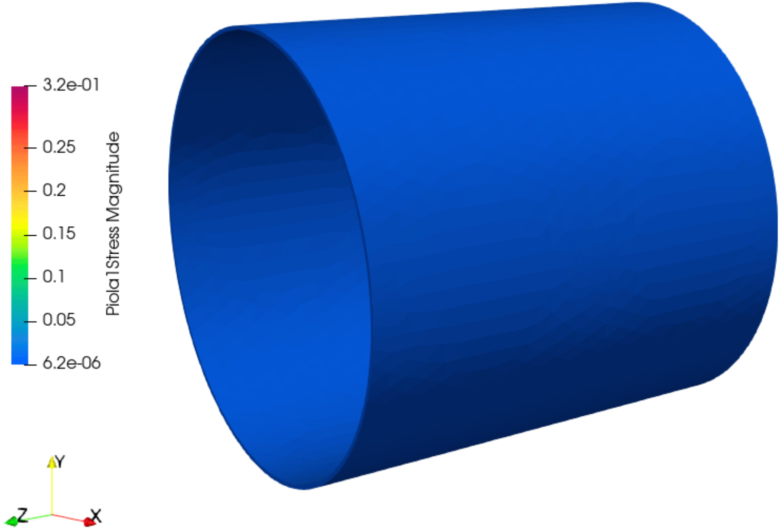
Pinched cylindrical shell

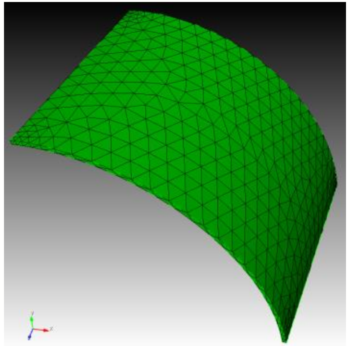


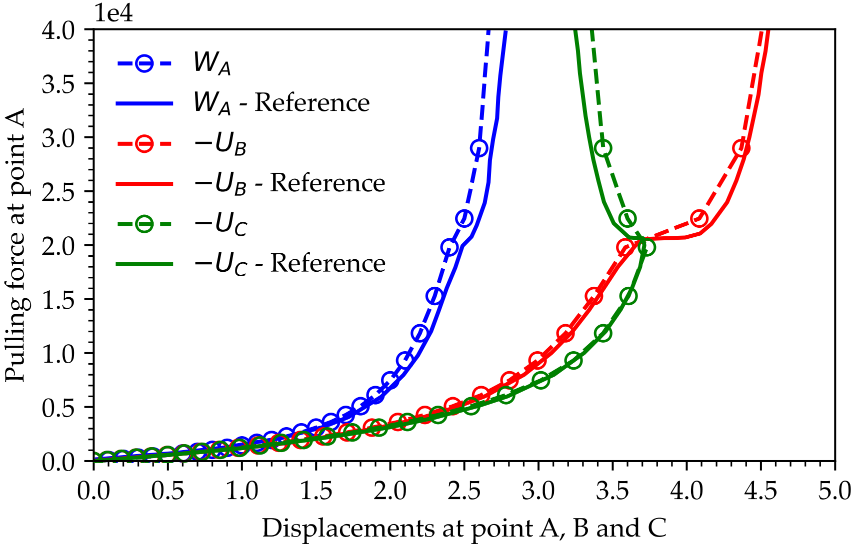




Pullout of an open-ended cylindrical shell

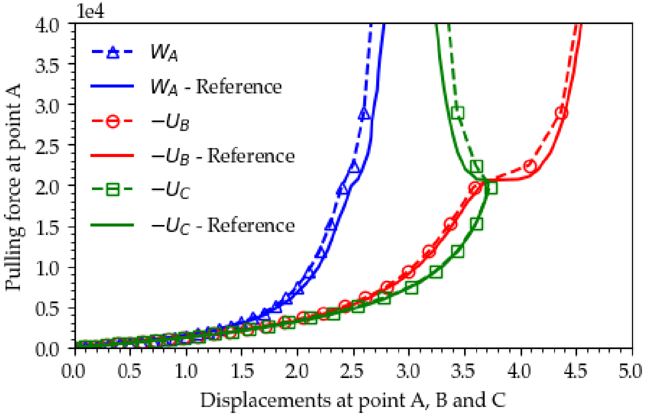




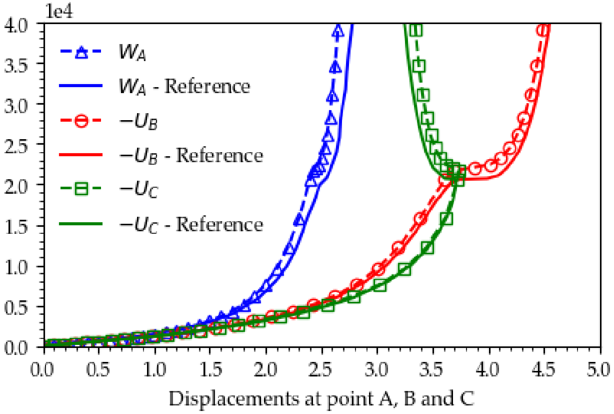


mofem.eng.gla.ac.uk

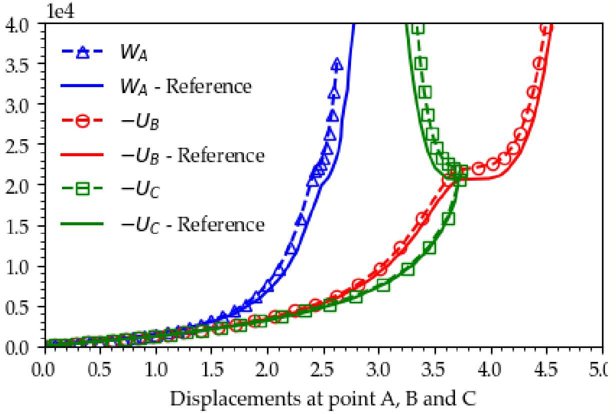
p-refinement



p=2



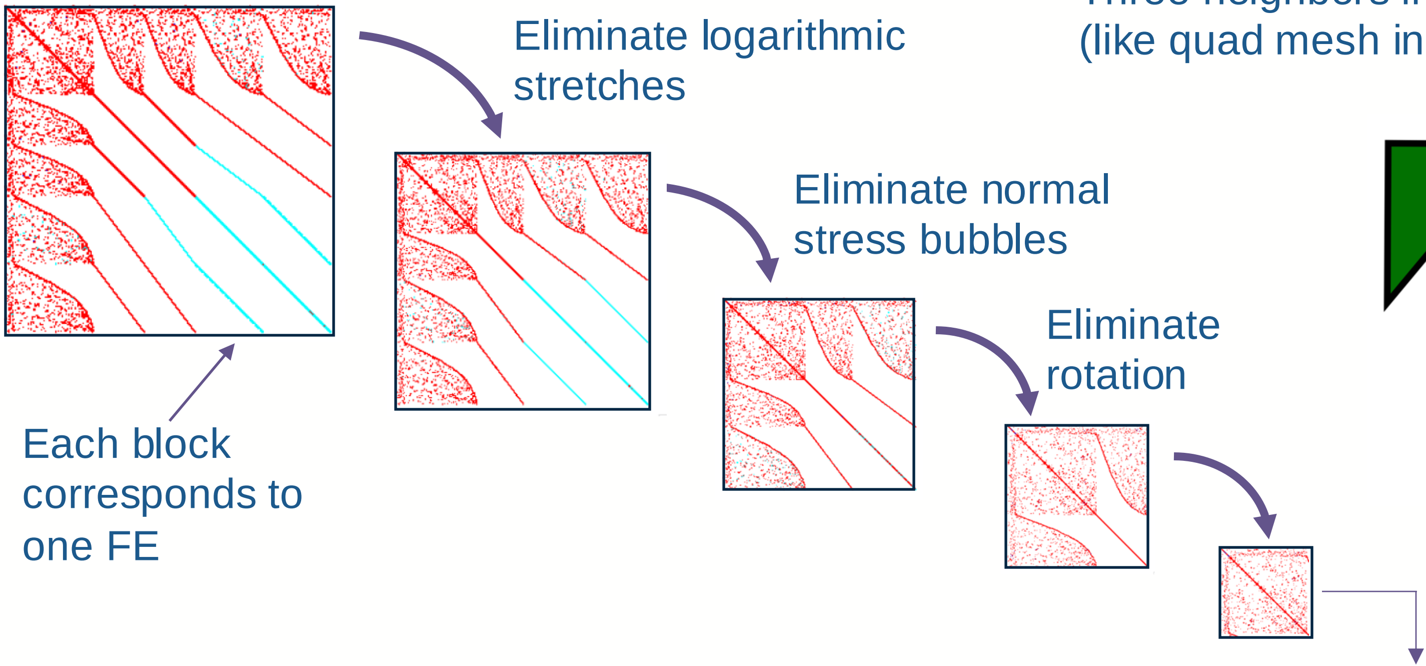
p=3



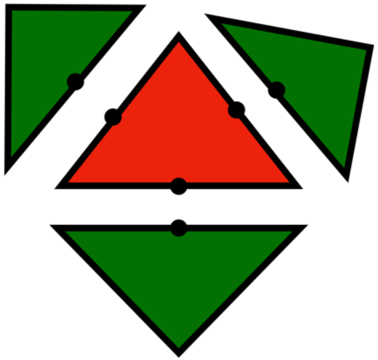
p=4

MOFEM
mofem.eng.gla.ac.uk

Exploiting block structure



Three neighbors in 2d and 4 in 3D
(like quad mesh in finite volume method)



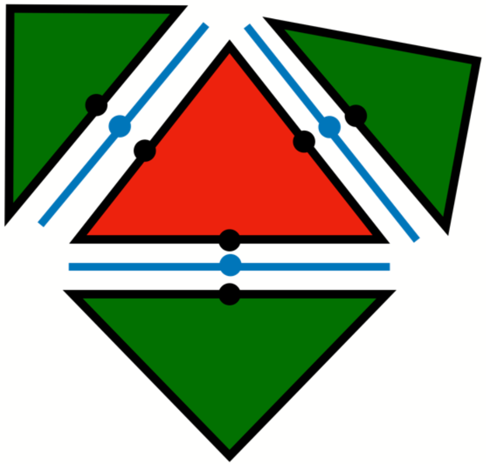
H-div data structure
Not well fit for of the shelf iterative solvers and their preconditioners
Multigrid is not trivial – Null Space – Neuman type problem

MOFEM
mofem.eng.gla.ac.uk

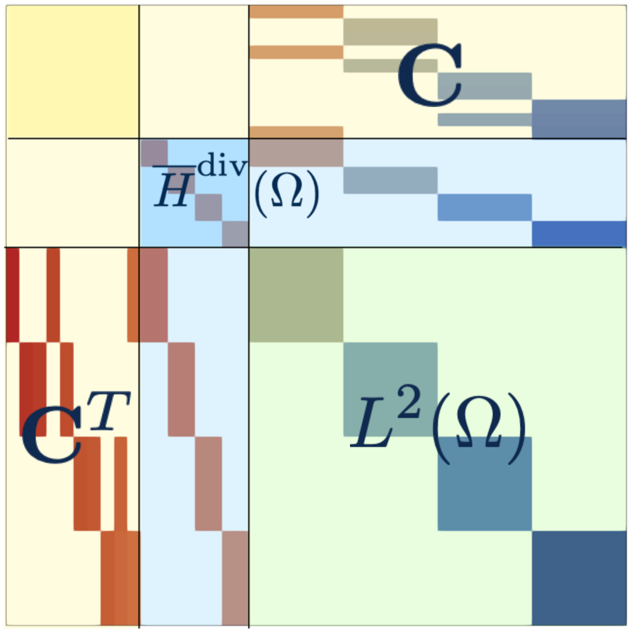
Hybridisation

$$\int_{\Gamma^S} \delta u_i^S \left(\mathbf{N}_J^+ \mathbf{P}_{iJ}^+ + \mathbf{N}_J^- \cdot \mathbf{P}_{iJ}^- \right) \mathrm{d}\Gamma = 0$$

Three neighbors in 2d and 4 in 3D
(like quad mesh in finite volume method)



$$\overline{H}^{\mathrm{div}}(\Omega_0^h) := \left\{ \mathbf{P} \in \sum_e H^{\mathrm{div}}(\Omega_0^e) \right\}$$

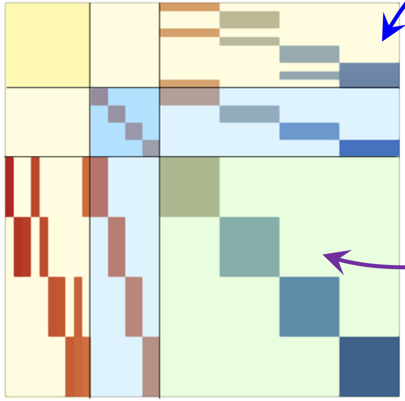


Boffi, Daniele, Franco Brezzi, and Michel Fortin. *Mixed finite element methods and applications*. Vol. 44. Heidelberg: Springer, 2013.

Dobrev, Veselin, et al. "Algebraic hybridization and static condensation with application to scalable H (div) preconditioning." *SIAM Journal on Scientific Computing* 41.3 (2019): B425-B447.

Block preconditioner – Exact Schur complement

$$\mathbf{S} = -\mathbf{C}^T\mathbf{D}^{-1}\mathbf{C}$$



$$\begin{bmatrix}\mathbf{A} & \mathbf{B}\\ \mathbf{C} & \mathbf{D}\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ \boldsymbol{\lambda}\end{bmatrix} = \begin{bmatrix}\mathbf{f_u}\\ \mathbf{f_\lambda}\end{bmatrix}$$

$$\begin{bmatrix}\mathbf{u}\\ \boldsymbol{\lambda}\end{bmatrix} = \begin{bmatrix}\mathbf{S}^{-1} & -\mathbf{S}^{-1}\mathbf{B}\mathbf{D}^{-1}\\ -\mathbf{D}^{-1}\mathbf{C}\mathbf{S}^{-1} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{C}\mathbf{S}^{-1}\mathbf{B}\mathbf{D}^{-1}\end{bmatrix}\begin{bmatrix}\mathbf{f_u}\\ \mathbf{f_\lambda}\end{bmatrix}$$

$$\begin{bmatrix}\mathbf{u}\\ \boldsymbol{\lambda}\end{bmatrix} = \begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \mathbf{D}^{-1}\end{bmatrix}\begin{bmatrix}\mathbf{I} & \mathbf{0}\\ -\mathbf{C} & \mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{S}^{-1} & \mathbf{0}\\ \mathbf{0} & \mathbf{D}\end{bmatrix}\begin{bmatrix}\mathbf{I} & -\mathbf{B}\\ \mathbf{0} & \mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \mathbf{D}^{-1}\end{bmatrix}\begin{bmatrix}\mathbf{f_u}\\ \mathbf{f_\lambda}\end{bmatrix}$$

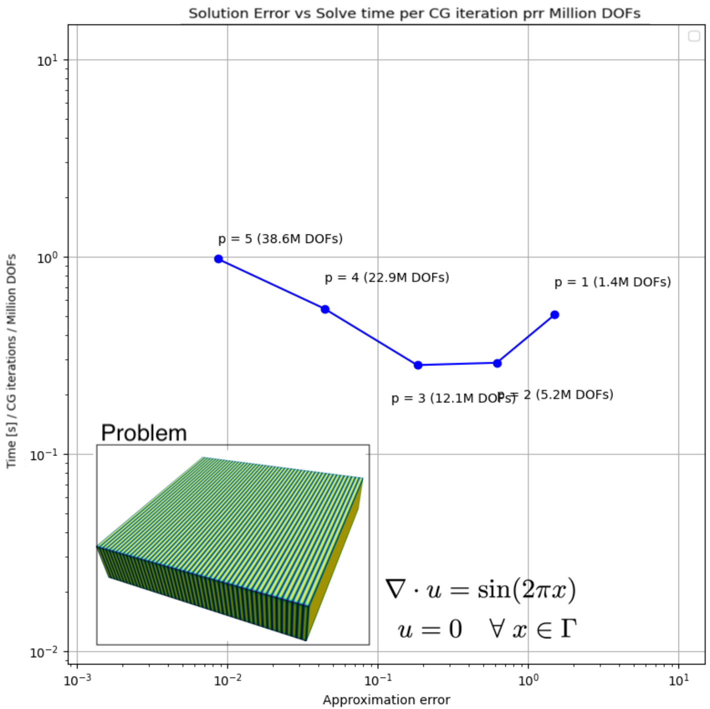
Use Algebraic Multigrid (AMG) to approximate S^{-1}

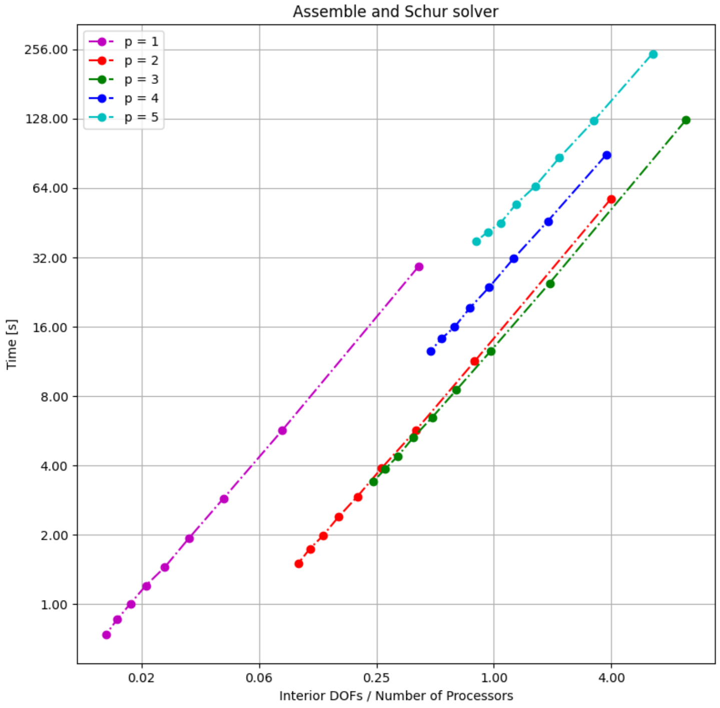
Invert exactly element-by-element

- Efficient block structure of Dense Block Matrices
- Block diagonal element by element
- Inverted exactly element by element
- Schur inversion is trivial
- Efficient to parallelize (GPU in perspective)

[10] PETSc/TAO Users Manual, https://petsc.org/

Hybridised solver





Stability of contact formulation

[3] Flemisch, B. and Wohlmuth, B.I. *Comput. Meth. Appl. Mech. Eng.*, *196*(8), 2007.
[4] Popp, A., et al., *SIAM J. Sci. Comput.*, 79(11), 2009.
[5] Boffi D, Brezzi F, Fortin M. Mixed finite element methods and applications (2013)

Stability of contact formulation

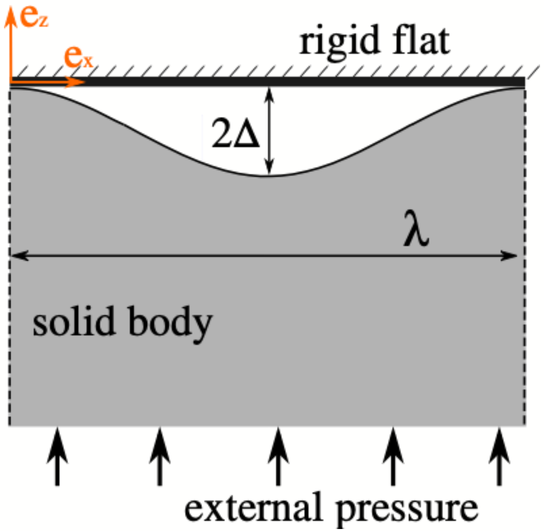
- Continuous functions $\mathcal{M} := H^1(\Gamma^c)$

[3] Flemisch, B. and Wohlmuth, B.I. *Comput. Meth. Appl. Mech. Eng.*, *196*(8), 2007.
[4] Popp, A., et al., *SIAM J. Sci. Comput.*, 79(11), 2009.
[5] Boffi D, Brezzi F, Fortin M. Mixed finite element methods and applications (2013)

Stability of contact formulation

- Continuous functions $\mathcal{M} := H^1(\Gamma^c)$

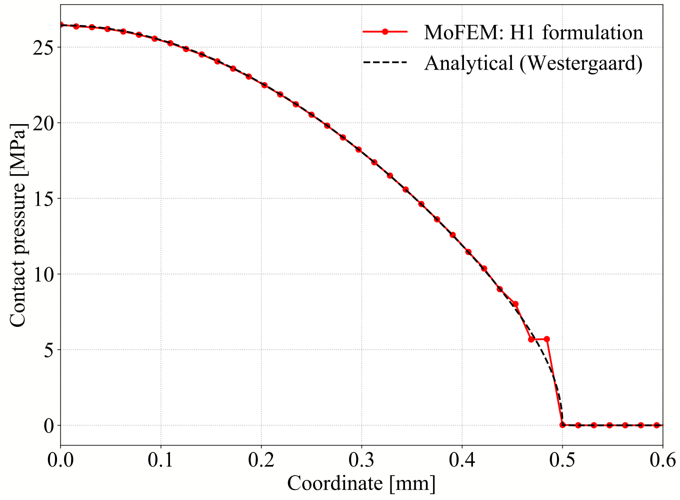
Test: 2D wavy surface contact



[3] Flemisch, B. and Wohlmuth, B.I. *Comput. Meth. Appl. Mech. Eng.*, *196*(8), 2007.
[4] Popp, A., et al., *SIAM J. Sci. Comput.*, 79(11), 2009.
[5] Boffi D, Brezzi F, Fortin M. Mixed finite element methods and applications (2013)

Stability of contact formulation

- Continuous functions $\mathcal{M} := H^1(\Gamma^c)$



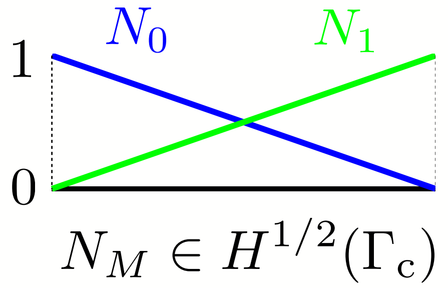
[3] Flemisch, B. and Wohlmuth, B.I. *Comput. Meth. Appl. Mech. Eng.*, *196*(8), 2007.
[4] Popp, A., et al., *SIAM J. Sci. Comput.*, 79(11), 2009.
[5] Boffi D, Brezzi F, Fortin M. Mixed finite element methods and applications (2013)

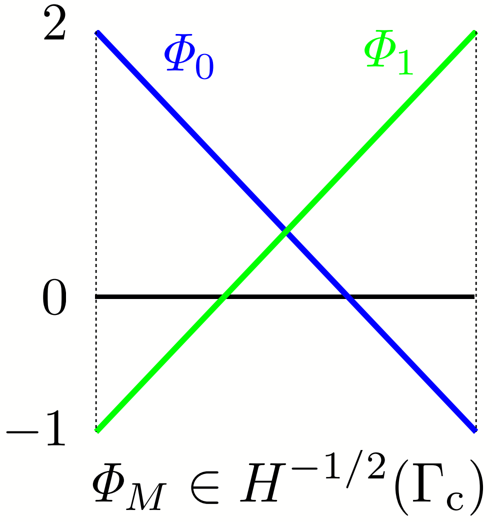
Stability of contact formulation

- Continuous functions $\mathcal{M} := H^1(\Gamma^c)$
- Dual space [3,4] $\mathcal{M} := H^{-1/2}(\Gamma^c)$

$$\text{trace} : H^1(\Omega) \to H^{1/2}(\Gamma^c)$$

dual space for $H^{1/2}(\Gamma^c)$ is denoted as $H^{-1/2}(\Gamma^c)$





[3] Flemisch, B. and Wohlmuth, B.I. *Comput. Meth. Appl. Mech. Eng.*, *196*(8), 2007.
[4] Popp, A., et al., *SIAM J. Sci. Comput.*, 79(11), 2009.
[5] Boffi D, Brezzi F, Fortin M. Mixed finite element methods and applications (2013)

Stability of contact formulation

- Continuous functions $\mathcal{M} := H^1(\Gamma^c)$

- Dual space [3,4] $\mathcal{M} := H^{-1/2}(\Gamma^c)$

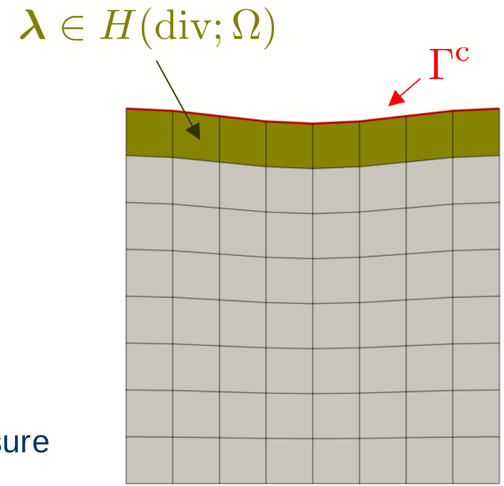
$$\text{trace} : H^1(\Omega) \to H^{1/2}(\Gamma^c)$$

dual space for $H^{1/2}(\Gamma^c)$ is denoted as $H^{-1/2}(\Gamma^c)$

- Raviart-Thomas space [5]

$$H(\text{div};\Omega) := \left\{ \mathbf{u} \in \left[L^2(\Omega)\right]^n \mid \text{div}\,\mathbf{u} \in L^2(\Omega) \right\}$$

$$\text{normal trace} : \boldsymbol{\lambda} \in \underbrace{H(\text{div};\Omega)}_{\text{natural space for stress}} \to \boldsymbol{\lambda} \cdot \mathbf{n}|_{\Gamma^c} \in \underbrace{H^{-1/2}(\Gamma^c)}_{\text{natural space for pressure}}$$



[3] Flemisch, B. and Wohlmuth, B.I. *Comput. Meth. Appl. Mech. Eng.*, *196*(8), 2007.
[4] Popp, A., et al., *SIAM J. Sci. Comput.*, 79(11), 2009.
[5] Boffi D, Brezzi F, Fortin M. Mixed finite element methods and applications (2013)

Stability of contact formulation

- Continuous functions $\mathcal{M} := H^1(\Gamma^c)$

- Dual space [3,4] $\mathcal{M} := H^{-1/2}(\Gamma^c)$

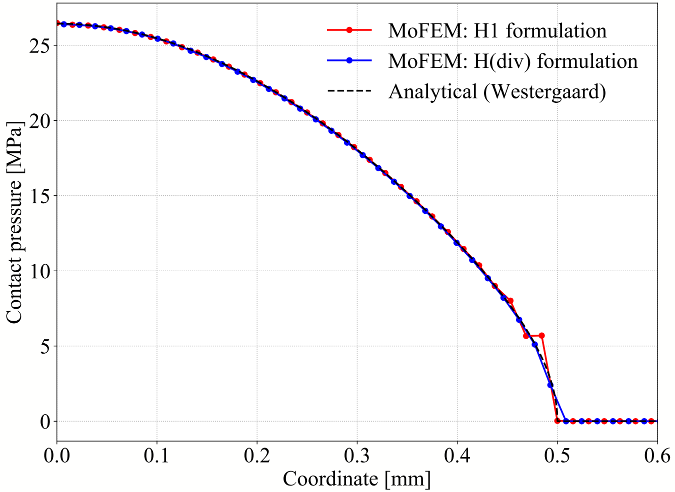
$$\text{trace} : H^1(\Omega) \to H^{1/2}(\Gamma^c)$$

dual space for $H^{1/2}(\Gamma^c)$ is denoted as $H^{-1/2}(\Gamma^c)$

- Raviart-Thomas space [5]

$$H(\text{div};\Omega) := \left\{ \mathbf{u} \in \left[L^2(\Omega)\right]^n \mid \text{div}\,\mathbf{u} \in L^2(\Omega) \right\}$$

$$\text{normal trace} : \boldsymbol{\lambda} \in \underbrace{H(\text{div};\Omega)}_{\text{natural space for stress}} \to \boldsymbol{\lambda} \cdot \mathbf{n}|_{\Gamma^c} \in \underbrace{H^{-1/2}(\Gamma^c)}_{\text{natural space for pressure}}$$



[3] Flemisch, B. and Wohlmuth, B.I. *Comput. Meth. Appl. Mech. Eng.*, *196*(8), 2007.
[4] Popp, A., et al., *SIAM J. Sci. Comput.*, 79(11), 2009.
[5] Boffi D, Brezzi F, Fortin M. Mixed finite element methods and applications (2013)

Stability of contact formulation

- Continuous functions $\mathcal{M} := H^1(\Gamma^c)$

- Dual space [3,4] $\mathcal{M} := H^{-1/2}(\Gamma^c)$

$$\text{trace} : H^1(\Omega) \to H^{1/2}(\Gamma^c)$$

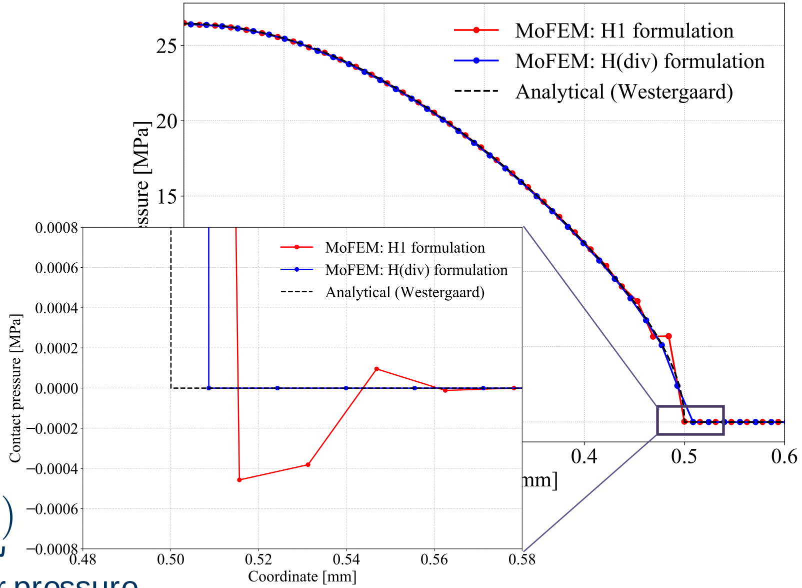
$$\text{dual space for } H^{1/2}(\Gamma^c) \text{ is denoted as } H^{-1/2}(\Gamma^c)$$

- Raviart-Thomas space [5]

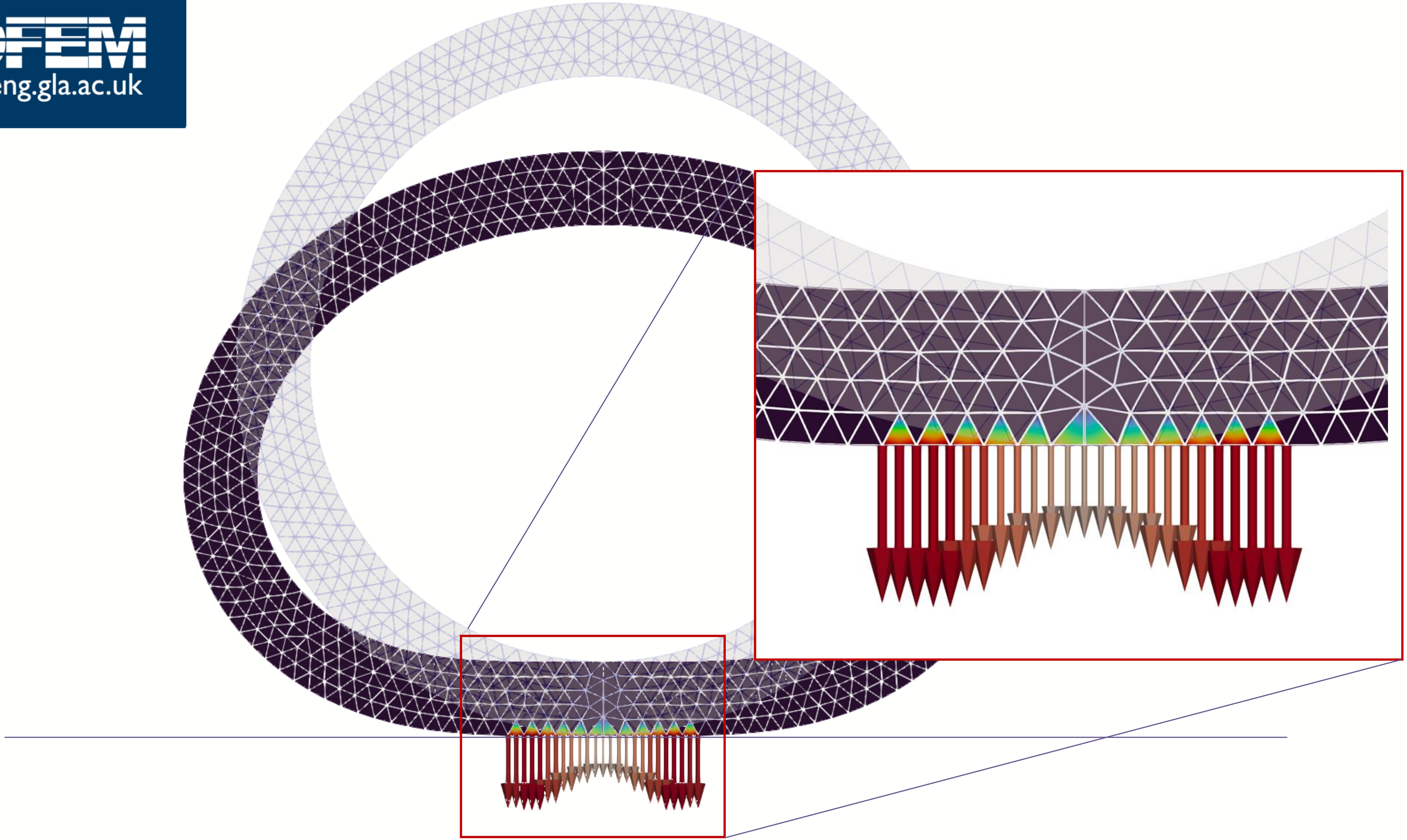
$$H(\text{div};\Omega) := \left\{ \mathbf{u} \in \left[L^2(\Omega)\right]^n \mid \text{div}\, \mathbf{u} \in L^2(\Omega) \right\}$$

$$\text{normal trace} : \boldsymbol{\lambda} \in \underbrace{H(\text{div};\Omega)}_{\text{natural space for stress}} \to \boldsymbol{\lambda} \cdot \mathbf{n}|_{\Gamma^c} \in \underbrace{H^{-1/2}(\Gamma^c)}_{\text{natural space for pressure}}$$

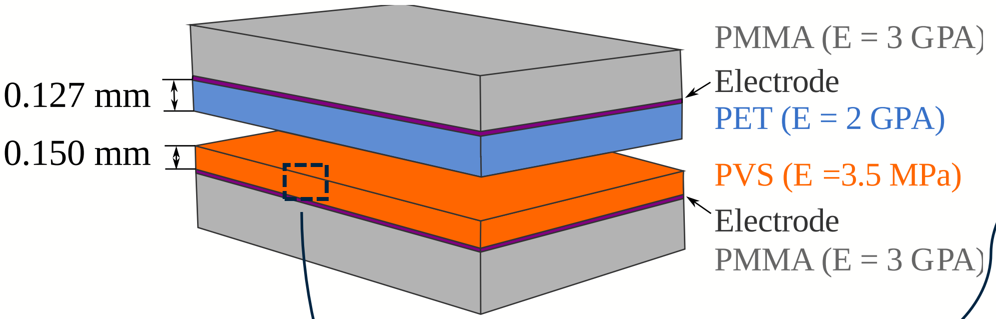
natural space for stress — natural space for pressure

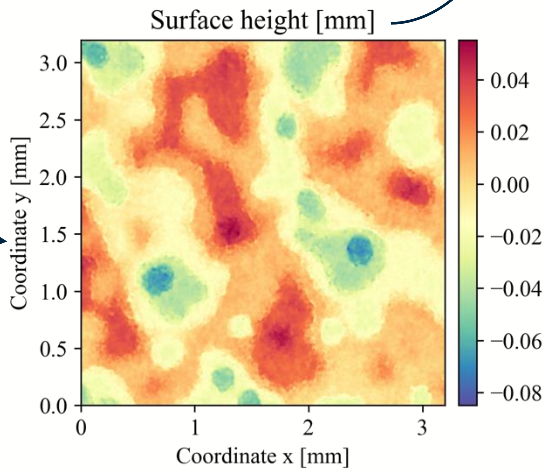


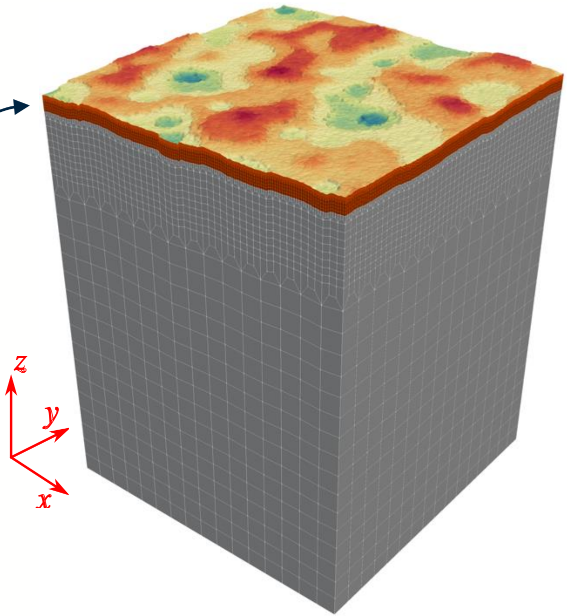
[3] Flemisch, B. and Wohlmuth, B.I. *Comput. Meth. Appl. Mech. Eng.*, *196*(8), 2007.
[4] Popp, A., et al., *SIAM J. Sci. Comput.*, 79(11), 2009.
[5] Boffi D, Brezzi F, Fortin M. Mixed finite element methods and applications (2013)



Stability is essential for contact area estimation







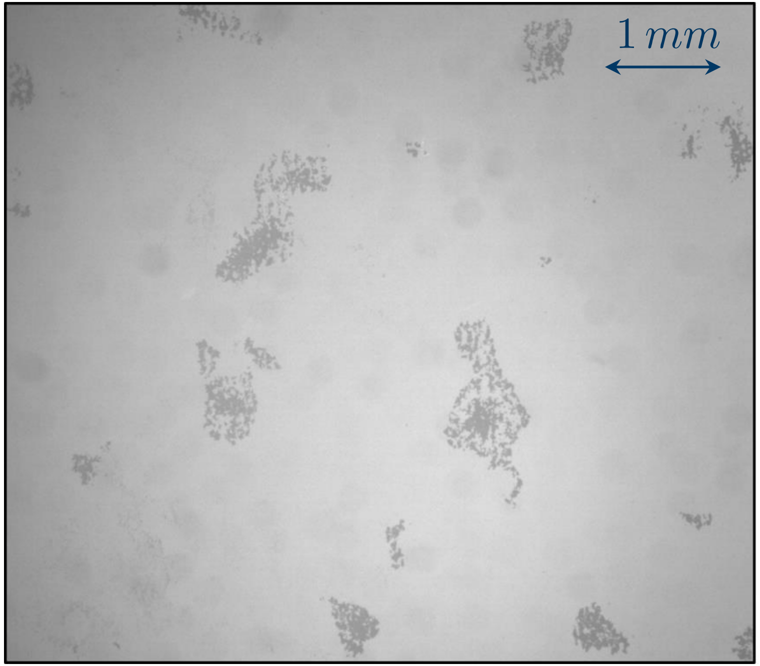
Andrei Shvarts

MD Tanzib Ehsan Sanglap

$S_q \approx 0.025$ mm

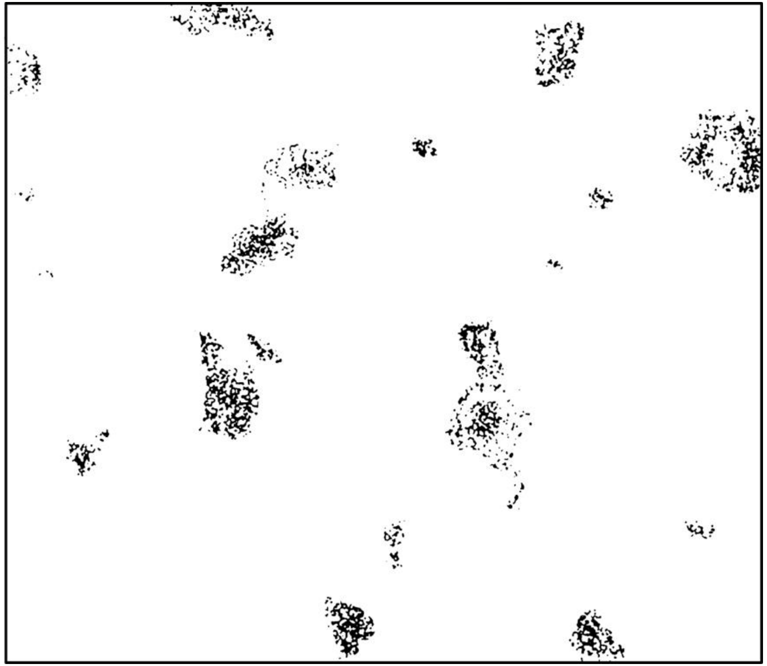
$S_{dq} \approx 0.3$

Contact area morphology (real roughness)



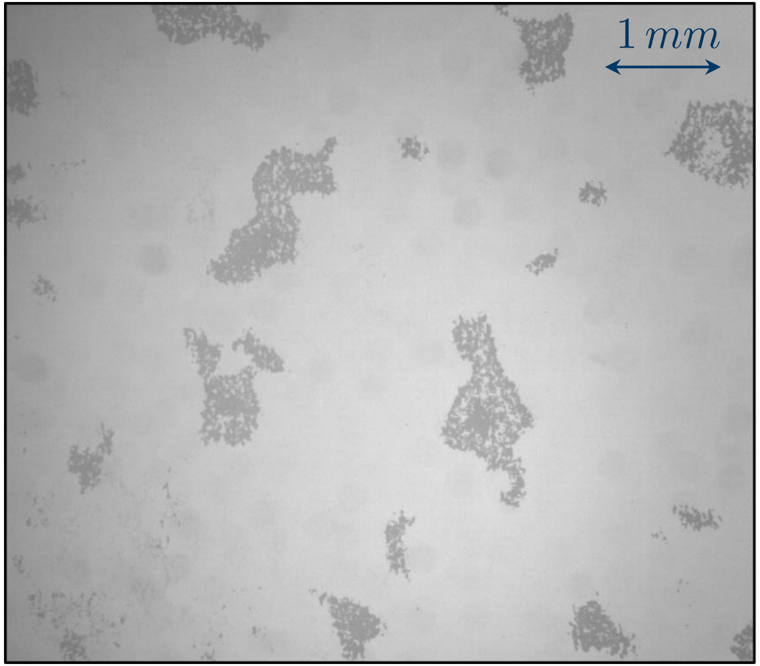
Experiment (interference reflection microscopy)

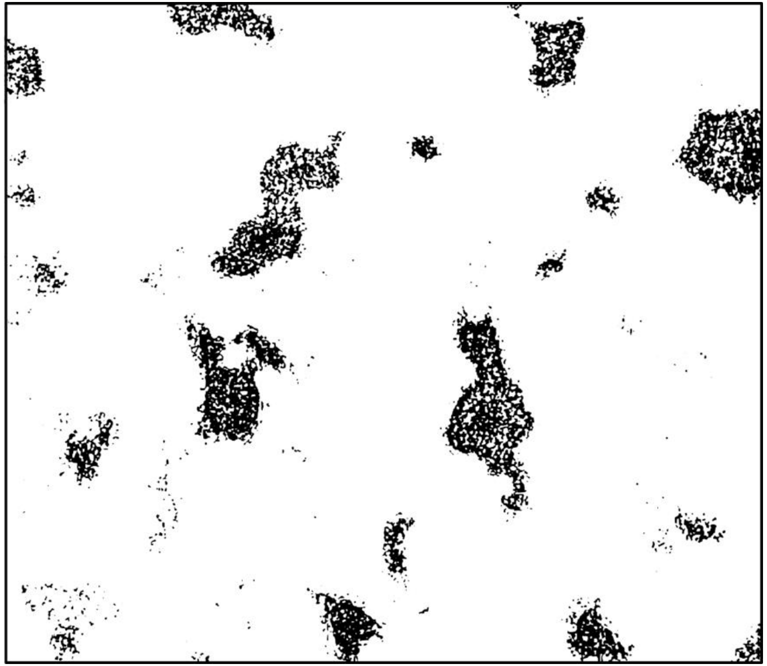
[8] Kumar C. et al. *Nano Energy* 107 (2023)



$p_{ext} \approx 0.01\,\text{MPa}$ Simulation

Contact area morphology (real roughness)



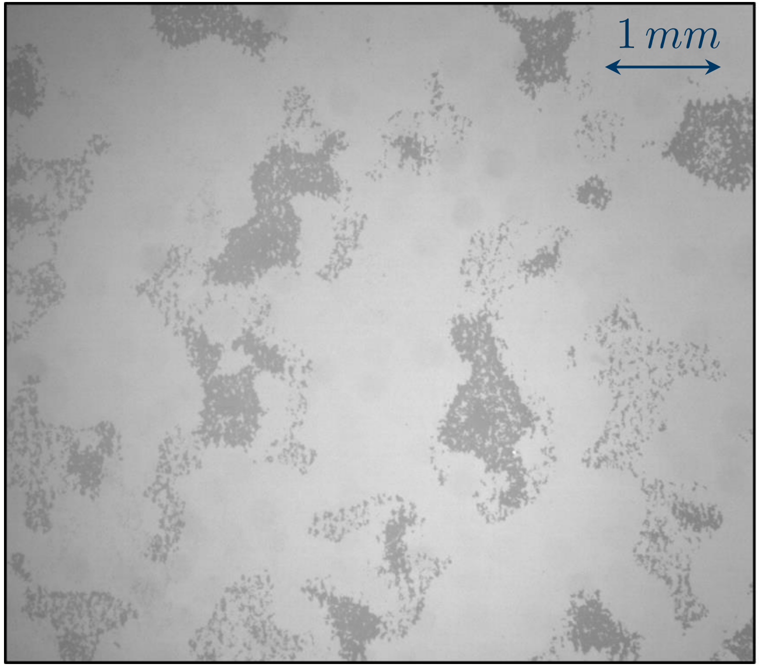


Experiment (interference reflection microscopy)

[8] Kumar C. et al. *Nano Energy* 107 (2023)

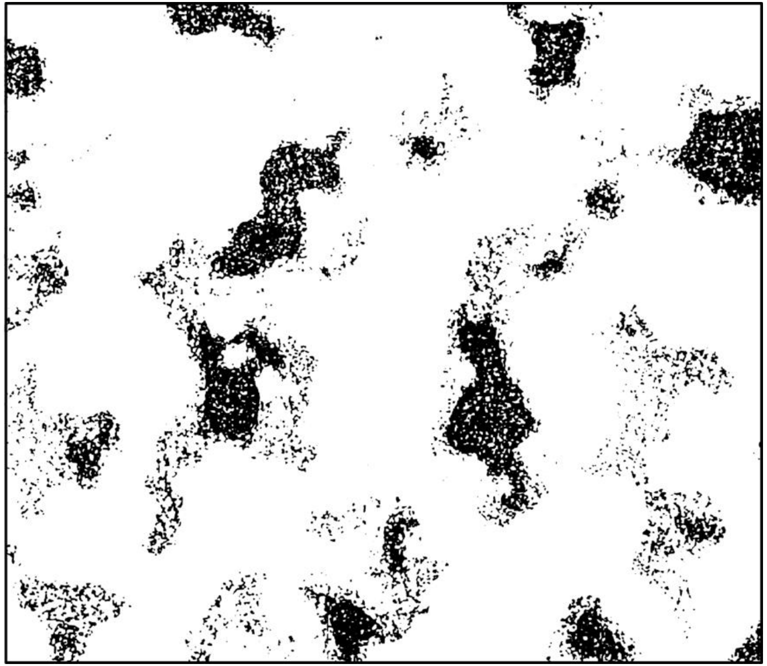
$p_{\text{ext}} \approx 0.04\,\text{MPa}$ Simulation

Contact area morphology (real roughness)



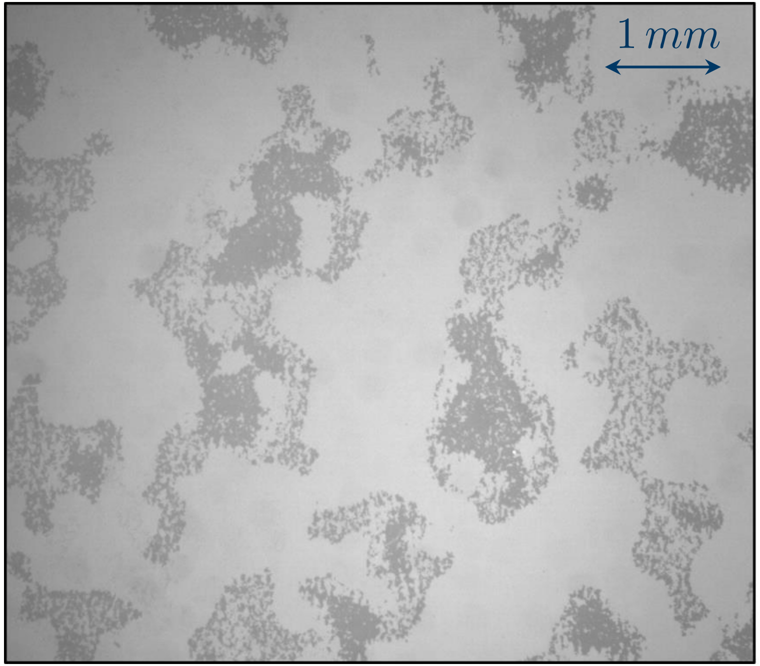
Experiment (interference reflection microscopy)

[8] Kumar C. et al. *Nano Energy* 107 (2023)



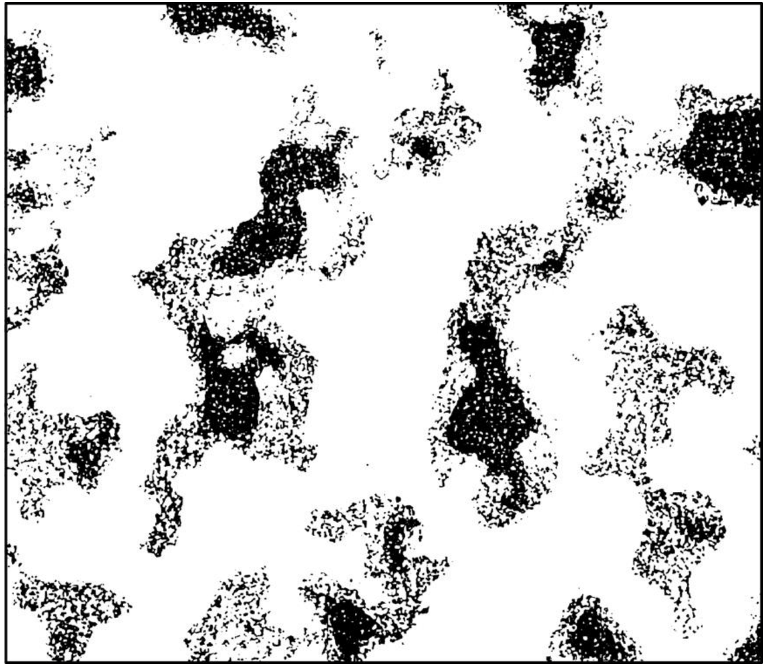
$p_{\text{ext}} \approx 0.07\,\text{MPa}$ Simulation

Contact area morphology (real roughness)



Experiment (interference reflection microscopy)

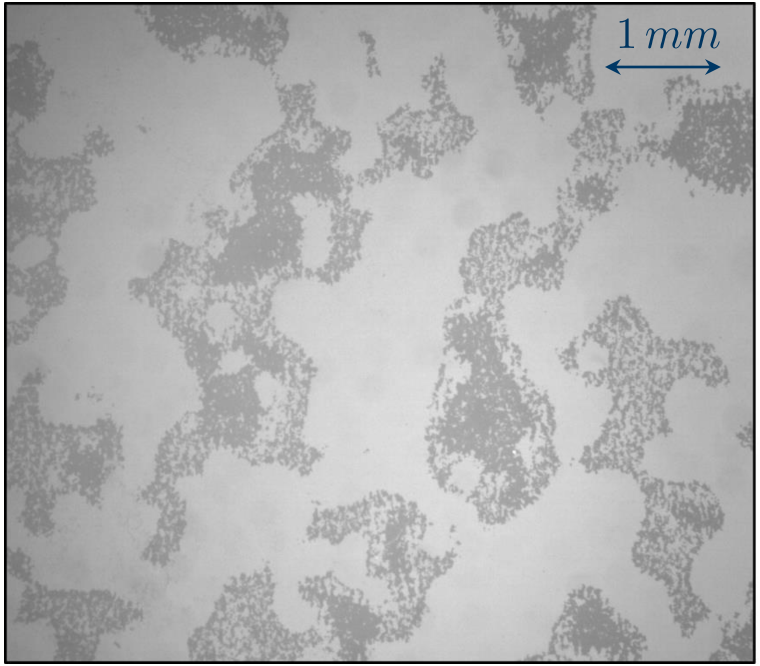
[8] Kumar C. et al. *Nano Energy* 107 (2023)



$p_{\text{ext}} \approx 0.1$ MPa

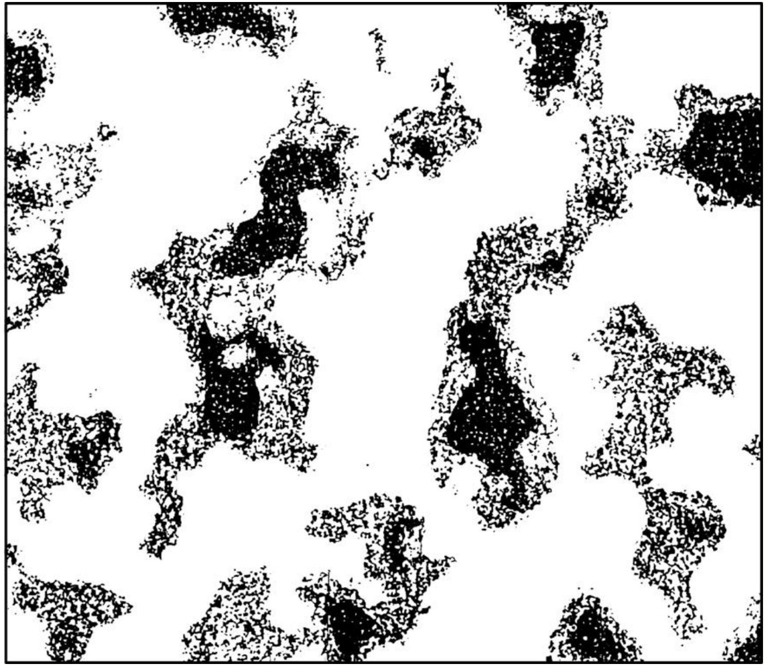
Simulation

Contact area morphology (real roughness)



Experiment (interference reflection microscopy)

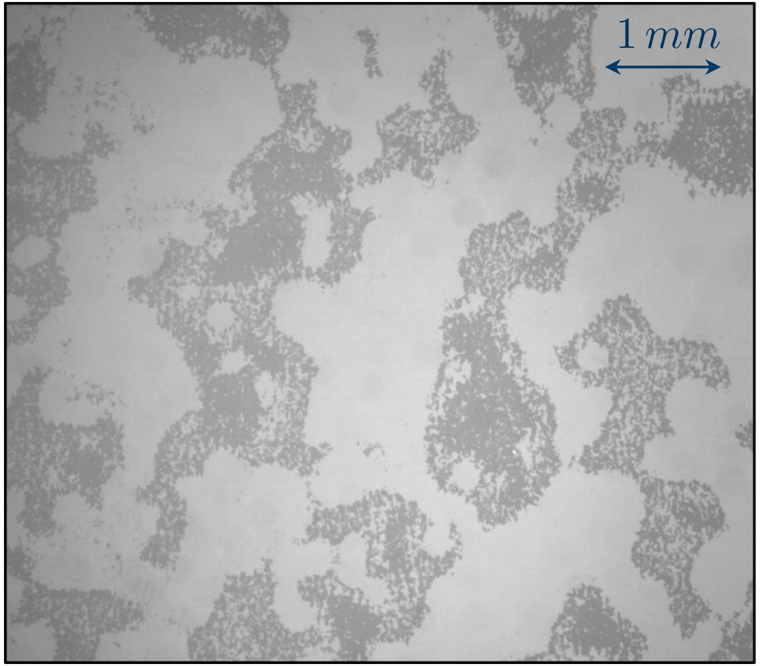
[8] Kumar C. et al. *Nano Energy* 107 (2023)



$p_{\text{ext}} \approx 0.13\,\text{MPa}$ Simulation

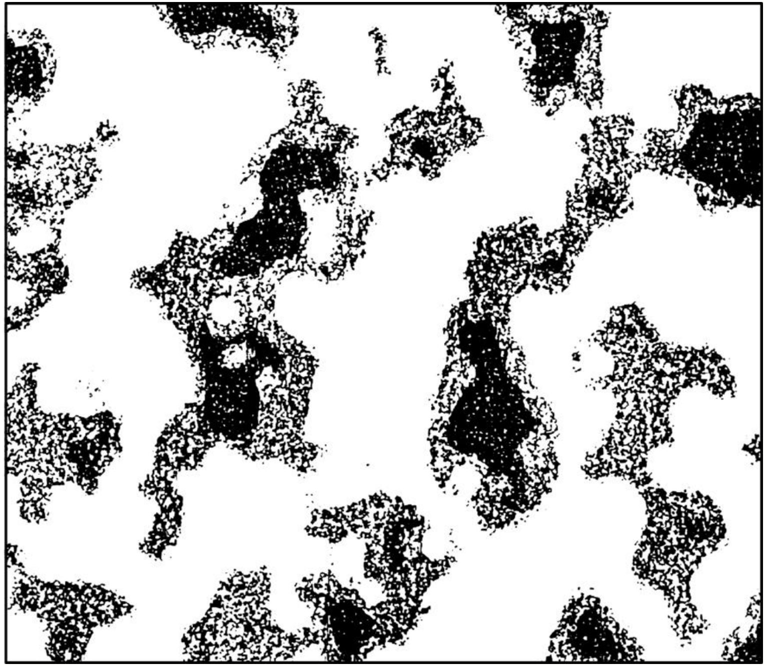
mofem.eng.gla.ac.uk

Contact area morphology (real roughness)



Experiment (interference reflection microscopy)

[8] Kumar C. et al. *Nano Energy* 107 (2023)



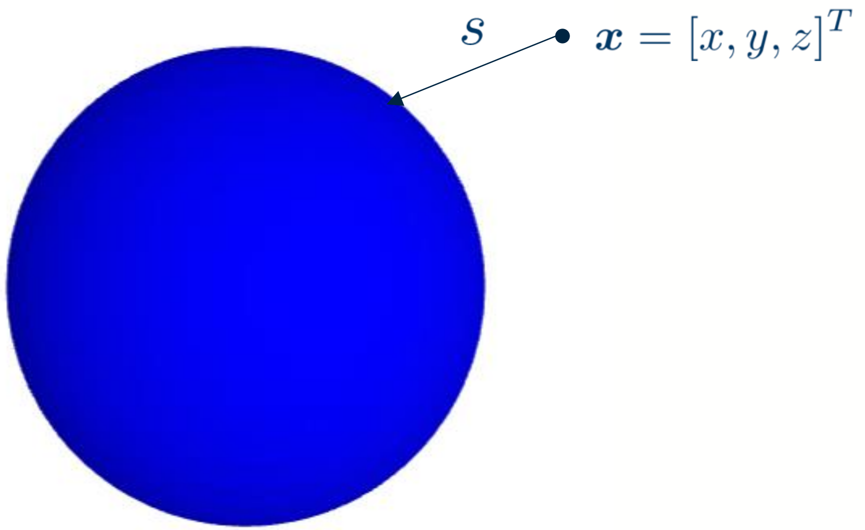
$p_{\text{ext}} \approx 0.16\,\text{MPa}$ Simulation

Signed distance function

Signed distance function defined for a domain Ω outside the surface

$$s(\boldsymbol{x}) = \begin{cases} d(\boldsymbol{x}, \partial\Omega) & \text{if } \boldsymbol{x} \in \Omega \\ -d(\boldsymbol{x}, \partial\Omega) & \text{if } \boldsymbol{x} \notin \Omega \end{cases}$$

$$||\nabla d(\boldsymbol{x}, \partial\Omega)|| = 1$$



Sphere with radius r and centroid:

$$\boldsymbol{x_c} = [x_c, y_c, z_c]^T$$

Signed distance function for a sphere:

$$s = \sqrt{(x - x_c)^2 + (y - y_c)^2 + (z - z_c)^2} - r$$

MOFEM
mofem.eng.gla.ac.uk

Contact formulation

One if positive gap, or positive traction, i.e. no contact

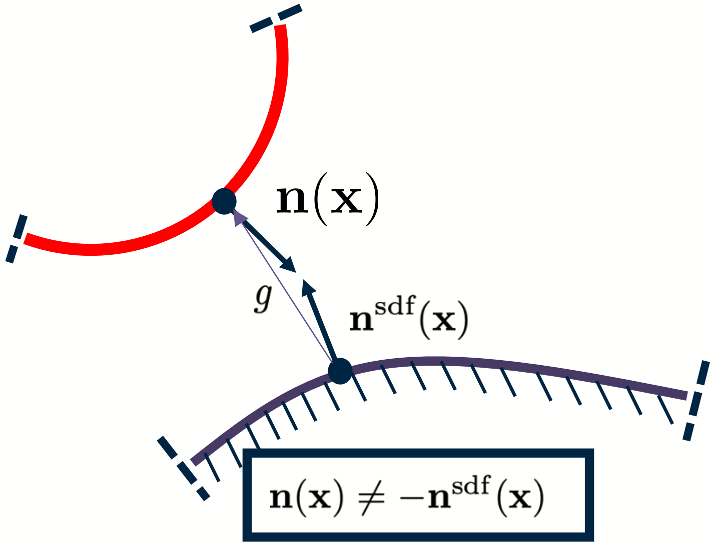
$$\mathcal{C}(g, t_n) = \frac{1}{2}(1 - \text{sign}(g - c_n t_n))$$

$$P_{ij}^{\mathcal{C}} = \mathcal{C}(n_i^{\text{sdf}} n_j^{\text{sdf}})$$ ← Contact projection operator

$$Q_{ij}^{\mathcal{C}} = \delta_{ij} - P_{ij}^{\mathcal{C}}$$ ← Tangent projection operator

$$f^{\mathcal{S}} = \int_{\Gamma^c} \delta u_i^{\mathcal{S}} \left(Q_{ij}^{\mathcal{C}} \left(N_J P_{jJ} \right) + \frac{\mathcal{C}}{c_n} n_i^{\text{sdf}} g \right) \text{d}\Gamma$$

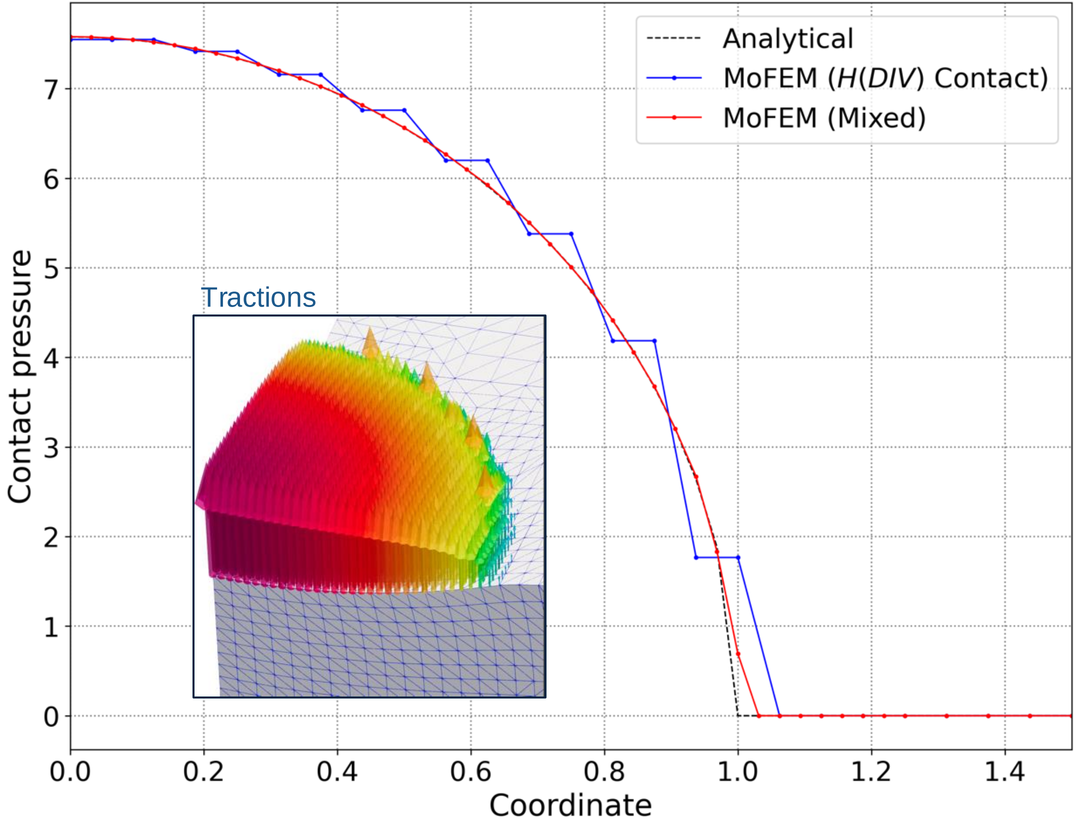
$$f^{\mathcal{P}} = \int_{\Gamma^c} \left(N_J \delta P_{iJ} \right) u_i^{\mathcal{S}} \text{d}\Gamma$$

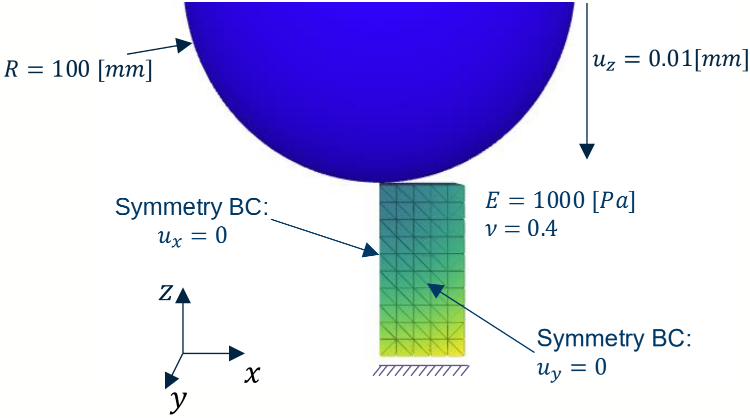


Note: Hybridised displacement on skeleton (contact boundary is part of it), is a Lagrange multiplier enforcing contact constraints.

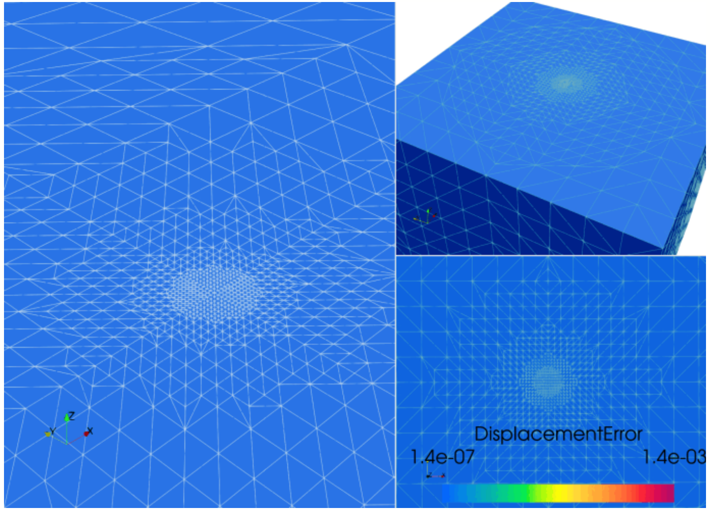
Hertz contact problem

Result for displacements order 2:





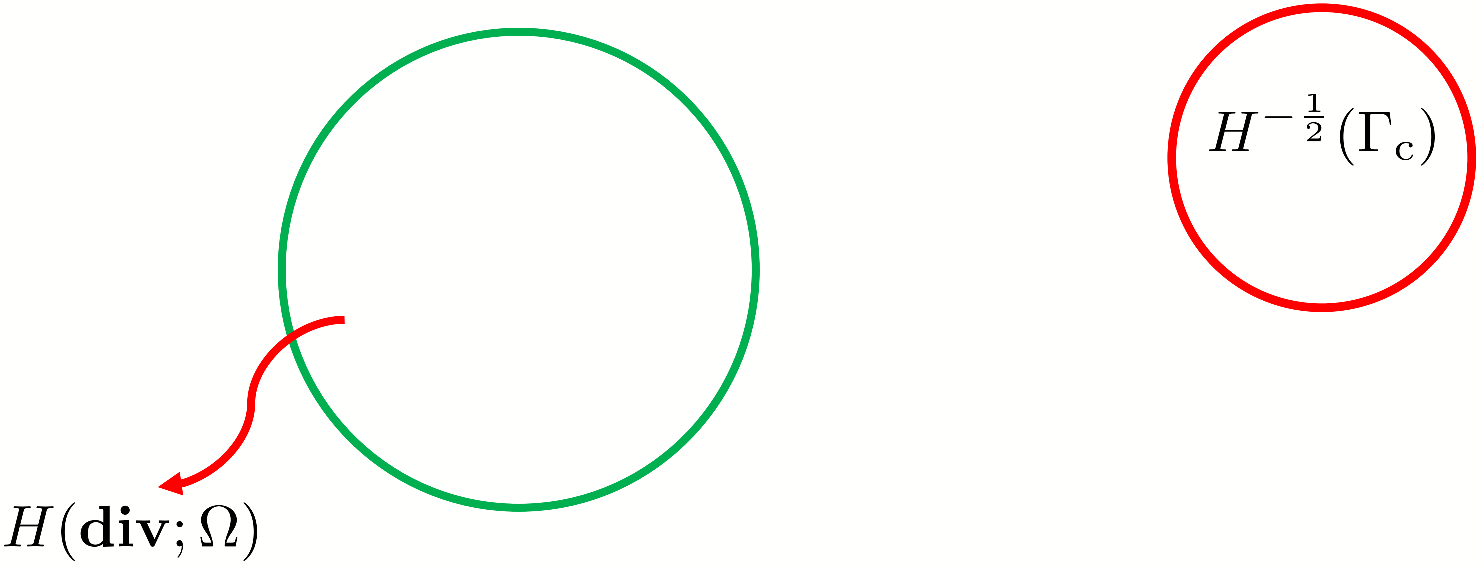
Displacement error



Restricting H(div; Ω) to RT

Boffi et al., 2013: **Lemma 2.1.2.**

The normal trace operator γ_{n}: $\boldsymbol{\lambda} \in H(\mathbf{div};\Omega) \rightarrow \boldsymbol{\lambda}\cdot\mathbf{n}|_{\Gamma} \in H^{-1/2}(\Gamma)$ is surjective

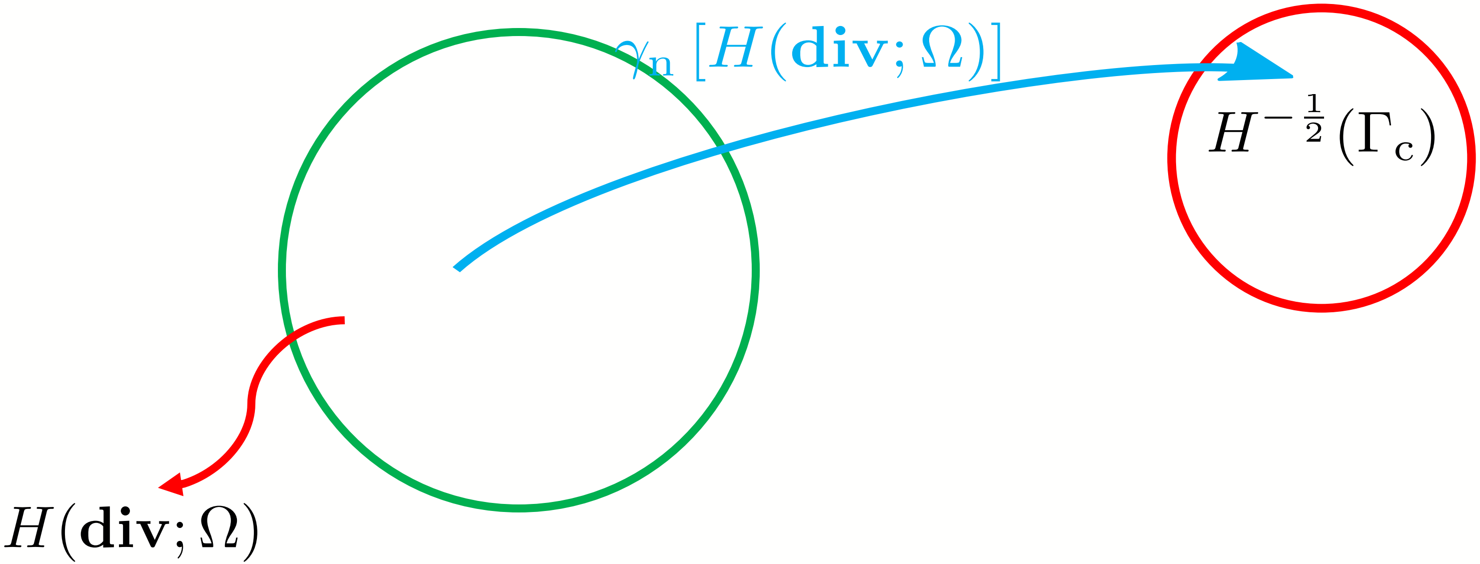


MOFEM
mofem.eng.gla.ac.uk

Restricting H(div; Ω) to RT

Boffi et al., 2013: **Lemma 2.1.2.**

The normal trace operator γ_{n}: $\boldsymbol{\lambda} \in H(\mathbf{div};\Omega) \rightarrow \boldsymbol{\lambda}\cdot\mathbf{n}|_{\Gamma} \in H^{-1/2}(\Gamma)$ is surjective

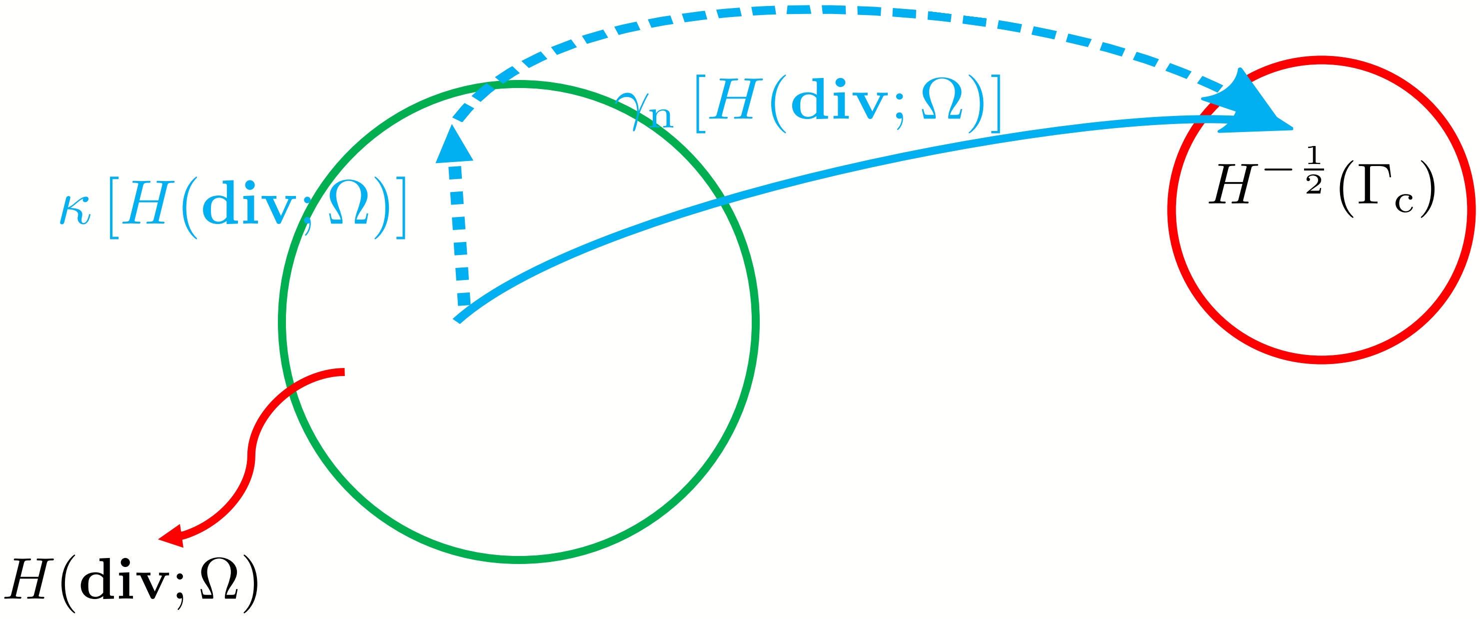


mofem.eng.gla.ac.uk

Restricting H(div; Ω) to RT

Boffi et al., 2013: **Lemma 2.1.2.**

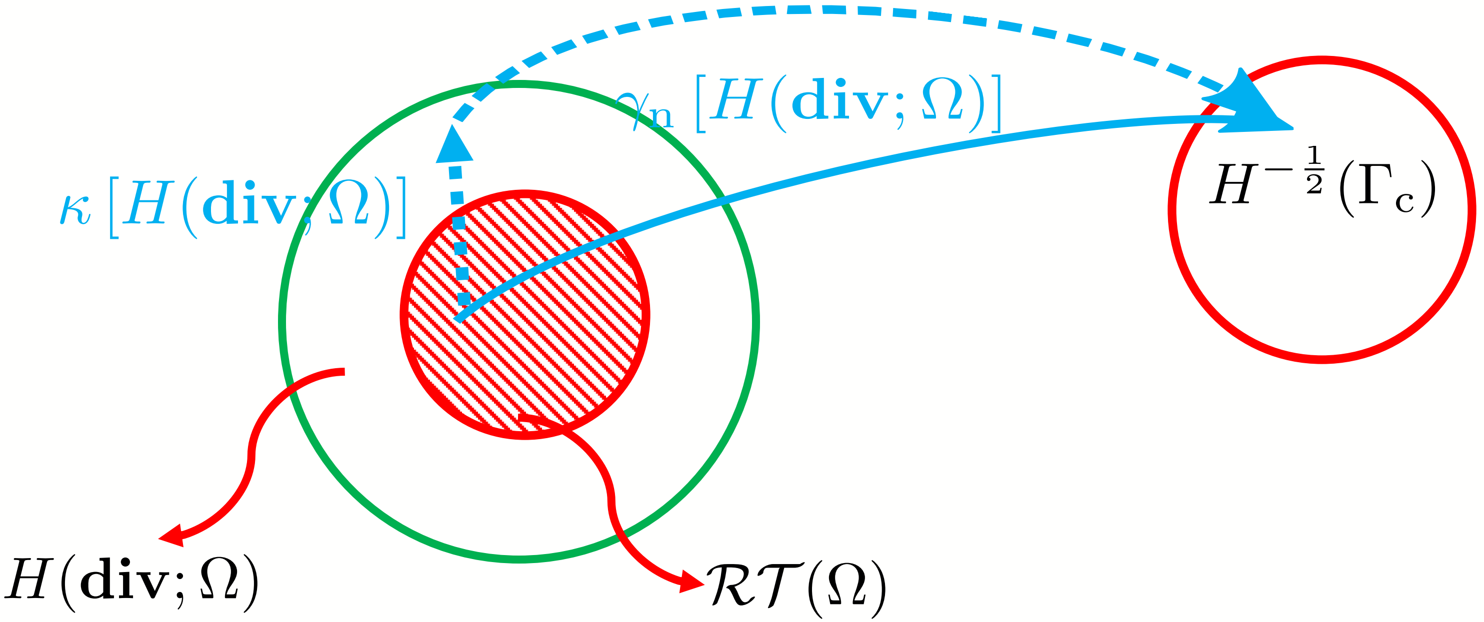
The normal trace operator γ_{n}: $\boldsymbol{\lambda} \in H(\mathbf{div};\Omega) \rightarrow \boldsymbol{\lambda}\cdot\mathbf{n}|_{\Gamma} \in H^{-1/2}(\Gamma)$ is surjective



Restricting H(div; Ω) to RT

Boffi et al., 2013: **Lemma 2.1.2.**

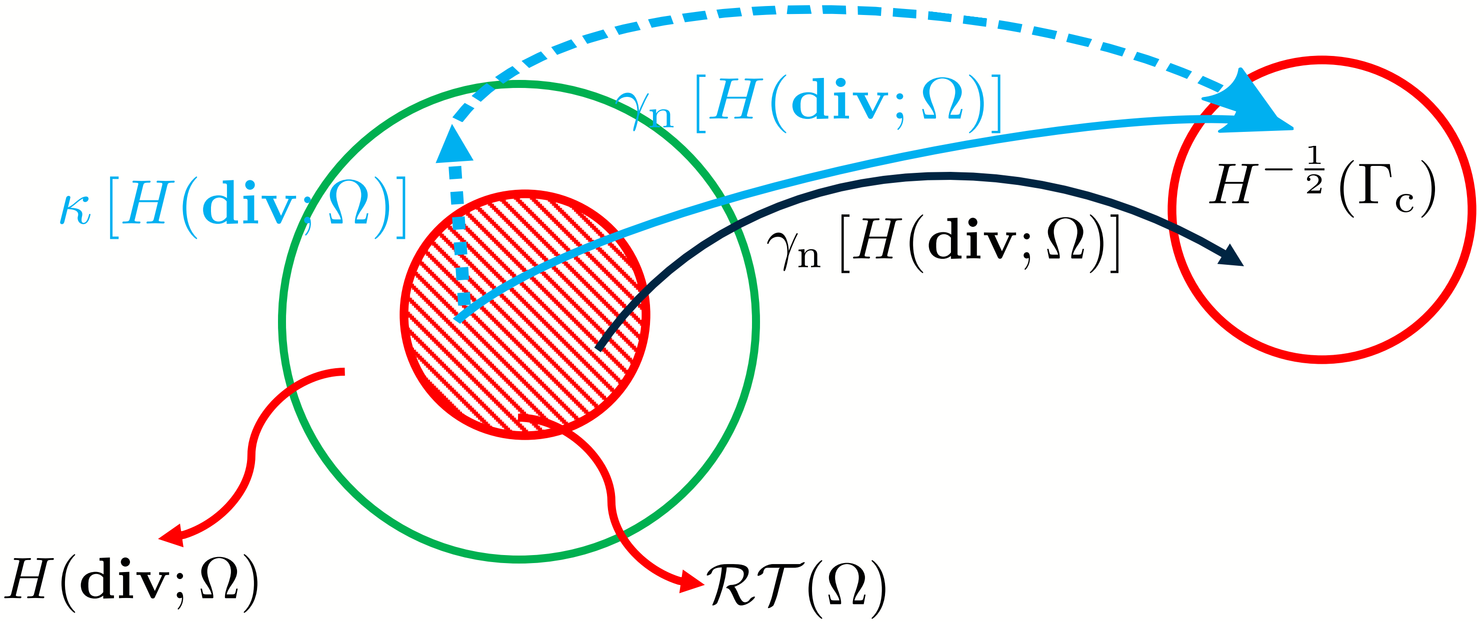
The normal trace operator $\gamma_{\mathrm{n}}\colon \boldsymbol{\lambda} \in H(\mathbf{div};\Omega) \to \boldsymbol{\lambda}\cdot\mathbf{n}|_\Gamma \in H^{-1/2}(\Gamma)$ is surjective



Restricting H(div; Ω) to RT

Boffi et al., 2013: **Lemma 2.1.2.**

The normal trace operator γ_{n}: $\boldsymbol{\lambda} \in H(\mathbf{div};\Omega) \rightarrow \boldsymbol{\lambda}\cdot\mathbf{n}|_{\Gamma} \in H^{-1/2}(\Gamma)$ is surjective

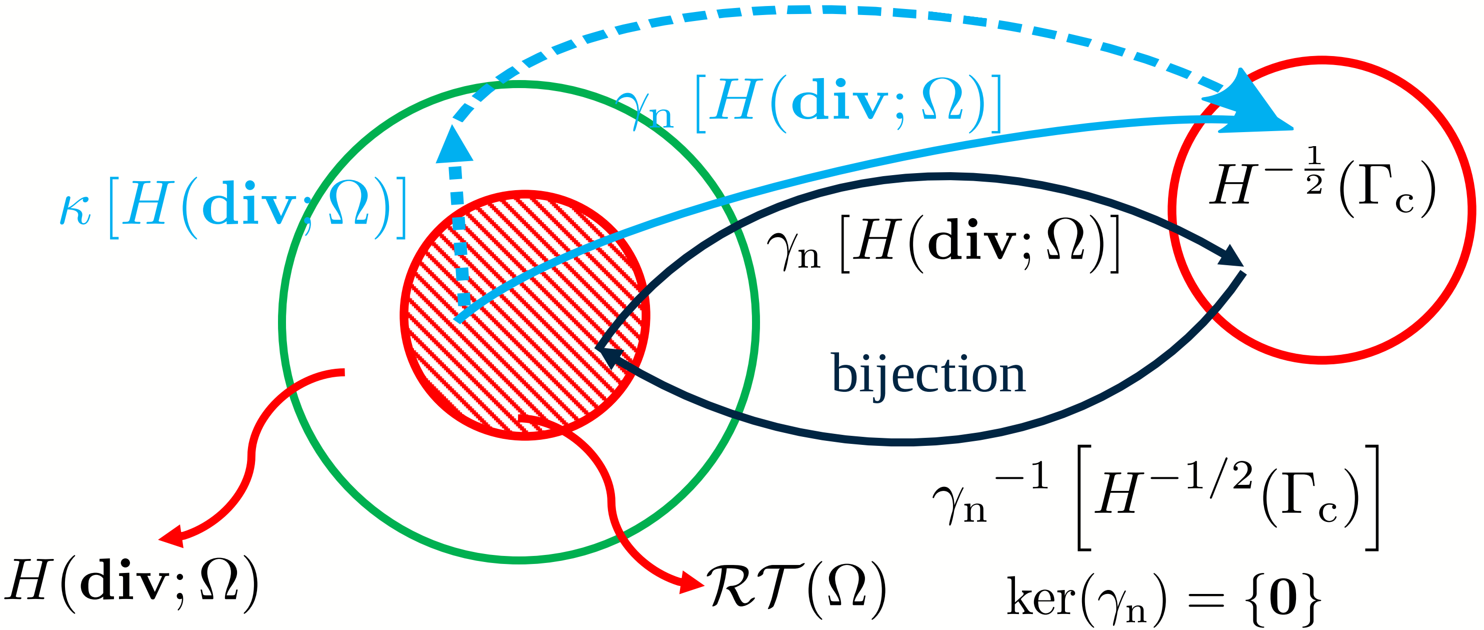


MOFEM mofem.eng.gla.ac.uk

Restricting H(div; Ω) to RT

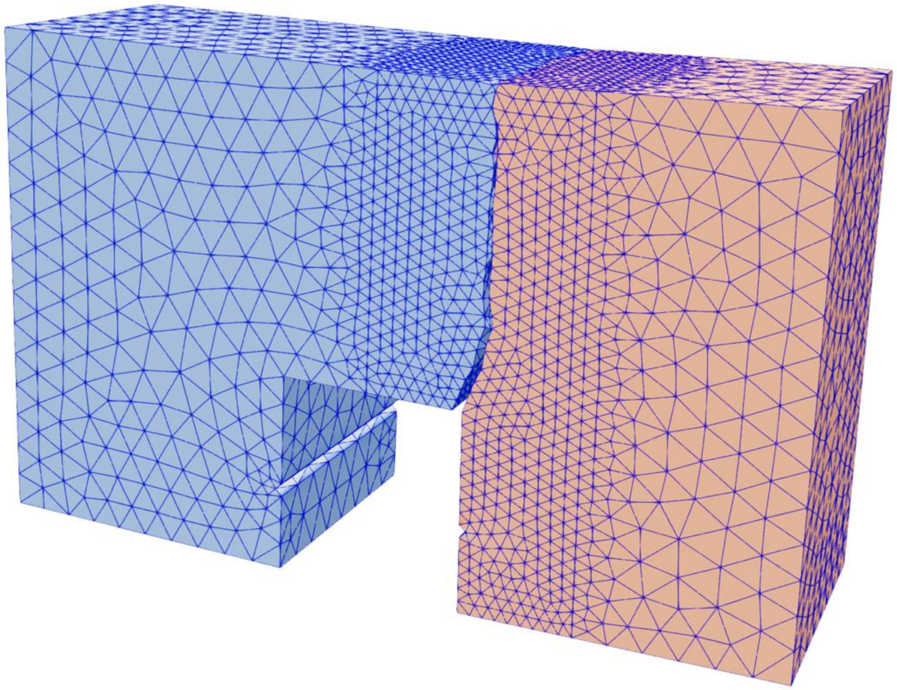
Boffi et al., 2013: **Lemma 2.1.2.**

The normal trace operator $\gamma_{\mathrm{n}}\colon \boldsymbol{\lambda} \in H(\mathbf{div};\Omega) \to \boldsymbol{\lambda}\cdot\mathbf{n}|_{\Gamma} \in H^{-1/2}(\Gamma)$ is surjective



Fracture is natural, for weakly enforced conformity

Color represents z-axis rotation



- Crack propagates by erasing rows and columns of the matrix. Matrix adjacency is fixed. That provides robustness
- Trace of H-div space is associated with faces, thus crack face energy can be easily estimated
- If crack propagate one face by one face, and iterative solver is deployed, crack propagation are resolved on linear solver level

$$\Psi^{\mathcal{F}} = \int_{\Omega} \sigma_{ij}^{\mathcal{F}} \varepsilon_{ij} \mathrm{d}\Omega$$

Extension of face trace

University of Glasgow

Thank you for your attention!

WORLD CHANGING GLASGOW

#UofGWorldChangers

@UofGlasgow