Applications in Solid Mechanics

Fifth deal.II Users and Developers Workshop
Texas A&M University

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A McBride

BD Reddy

S Bartle, A de Villiers, B Grieshaber, M Hamed, J-P Pelteret, T Povall, N Richardson

Centre for Research in Computational and Applied Mechanics, University of Cape Town, South Africa

DEAL.II AND CERECAM

Centre for Research in Computational and Applied Mechanics:

- multidisciplinary research centre with 12 members from various faculties and departments
- postgraduate eduction in mechanics is a key objective
  - 6 courses in FE, continuum mechanics, C++, deal.II (computational FEA)
  - MSc and PhD supervision
  - unique facility in (South) Africa

deal.II and CERECAM

- decision made in 2008 to use deal.II as base for code development
  - SIAM news article on deal.II winning the Wilkinson Prize in 2007
  - lacked the critical mass to develop own in-house code
  - even if we had the mass, we would be small number of isolated individuals reinventing the wheel in a country far away…
- 5 MSc projects and 8 PhD projects used deal.II in CERECAM to date

Overview of Presentation

- Overview of several of the research projects using deal.II
    1. IP methods for problems in elasticity
    2. Thin-shells with applications in biomechanics
    3. Patient-specific FSI for vascular access in haemodialysis patients
    4. Surface elasticity
    5. Single crystal plasticity
    6. Homogenisation of material layers
    7. Friction-stir welding
- What would I like to see (or be encouraged to implement) in deal.II

IP Methods for Problems in Elasticity

or Why it's good NOT to have tetrahedral elements in deal.II

- Locking:
  - The poor behaviour of low-order conforming finite element approximations for problems of near-incompressible or incompressible elasticity

$$-\mathrm{div}\,\boldsymbol{\sigma}(\mathbf{u}) = \mathbf{f}$$

$$\boldsymbol{\sigma}(\mathbf{u}) := 2\mu\boldsymbol{\varepsilon}(\mathbf{u}) + \lambda \mathrm{tr}\,\boldsymbol{\varepsilon}(\mathbf{u})\,\mathbf{1} = 2\mu\boldsymbol{\varepsilon}(\mathbf{u}) + \lambda(\nabla\cdot\mathbf{u})\,\mathbf{1},$$

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

- Some remedies:
  - selective reduced integration (SRI)
  - mixed DG methods for meshes of low-order quadrilateral or hexahedral cells
  - primal DG methods for triangular elements…convergence analysis similarly restrictive
- Context:
  - we assumed we could simply use a primal DG formulation in deal.II, circumvent locking and move on to the actual problem…

> Contrary to initial expectations, numerical experiments with the IP methods show that bilinear quadrilateral elements, while performing very well for highly compressible materials, perform poorly for the nearly incompressible case, unlike their triangular counterparts.

- our remedy: SRI on edge terms for IP methods

- Grieshaber (2013) PhD
- Grieshaber, McB, Reddy (accepted), SINUM

DG Formulation

$$a_h^{\mathrm{UI}}\left(\mathbf{u}_h, \mathbf{v}\right) = l_h^{\mathrm{UI}}\left(\mathbf{v}\right)$$

$$
\begin{aligned}
a_h^{\mathrm{UI}}\left(\mathbf{u}, \mathbf{v}\right) = & \sum_{\Omega_e \in \mathcal{T}_h} \int_{\Omega_e} \boldsymbol{\sigma}\left(\mathbf{u}\right) : \boldsymbol{\varepsilon}\left(\mathbf{v}\right) dx \\
& + \theta\, 2\mu \sum_{E \in \Gamma_{iD}} \int_E [\![\mathbf{u}]\!] : \{\boldsymbol{\varepsilon}\left(\mathbf{v}\right)\} ds + \theta\, \lambda \sum_{E \in \Gamma_{iD}} \sum_{i=1}^{ngp} [[\![\mathbf{u}]\!] : \{\nabla \cdot \mathbf{v} \mathbf{1}\}] |_{\mathrm{p_i}} w_i \\
& - 2\mu \sum_{E \in \Gamma_{iD}} \int_E \{\boldsymbol{\varepsilon}\left(\mathbf{u}\right)\} : [\![\mathbf{v}]\!] ds - \lambda \sum_{E \in \Gamma_{iD}} \sum_{i=1}^{ngp} [\{\nabla \cdot \mathbf{u} \mathbf{1}\} : [\![\mathbf{v}]\!]] |_{\mathrm{p_i}} w_i \\
& + k_\mu\, \mu \sum_{E \in \Gamma_{iD}} \frac{1}{h_E} \int_E [\![\mathbf{u}]\!] : [\![\mathbf{v}]\!]\, ds + k_\lambda\, \lambda \sum_{E \in \Gamma_{iD}} \frac{1}{h_E} \sum_{i=1}^{ngp} [[\![\mathbf{u}]\!] [\![\mathbf{v}]\!]] |_{\mathrm{p_i}} w_i,
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{u} &= \mathbf{g} && \text{on } \Gamma_D \\
\boldsymbol{\sigma}\left(\mathbf{u}\right)\mathbf{n} &= \mathbf{h} && \text{on } \Gamma_N
\end{aligned}
$$

$$
\begin{aligned}
l_h^{\mathrm{UI}}\left(\mathbf{v}\right) = & \sum_{\Omega_e \in \mathcal{T}_h} \int_{\Omega_e} \mathbf{f} \cdot \mathbf{v}\, dx + \theta\, 2\mu \sum_{E \in \Gamma_D} \int_E \left(\mathbf{g} \otimes \mathbf{n}\right) : \boldsymbol{\varepsilon}\left(\mathbf{v}\right)\, ds \\
& + \theta\, \lambda \sum_{E \in \Gamma_D} \sum_{i=1}^{ngp} [\left(\mathbf{g} \otimes \mathbf{n}\right) : \left(\nabla \cdot \mathbf{v}\, \mathbf{1}\right)] |_{\mathrm{p_i}} w_i \\
& + k_\mu\, \mu \sum_{E \in \Gamma_D} \frac{1}{h_E} \int_E \left(\mathbf{g} \otimes \mathbf{n}\right) : \left(\mathbf{v} \otimes \mathbf{n}\right)\, ds \\
& + k_\lambda\, \lambda \sum_{E \in \Gamma_D} \frac{1}{h_E} \sum_{i=1}^{ngp} [\left(\mathbf{g} \cdot \mathbf{n}\right)\left(\mathbf{v} \cdot \mathbf{n}\right)] |_{\mathrm{p_i}} w_i + \sum_{E \in \Gamma_N} \int_E \mathbf{h} \cdot \mathbf{v}\, ds
\end{aligned}
$$

standard formulation: $ngp = 2$

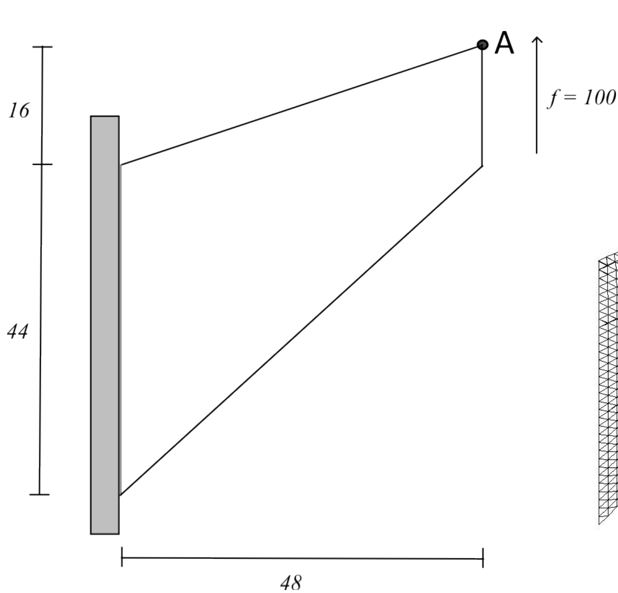
NIPG: $\theta = 1$

SIPG: $\theta = -1$

IIPG: $\theta = 0$

❖ Grieshaber, McB, Reddy (accepted), SINUM

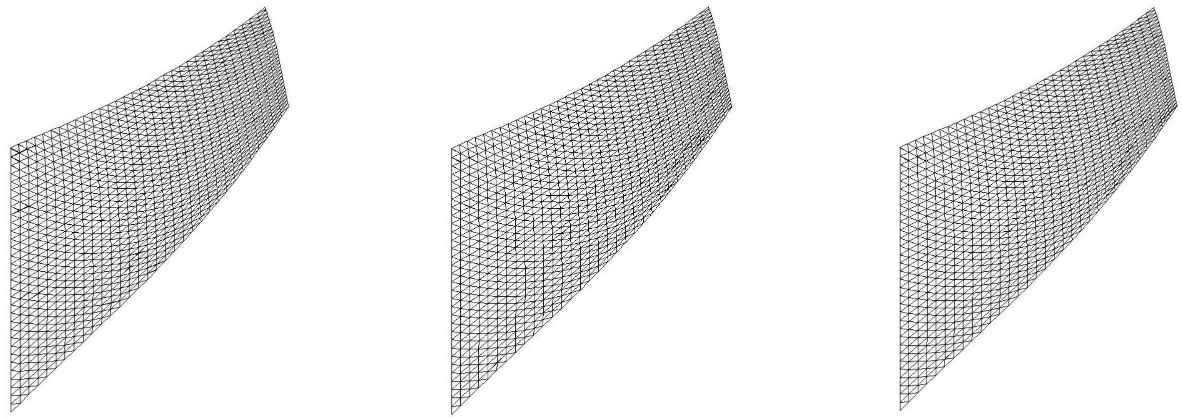
Cook's Membrane Problem



$\nu = 0.49995$

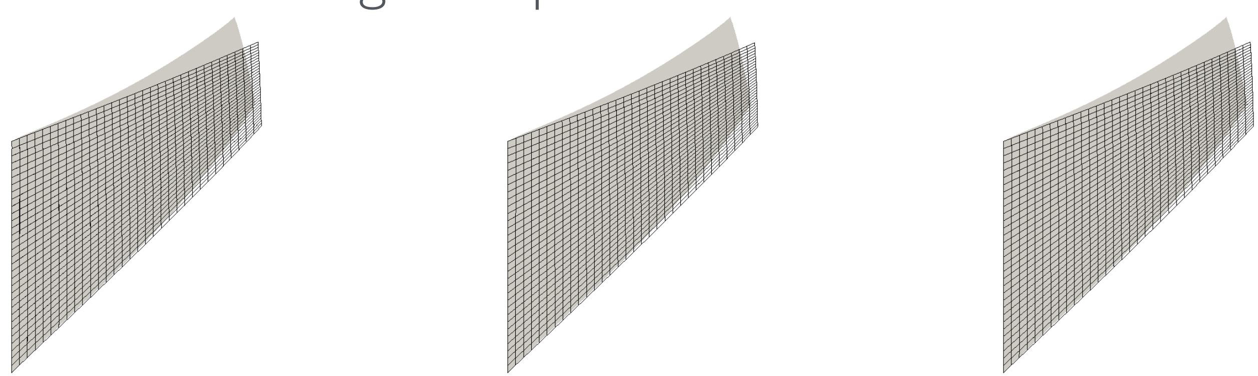
$E = 250$

locking-free response for triangular elements



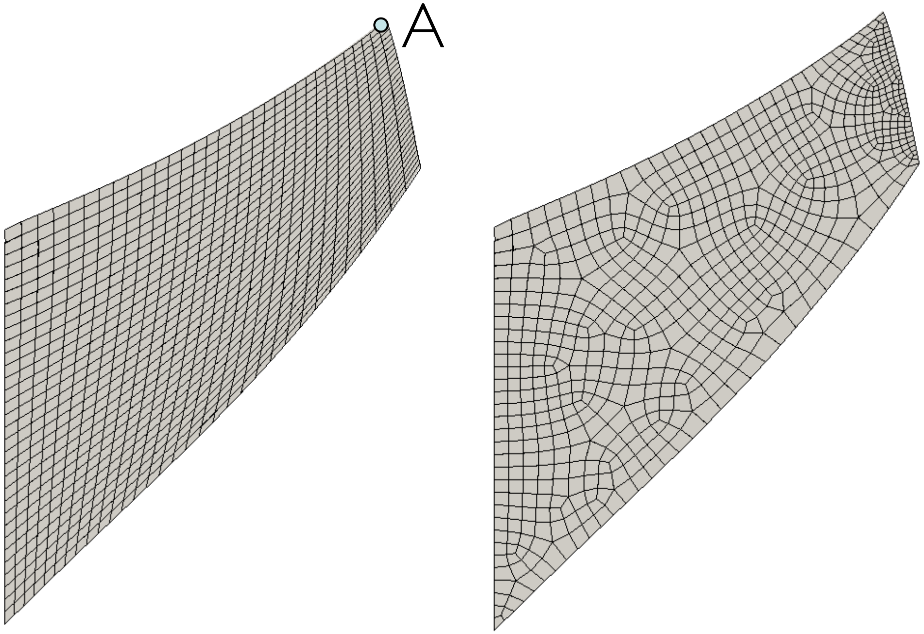
(a) NIPG (b) IIPG (c) SIPG

locking for quadrilateral element



(a) NIPG (b) IIPG (c) SIPG

Cook's Membrane Problem



(a) Modified SIPG

(b) Modified IIPG

locking-free response for quadrilateral elements using modified formulation

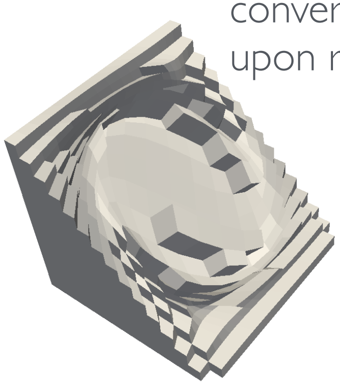
neps	SG	SG Q2	NIPG	— UI	IIPG	— UI	SIPG	— UI
Skewed mesh								
4	1.3855	5.99901	2.07077	4.67802	2.08011	4.6961	2.21427	4.72803
8	1.95749	7.06822	2.12496	6.13406	2.08011	4.6961	2.21427	4.72803
16	2.01279	7.49608	2.24957	7.14275	2.15449	7.14171	2.28465	7.14403
32	2.19539	7.64827	2.633127	7.54839	2.38855	7.54625	2.50211	7.54509
Unstructured mesh								
32	3.054	7.66333	5.44538	7.61069	4.42923	7.60888	4.5467	7.60599

vertical deflection of point A

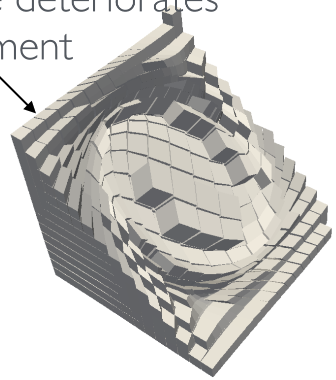
3D Cube Subject to Body Force

locking for quadrilateral element

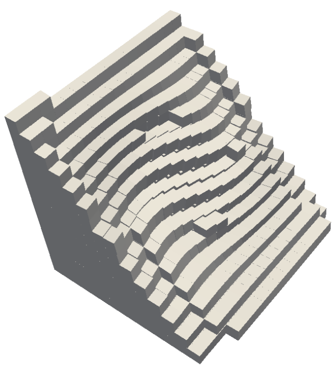
convergence deteriorates upon refinement



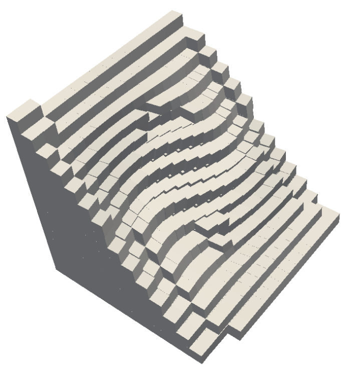
(a) Exact solution



(b) NIPG

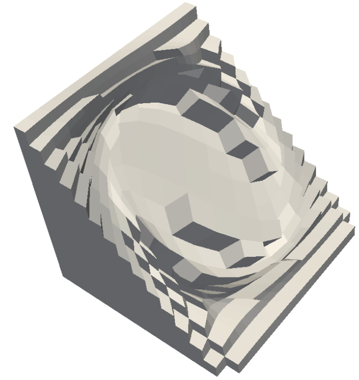


(c) IIPG

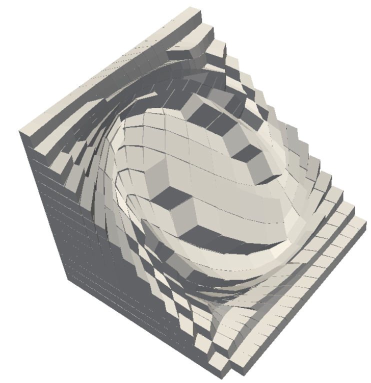


(d) SIPG

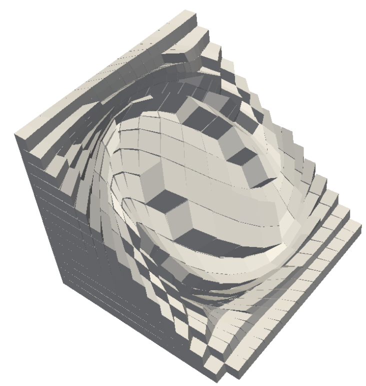
locking-free response for quadrilateral elements using modified formulation



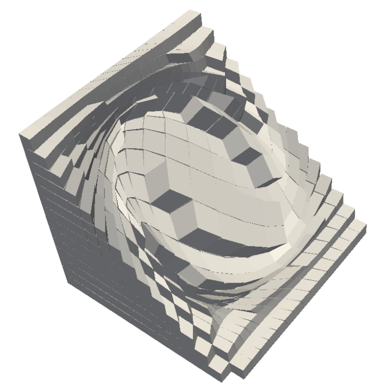
(a) Exact solution



(b) Modified NIPG



(c) Modified IIPG



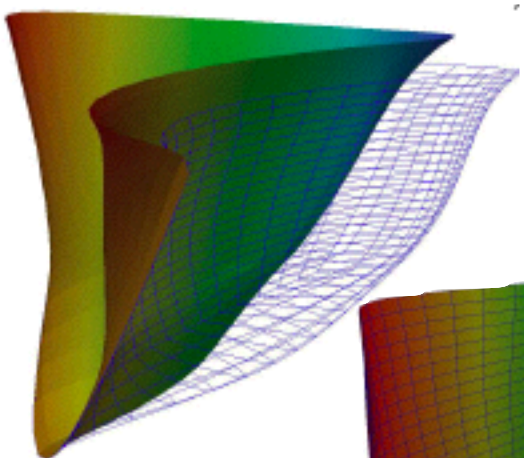
(d) Modified SIPG

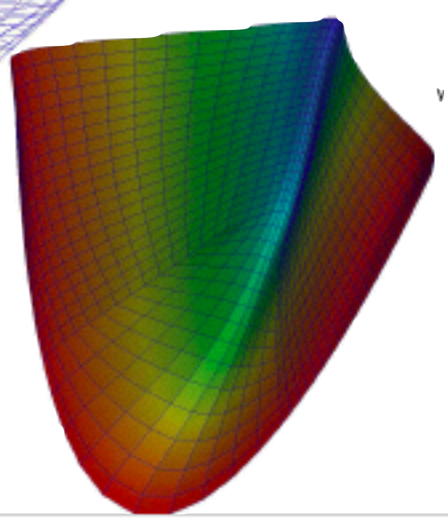
❖ Grieshaber, McB, Reddy (in review)

Applications of Thin Shell Theory in Biomechanics

or How to trick deal.II to handle lower-dimensional manifolds prior to codimension one and manifolds

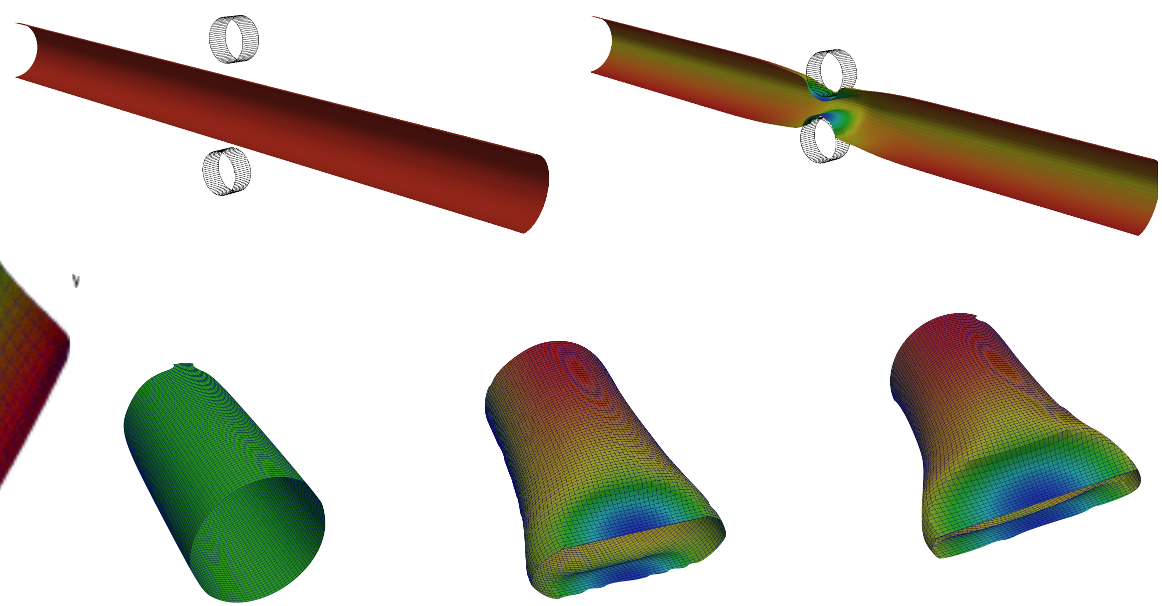
- Treat the 3D body as a 2D surface with a director at each point
- Formulate problem in terms of quantities averaged through the thickness (see Simo & Fox)
  - SRI through the thickness to prevent membrane locking
  - account for transverse isotropy and incompressibility





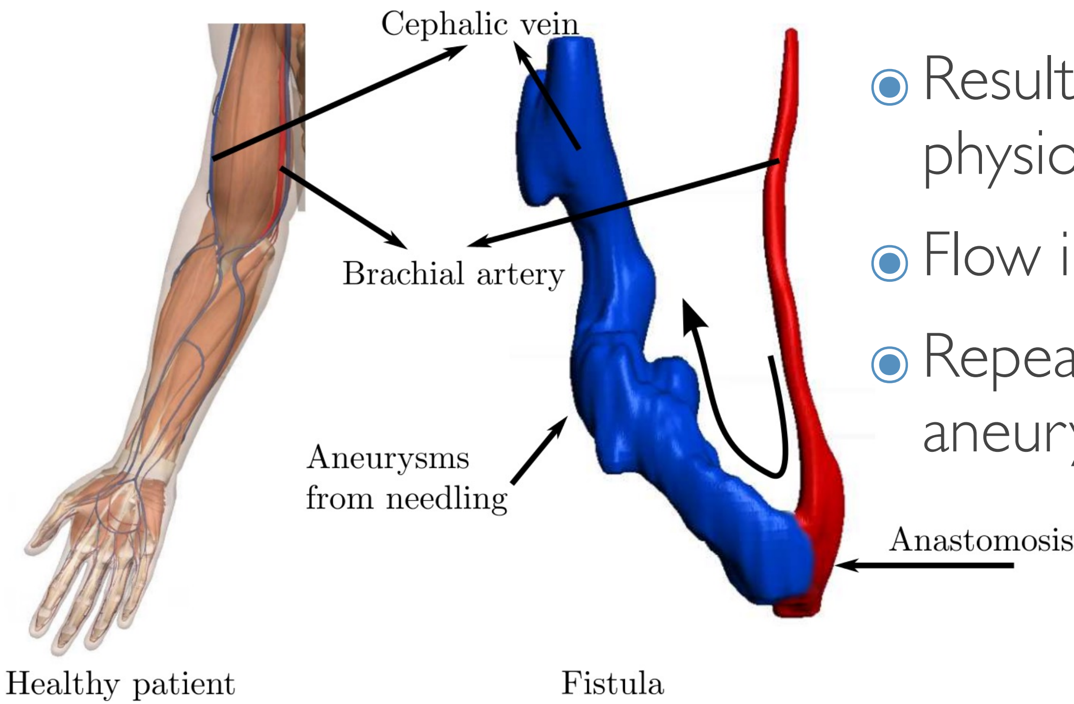
artificial heart valves

- ❖ Bartle (2009) MSc



aortic clamping

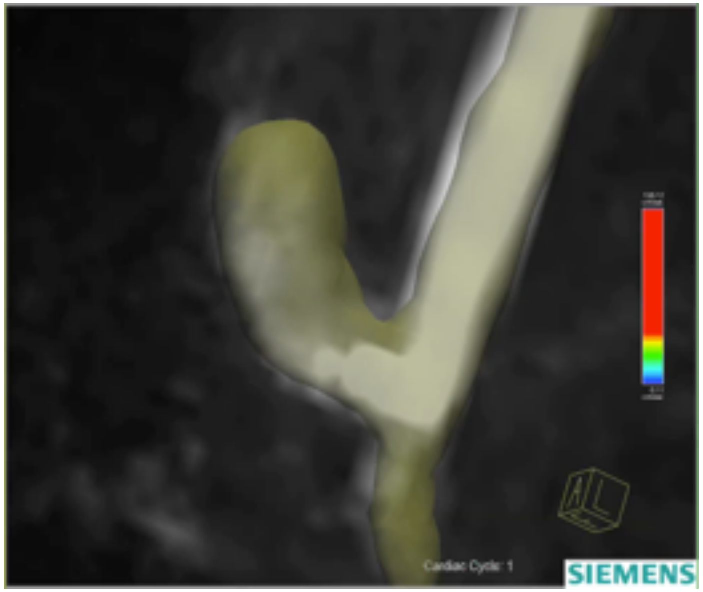
Patient-specific FSI for vascular access in haemodialysis patients



- Resulting flow rates up to 30 times physiological norms
- Flow in vein significantly altered
- Repeated needling leads to pseudo aneurysms

Objective:

- Develop a patient specific FSI model of arteriovenous vascular access configurations, verified by in vivo MRI data

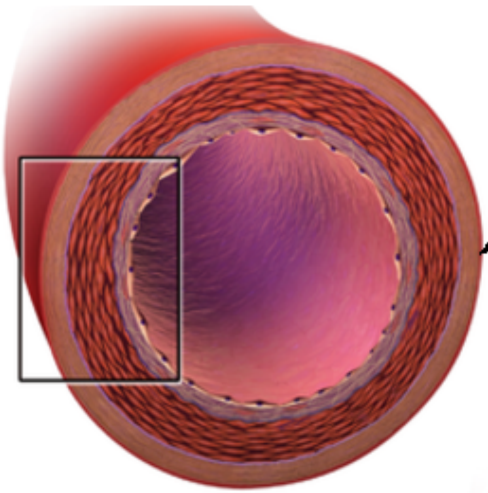


❖ de Villiers (current) PhD

FSI Model

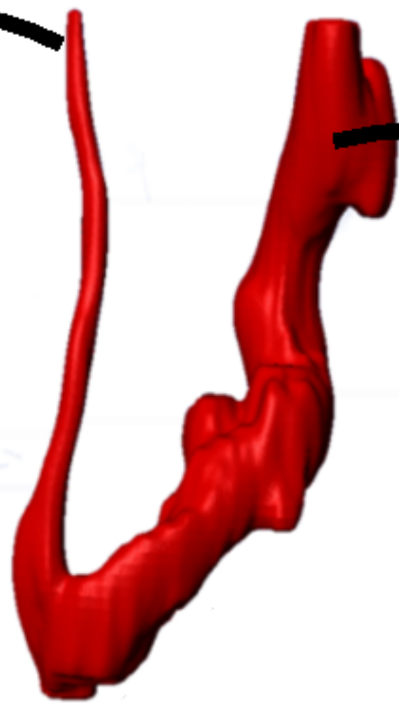
Transverse isotropy

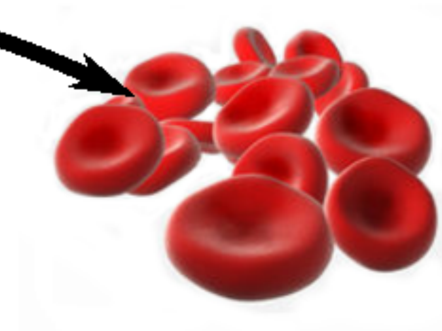
$$\Psi(\mathbf{C}, \mathbf{A}_1, \mathbf{A}_2) = U(J) + \overline{\Psi}(\overline{\mathbf{C}}, \mathbf{A}_1, \mathbf{A}_2)$$



Navier-Stokes in ALE setting

$$\begin{aligned} \rho_\mathrm{f}\partial_\mathrm{t}\mathbf{v}_\mathrm{f}\,|_\mathbf{x} + \rho_\mathrm{f}\mathbf{c}\cdot\nabla\mathbf{v}_\mathrm{f} - \mathrm{div}\boldsymbol{\sigma}_\mathrm{f} &= \mathbf{0} \\ \mathrm{div}\mathbf{v}_\mathrm{f} &= \mathbf{0} \end{aligned}$$





Balance linear momentum (solid)

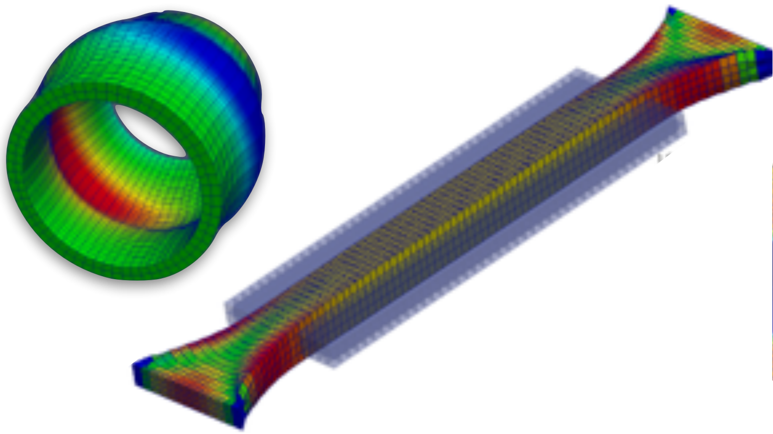
$$\rho_\mathrm{s}\partial_\mathrm{t}^2\mathbf{U}_\mathrm{s} - \mathrm{Div}(\mathbf{P}_\mathrm{s}) = \mathbf{0}$$

- Wick (2011) Fluid-structure interactions using different mesh motion techniques. Computers & Structures
- Wick (2013). Solving monolithic fluid-structure interaction problems in Arbitrary Lagrangian Eulerian co-ordinates with the deal.II library. Archive of Numerical Software

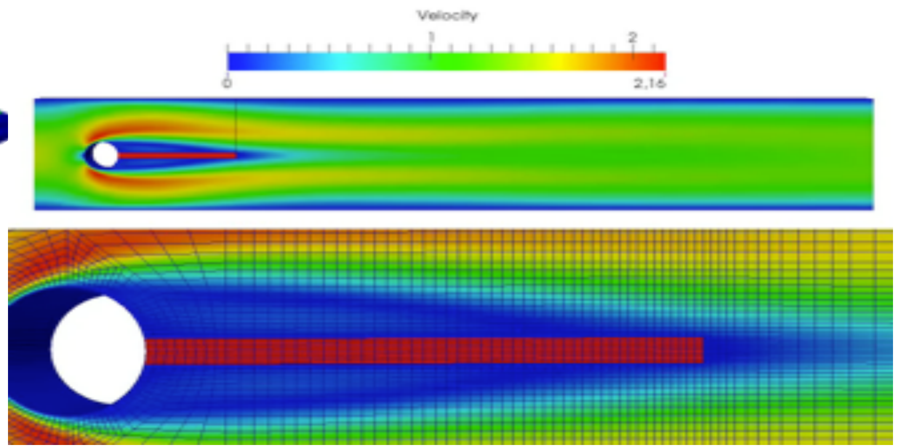
Harmonic mesh motion

$$\begin{aligned} -\mathrm{div}\boldsymbol{\sigma}_\mathrm{m} &= \mathbf{0} \\ \boldsymbol{\sigma}_\mathrm{m} &= \alpha_u\nabla\mathbf{U}_f \end{aligned}$$

Validation and Extensions

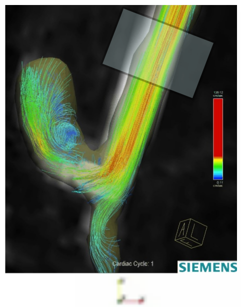


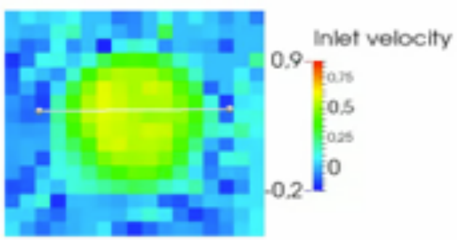
Incompressible finite elasticity
with transverse isotropy

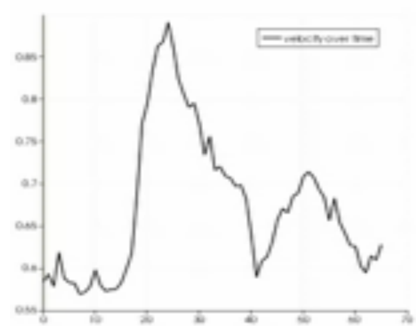


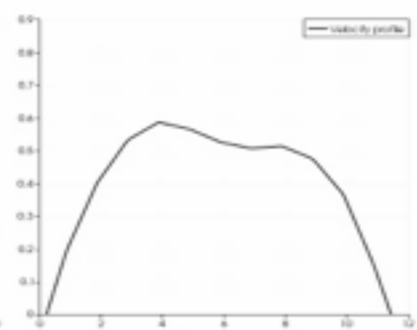
Turek flag

- Extended model to 3D
- Parallel direct solver (SuperLU)
- Windkessel outlet boundary condition for physiologically meaningful flow split

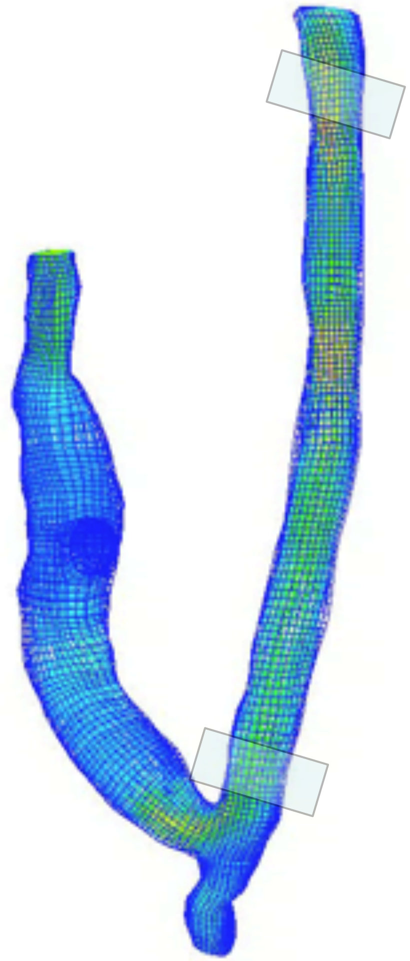


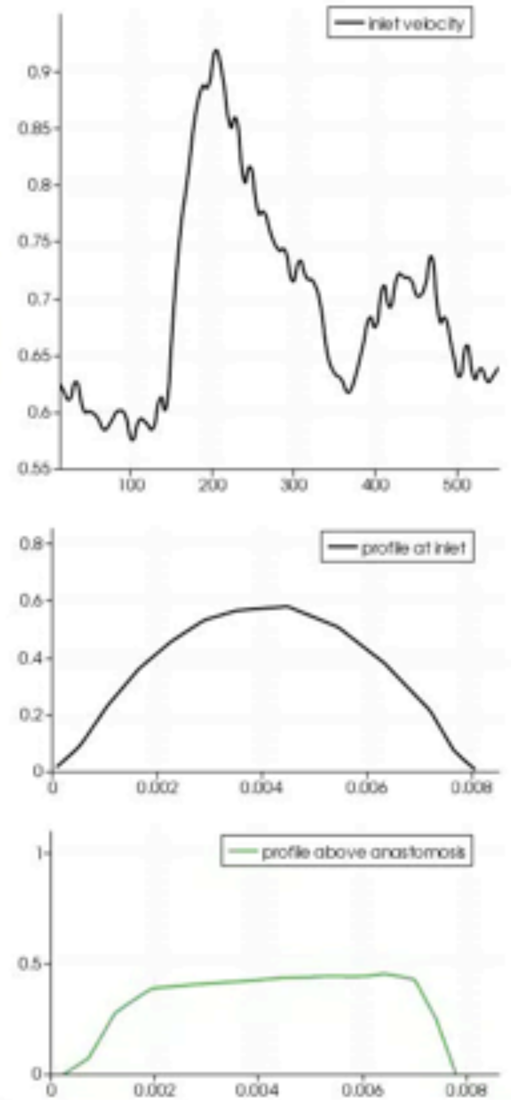






Current State: CFD Model





simpleware + ANSA

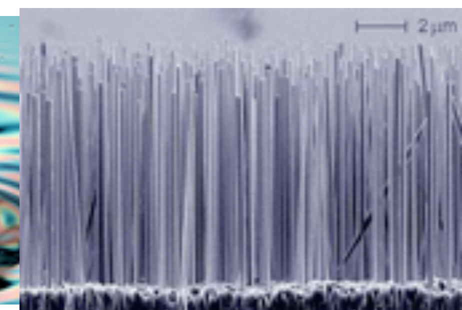
SURFACE ELASTICITY

- Surfaces behave differently from the bulk
  - broken bonds on surface, coatings, oxidation, …
- Are surface effects significant?

$$\frac{\text{surface energy}}{\text{bulk energy}} \propto \frac{\widehat{\Psi}}{\Psi}\,\frac{\mathrm{d}A}{\mathrm{d}V}$$

- Objective: capture surface effects within a continuum model
  - accounting for surface using surface elasticity theory of GURTIN & MURDOCH (1975)
  - solid and fluid-like surfaces
  - fully nonlinear theory
  - to provide details of numerical implementation
    - generally restricted to linear theory

surface tension H_20



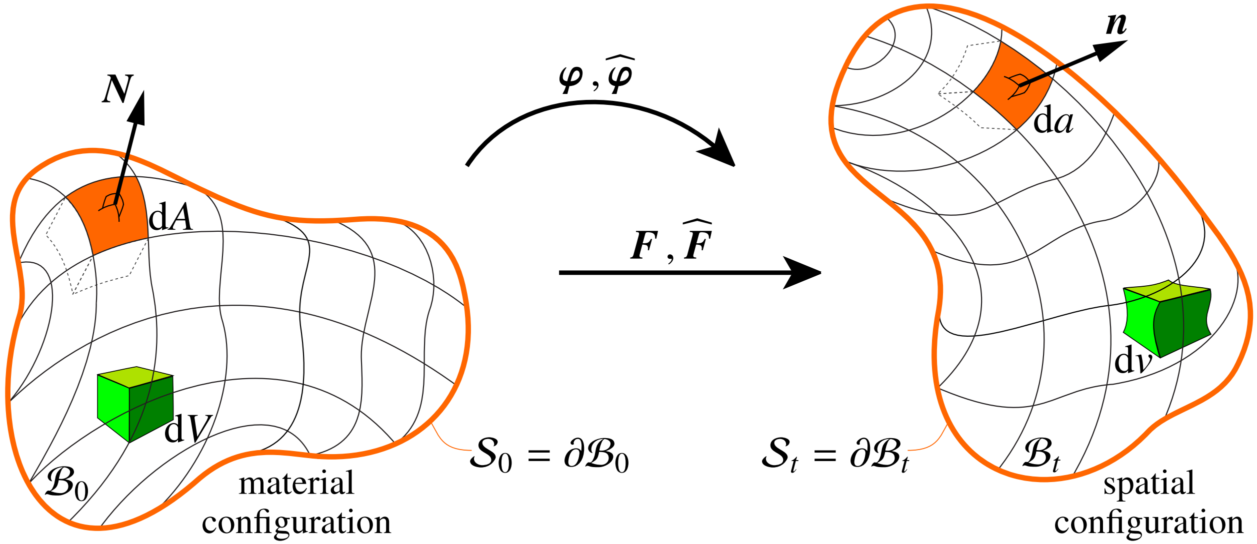
carbon nanotubes

❖ JAVILI, MCB, STEINMANN & REDDY (2014), COMP MECH

❖ SURFACE ELASTICITY ON bitbucket.org

❖ Davydov, Javili, Steinmann, McB (2013), in Surface Effects in Solid Mechanics

Kinematics of Surface Elasticity



$$X \bullet \xrightarrow{F} \bullet\, x \qquad (\varphi)$$

$$F := \partial x / \partial X \qquad f := \partial X / \partial x$$

$$\widehat{X} \bullet \xrightarrow{\widehat{F}} \bullet\, \widehat{x} \qquad (\widehat{\varphi})$$

$$\widehat{F} := \partial \widehat{x} / \partial \widehat{X} \qquad \widehat{f} := \partial \widehat{X} / \partial \widehat{x}$$

- Surface is coherent: $\widehat{\varphi} = \varphi|_{\partial\mathcal{B}_0}$
- Surface deformation gradient is rank deficient
  - inverse defined via relations:

$$\widehat{f} \cdot \widehat{F} = \widehat{I} =: I - N \otimes N \qquad \text{and} \qquad \widehat{F} \cdot \widehat{f} = \widehat{i} =: i - n \otimes n\,.$$

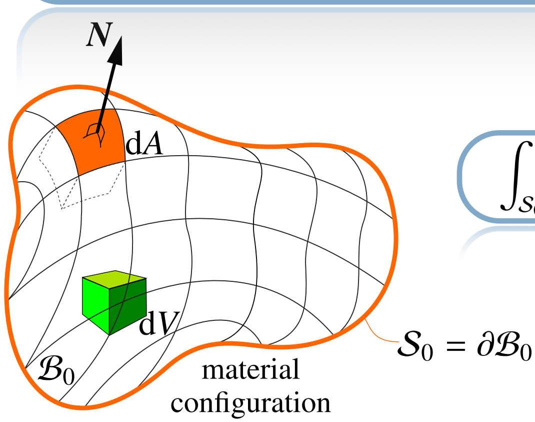
GOVERNING EQUATIONS

Strong form:

balance of linear momentum		balance of angular momentum	
$\boxed{\mathrm{Div}\boldsymbol{P} + \boldsymbol{b}_0^{\mathrm{p}} = \boldsymbol{0}}$	,	$\boldsymbol{F}\cdot\boldsymbol{P}^{\mathrm{t}} = \boldsymbol{P}\cdot\boldsymbol{F}^{\mathrm{t}}$	in $\mathcal{B}_0$
$\boxed{\widehat{\mathrm{Div}}\widehat{\boldsymbol{P}} + \widehat{\boldsymbol{b}}_0^{\mathrm{p}} - \boldsymbol{P}\cdot\boldsymbol{N} = \boldsymbol{0}}$	,	$\widehat{\boldsymbol{F}}\cdot\widehat{\boldsymbol{P}}^{\mathrm{t}} = \widehat{\boldsymbol{P}}\cdot\widehat{\boldsymbol{F}}^{\mathrm{t}}$	on $\mathcal{S}_0$

Weak form:

$$\int_{\mathcal{B}_0}\boldsymbol{P} : \mathrm{Grad}\delta\boldsymbol{\varphi}\,\mathrm{d}V + \int_{\mathcal{S}_0}\widehat{\boldsymbol{P}} : \widehat{\mathrm{Grad}}\delta\widehat{\boldsymbol{\varphi}}\,\mathrm{d}A - \int_{\mathcal{B}_0}\delta\boldsymbol{\varphi}\cdot\boldsymbol{b}_0^{\mathrm{p}}\,\mathrm{d}V - \int_{\mathcal{S}_0^{\mathrm{N}}}\delta\widehat{\boldsymbol{\varphi}}\cdot\widehat{\boldsymbol{b}}_0^{\mathrm{p}}\,\mathrm{d}A = 0 \qquad \forall\delta\boldsymbol{\varphi}\in\mathcal{H}_0^1(\mathcal{B}_0)\,,\ \forall\delta\widehat{\boldsymbol{\varphi}}\in\mathcal{H}_0^1(\mathcal{S}_0)$$



surface divergence theorem

$$\boxed{\int_{\mathcal{S}_0}\widehat{\mathrm{Div}}\{\widehat{\bullet}\}\,\mathrm{d}A = \int_{\mathcal{C}_0}\{\widehat{\bullet}\}\cdot\widehat{\boldsymbol{N}}\,\mathrm{d}L - \int_{\mathcal{S}_0}\widehat{C}\{\widehat{\bullet}\}\cdot\boldsymbol{N}\,\mathrm{d}A}$$

superficial tensor

$$\boxed{\widehat{\boldsymbol{P}}\cdot\boldsymbol{N} = \boldsymbol{0}}$$

twice mean surface curvature

$$\boxed{\widehat{C} = -\widehat{\mathrm{Div}}\boldsymbol{N}}$$

Constitutive Relations

bulk

$J := \mathrm{Det}\boldsymbol{F}$: Jacobian determinant

$\mu\,,\lambda$: Lamé constants

Free energy $\quad \Psi(\boldsymbol{F}) = \frac{1}{2}\,\lambda \ln^2 J + \frac{1}{2}\,\mu\,[\boldsymbol{F} : \boldsymbol{F} - 3 - 2\ln J]$

Piola stress $\quad \boldsymbol{P}(\boldsymbol{F}) = \dfrac{\partial \Psi}{\partial \boldsymbol{F}} = \lambda \ln J\, \boldsymbol{f}^{\mathrm{t}} + \mu\,[\boldsymbol{F} - \boldsymbol{f}^{\mathrm{t}}]$

surface

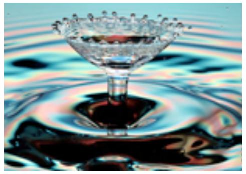
$\widehat{J} := \widehat{\mathrm{Det}\boldsymbol{F}}$: Surface Jacobian determinant

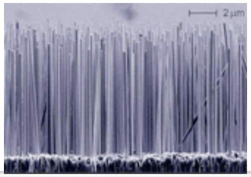
$\widehat{\mu}\,,\widehat{\lambda}$: Surface Lamé constants

$\widehat{\gamma}$: Surface tension

Surface Free energy $\quad \widehat{\Psi}(\widehat{\boldsymbol{F}}) = \frac{1}{2}\,\widehat{\lambda} \ln^2 \widehat{J} + \frac{1}{2}\,\widehat{\mu}\,[\widehat{\boldsymbol{F}} : \widehat{\boldsymbol{F}} - 2 - 2\ln \widehat{J}] + \widehat{\gamma}\,\widehat{J}$

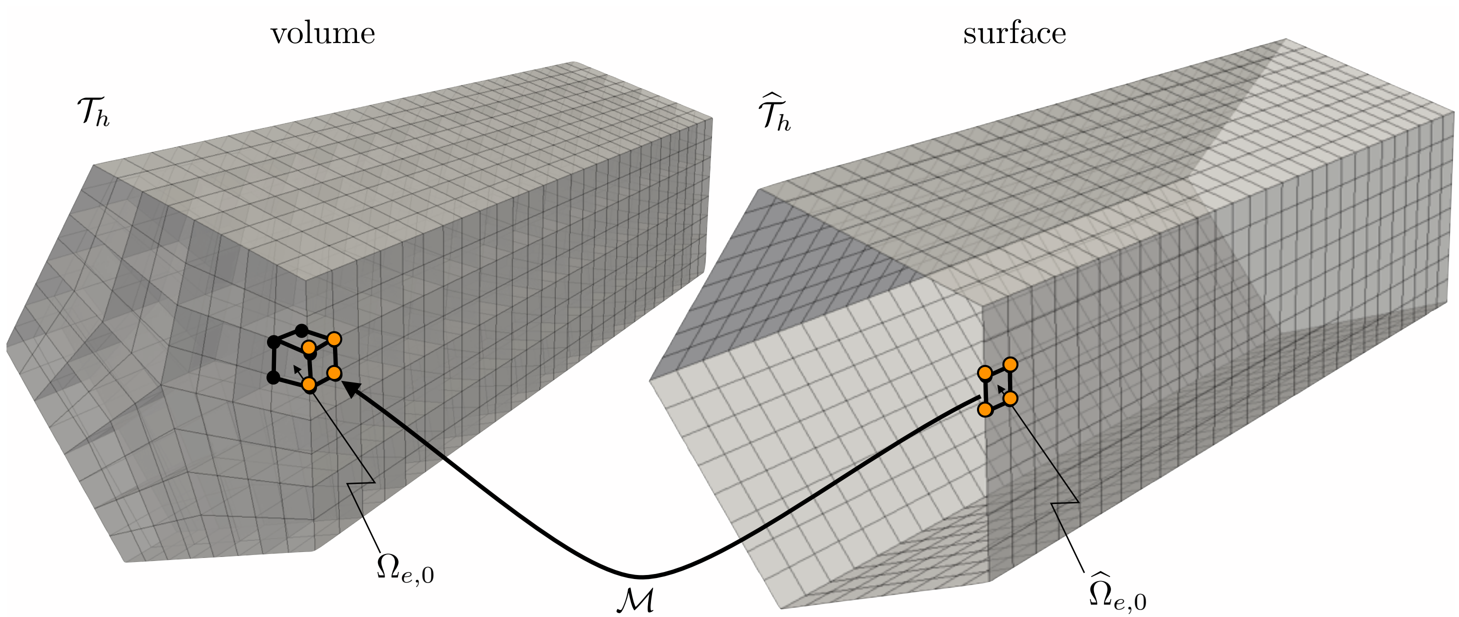
Surface Piola stress $\quad \widehat{\boldsymbol{P}}(\widehat{\boldsymbol{F}}) = \dfrac{\partial \widehat{\Psi}}{\partial \widehat{\boldsymbol{F}}} = \widehat{\lambda} \ln \widehat{J}\, \widehat{\boldsymbol{f}}^{\mathrm{t}} + \widehat{\mu}\,[\widehat{\boldsymbol{F}} - \widehat{\boldsymbol{f}}^{\mathrm{t}}] + \widehat{\gamma}\,\widehat{J}\,\widehat{\boldsymbol{f}}^{\mathrm{t}}$





Numerical Implementation

- manifolds: set of routines to compute on lower-dimensional manifolds (surface) embedded in higher-dimensional space
- independent volume and surface meshes, dof linked via map
- coherent surface: surface dof are not independent
- large portions of user code parallelized (shared) using TBB
- Newton-Raphson strategy with exact tangent computation
- Q1 elements in volume and on surface



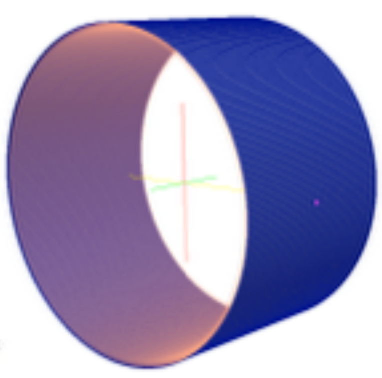
Example Problem: Surface Tension

- Membrane with surface tension acting in material configuration
- Volume with vanishing strength
- Incrementally increase surface tension

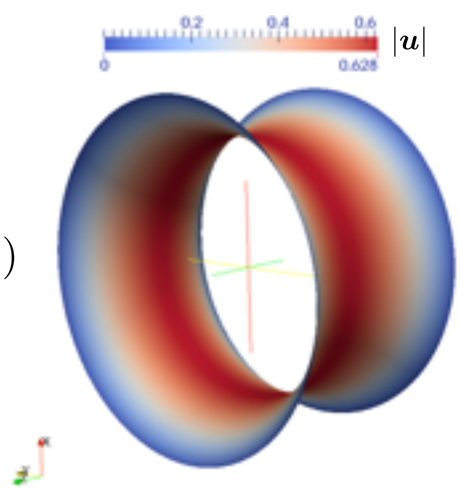
$$\Psi(\boldsymbol{F}) = \cancel{\tfrac{1}{2}\lambda \ln^2 J} + \tfrac{1}{2}\mu\,[\boldsymbol{F} : \boldsymbol{F} - 3 - 2\ln J]$$

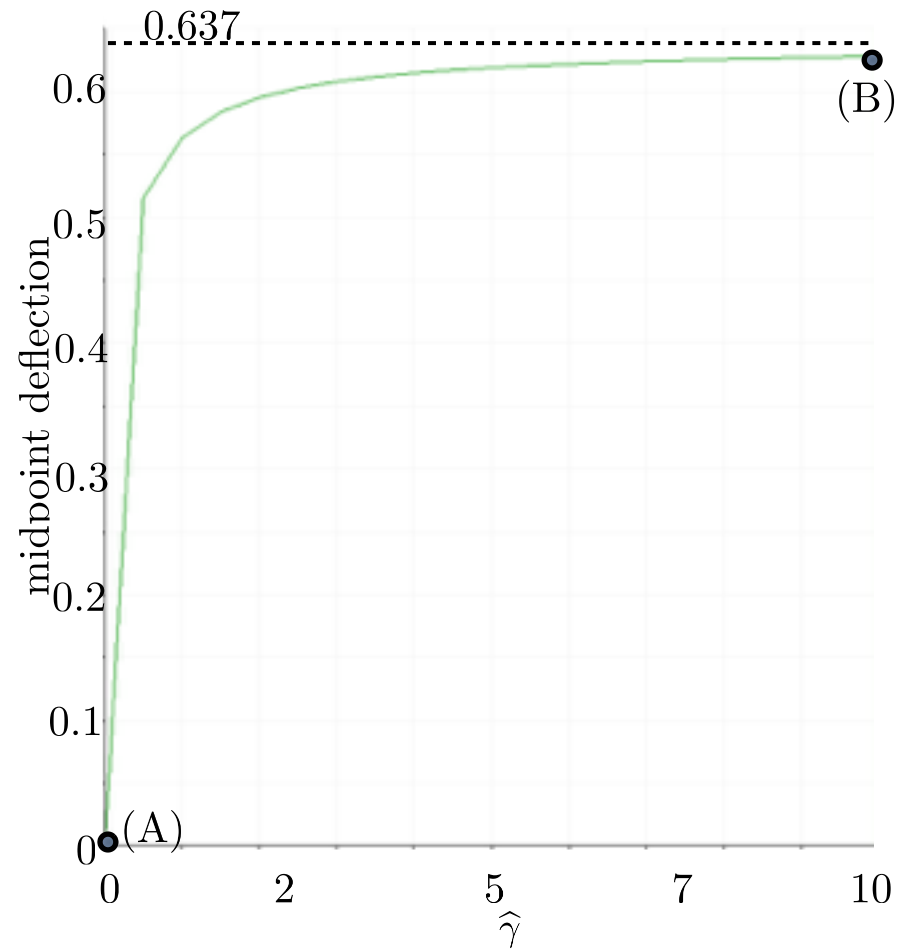
$$\widehat{\Psi}(\widehat{\boldsymbol{F}}) = \cancel{\tfrac{1}{2}\widehat{\lambda}\ln^2 \widehat{J}} + \tfrac{1}{2}\widehat{\mu}\cancel{[\widehat{\boldsymbol{F}} : \widehat{\boldsymbol{F}} - 2 - 2\ln \widehat{J}]} + \widehat{\gamma}\,\widehat{J}$$

(A)



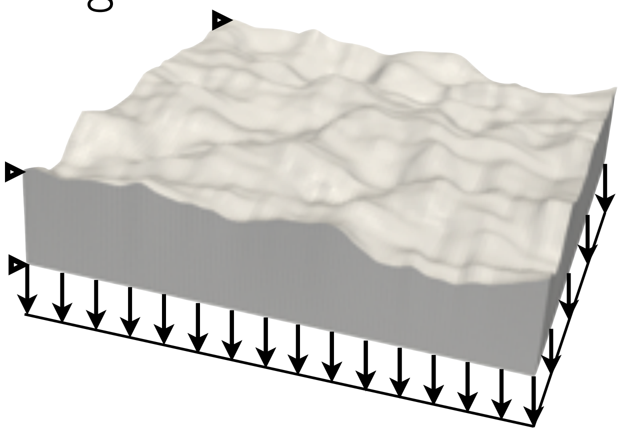
(B)

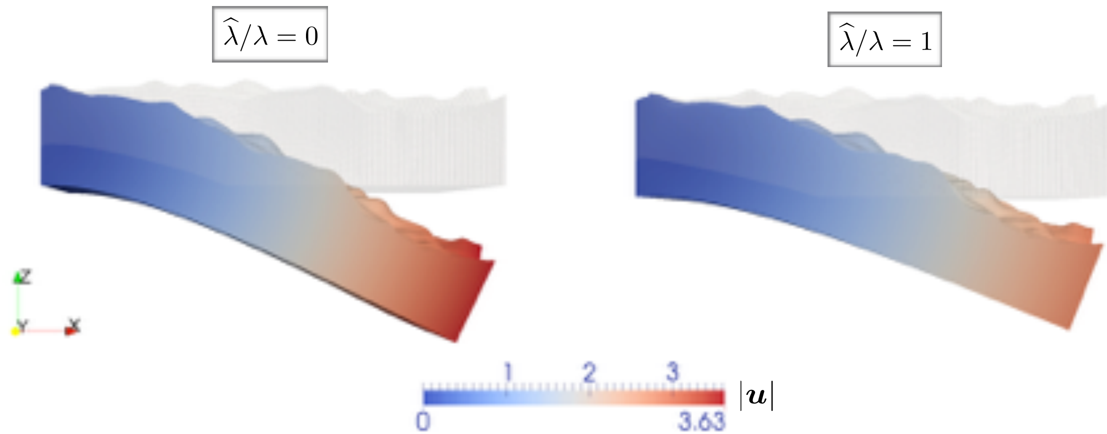




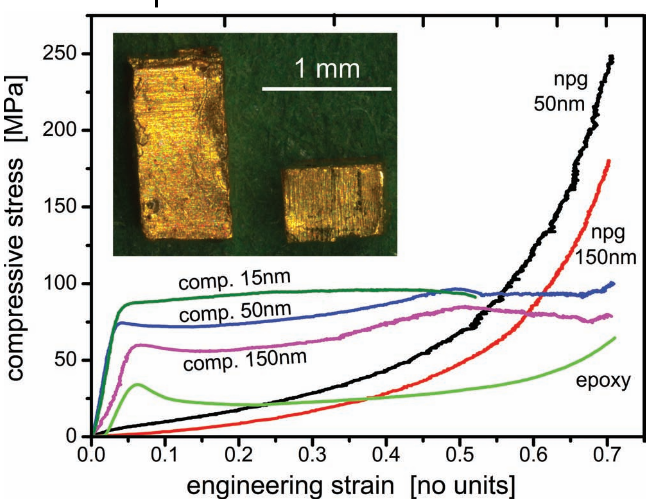
Example problem: Small Structures

rough surfaces:

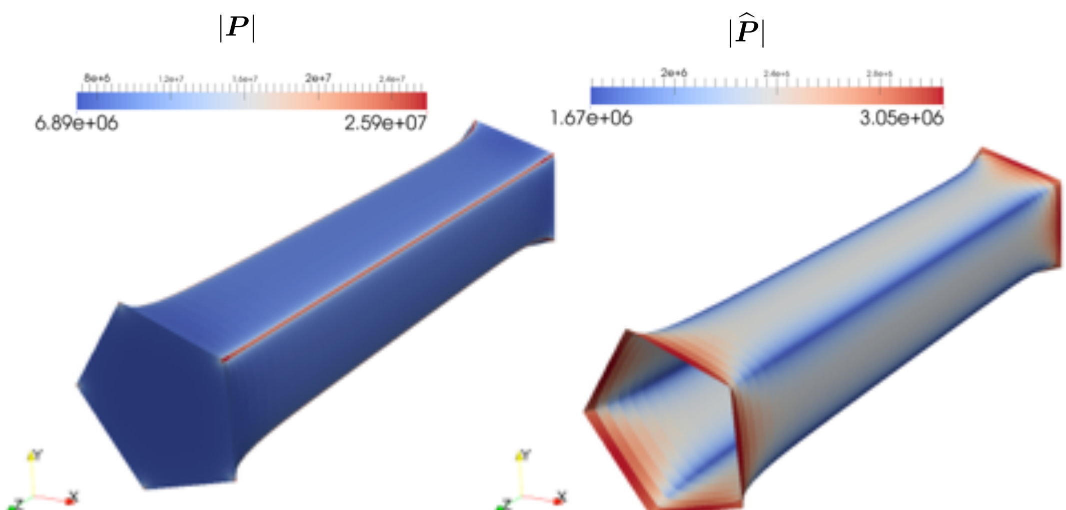




Interface elasticity in polymer-filled nanoporous metals



nano-wires:



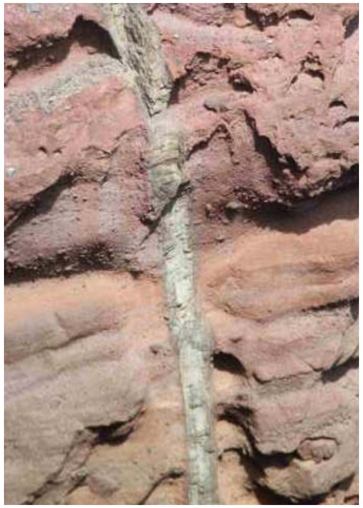
❖ Bargmann, Wilners (TUHH, Helmholtz Geesthacht)

HETEROGENEOUS MATERIAL LAYERS

Objectives:

- Describe material layers within a continuum
  - adhesive bonding, laminated composites, geomaterials, masonry structures, etc.
- Layer has distinct material properties and heterogeneous microstructure
- dictate the overall response of the continuum

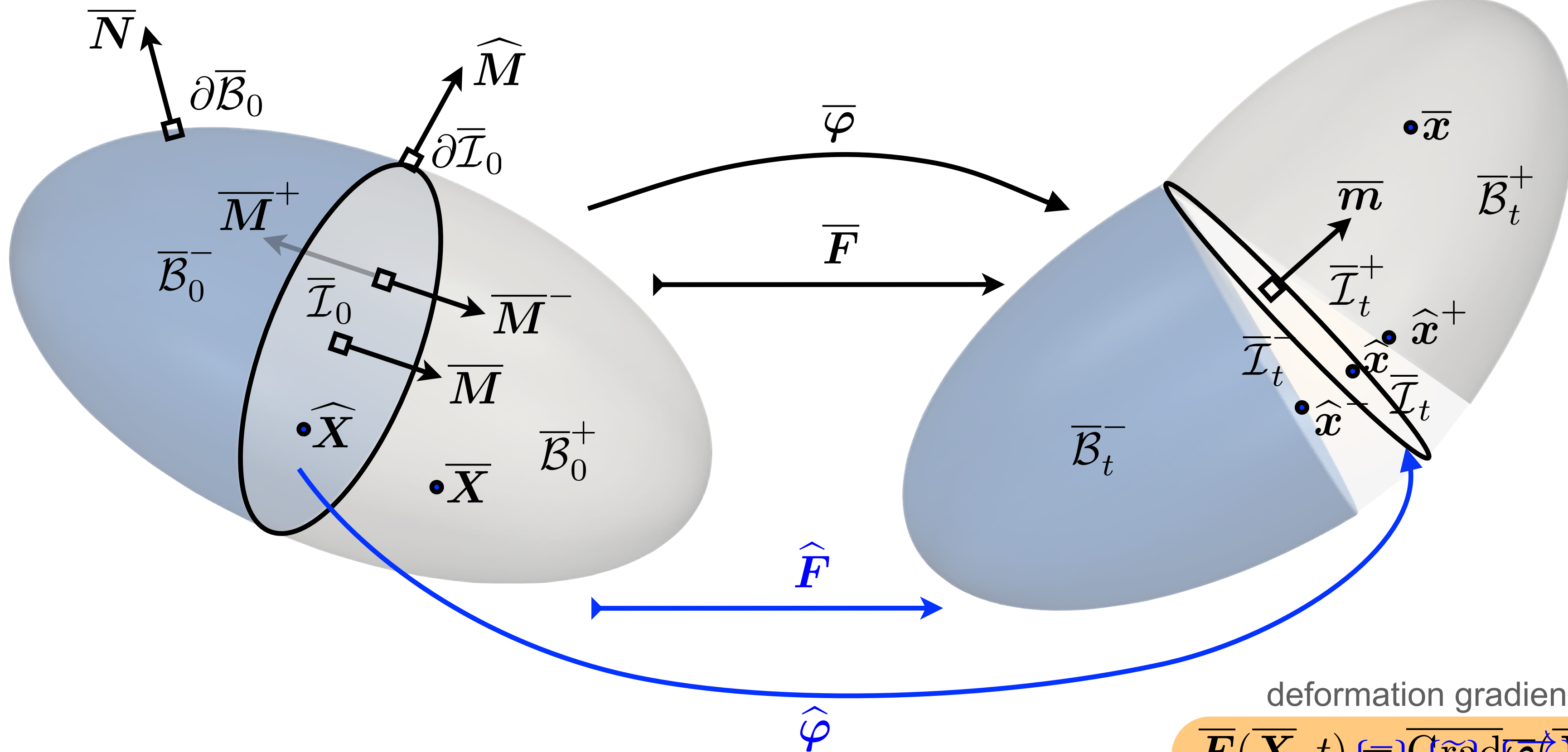
- To determine the constitutive response of the layer using computational homogenisation
  - accounting for in-plane deformation of layer



layer in geological material
HIRSCHBERGER ET AL (2009)

❖ MCB, MERGHEIM, JAVILI, STEINMANN, BARGMANN (2012), JMPS

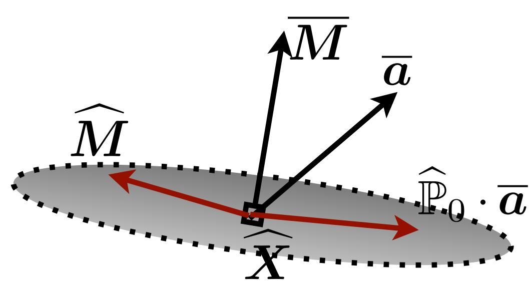
Kinematics of Material Layers



projection and surface gradient

$$\widehat{\boldsymbol{I}} = \widehat{\mathbb{P}}_0 = \overline{\boldsymbol{I}} - \overline{\boldsymbol{M}} \otimes \overline{\boldsymbol{M}}$$

$$\widehat{\mathrm{Grad}}\,\{\widehat{\bullet}\} := \overline{\mathrm{Grad}}\,\{\widehat{\bullet}\} \cdot \widehat{\boldsymbol{I}}$$



deformation gradients

$$\overline{\boldsymbol{F}}(\overline{\boldsymbol{X}}, t) := \overline{\mathrm{Grad}}\,\overline{\boldsymbol{\varphi}}(\overline{\boldsymbol{X}}, t)$$

$$\widehat{\boldsymbol{F}} := \widehat{\mathrm{Grad}}\,\widehat{\boldsymbol{\varphi}}(\widehat{\boldsymbol{X}}, t)$$

overbar : macro

otherwise

micro

$\{\bullet\}$

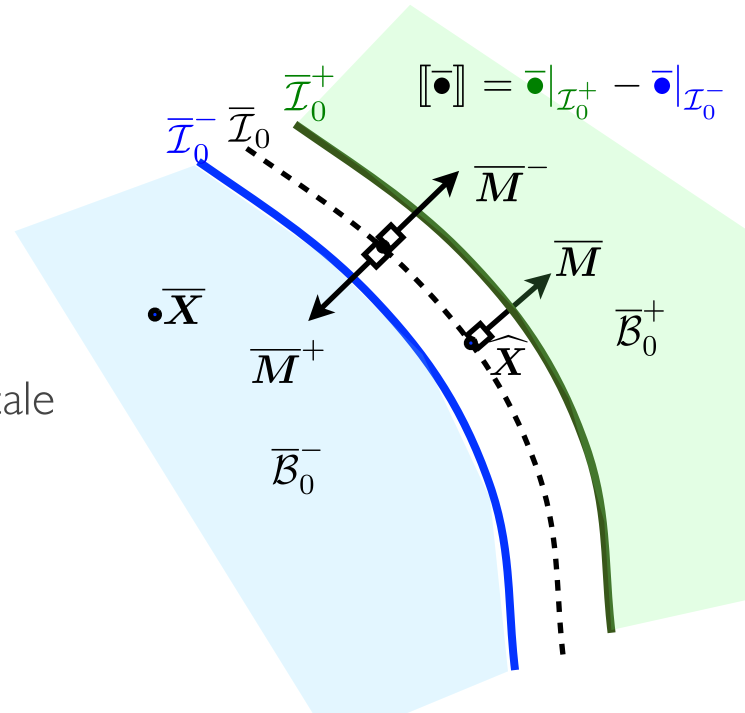
Homogenisation

- Standard approach
  - constitutive traction separation law*

$[\![\overline{\varphi}]\!] \rightarrow$ **constitutive law** $\rightarrow \widetilde{\boldsymbol{t}}_0$

- Approach of Hirschberger et al (2009)
  - constitutive traction separation law replaced by micro-scale simulation to capture heterogeneities

$[\![\overline{\varphi}]\!] \rightarrow$ **microscale** $\rightarrow \widetilde{\boldsymbol{t}}_0$

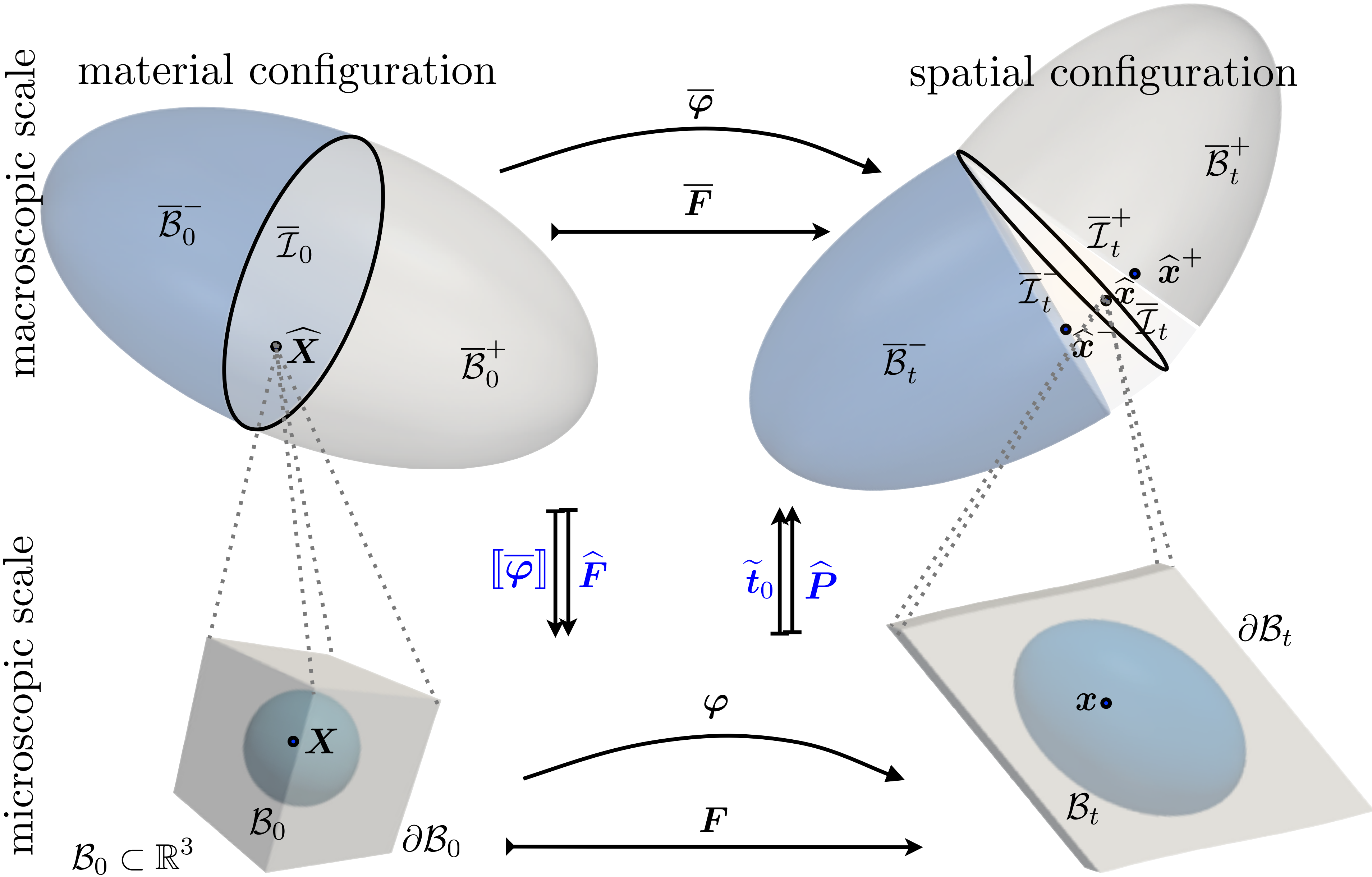


- extend above using interface theory of Gurtin & Murdoch (1975)
  - interface has own energetic structures (Helmholtz energy): $\widehat{\boldsymbol{P}} = 2\widehat{\boldsymbol{F}} \cdot \partial_{\widehat{\boldsymbol{C}}} \widehat{\psi}_0$
  - account for in-plane deformation

$[\![\overline{\varphi}]\!]$, $\widehat{\boldsymbol{F}} \rightarrow$ **microscale** $\rightarrow \widetilde{\boldsymbol{t}}_0$, $\widehat{\boldsymbol{P}}$

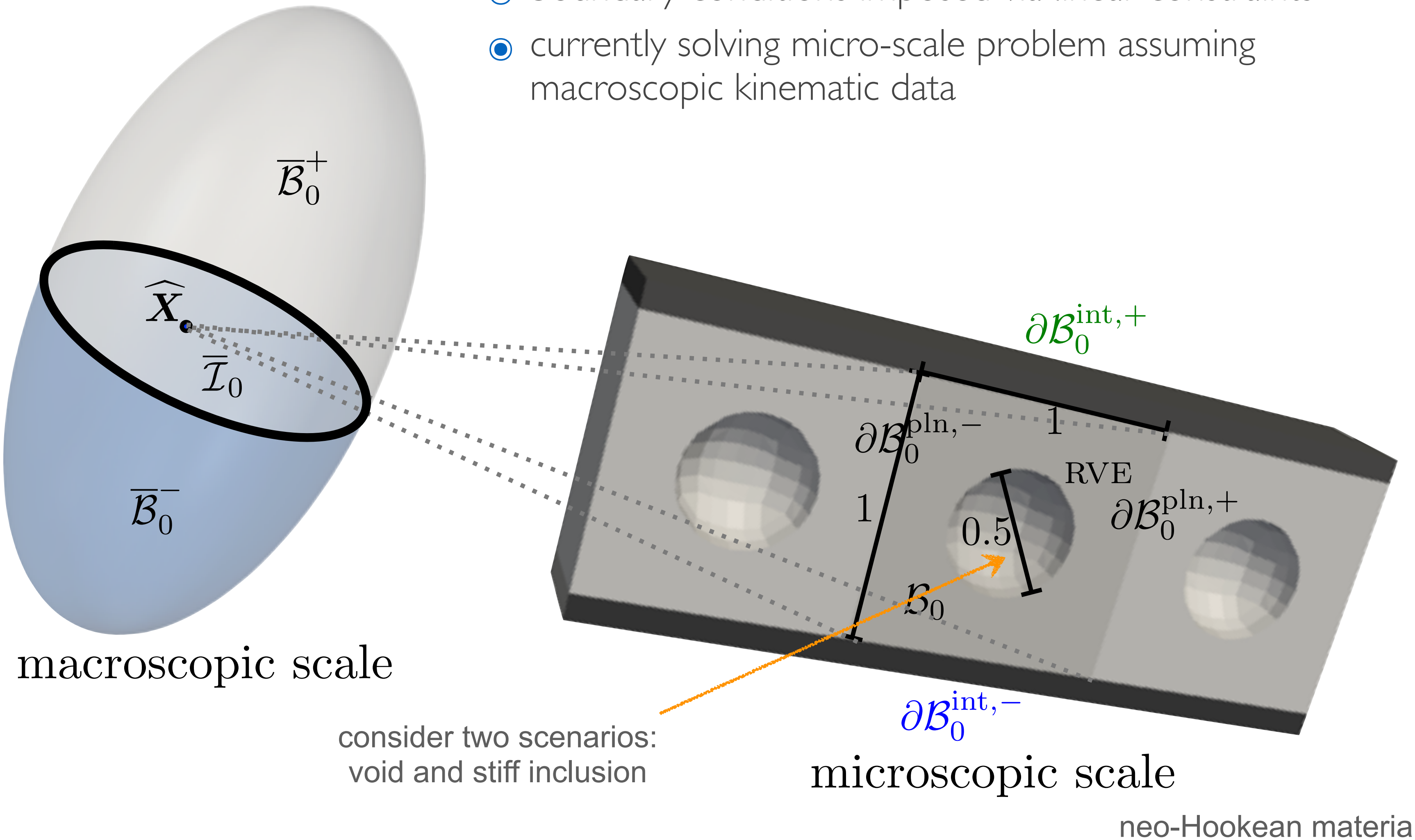
*see e.g. Needleman et al (1987,1993), Mosler & Scheider (2011)

Micro-to-Macro Transitions

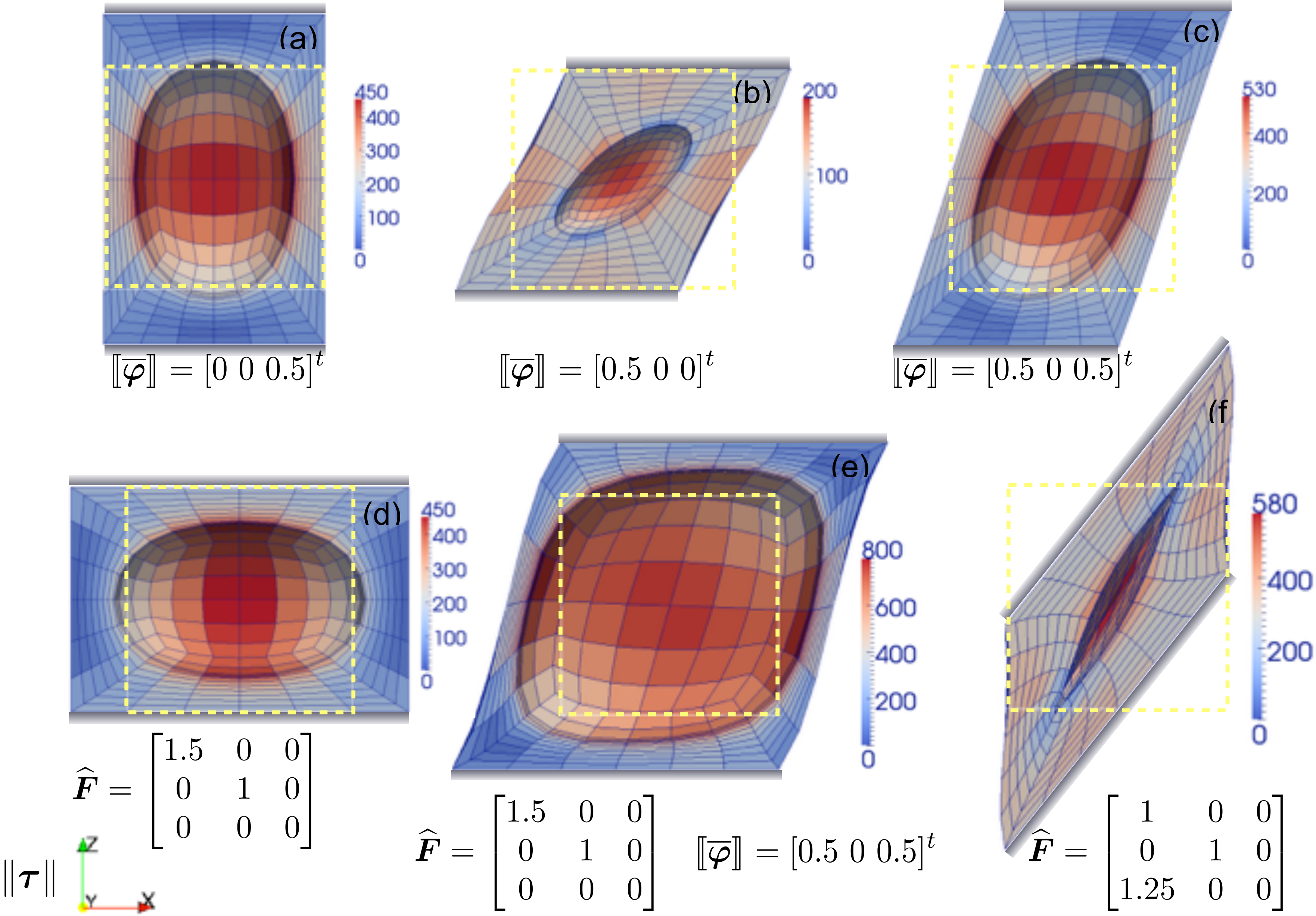


Example Problem

- boundary conditions imposed via linear constraints
- currently solving micro-scale problem assuming macroscopic kinematic data



Numerical Results



(a) $[\![\overline{\varphi}]\!] = [0\ 0\ 0.5]^t$

(b) $[\![\overline{\varphi}]\!] = [0.5\ 0\ 0]^t$

(c) $[\![\overline{\varphi}]\!] = [0.5\ 0\ 0.5]^t$

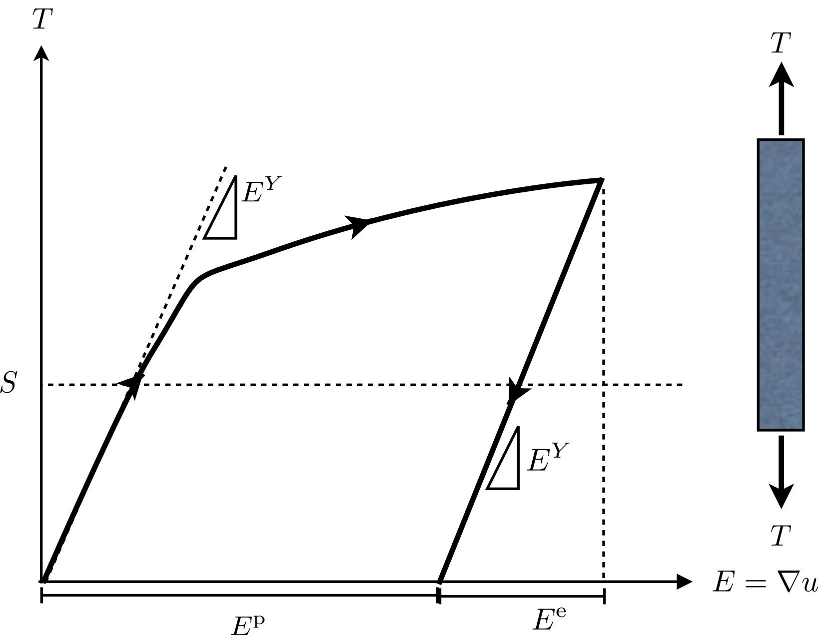
(d) $$\widehat{\boldsymbol{F}} = \begin{bmatrix} 1.5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

(e) $$\widehat{\boldsymbol{F}} = \begin{bmatrix} 1.5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad [\![\overline{\varphi}]\!] = [0.5\ 0\ 0.5]^t$$

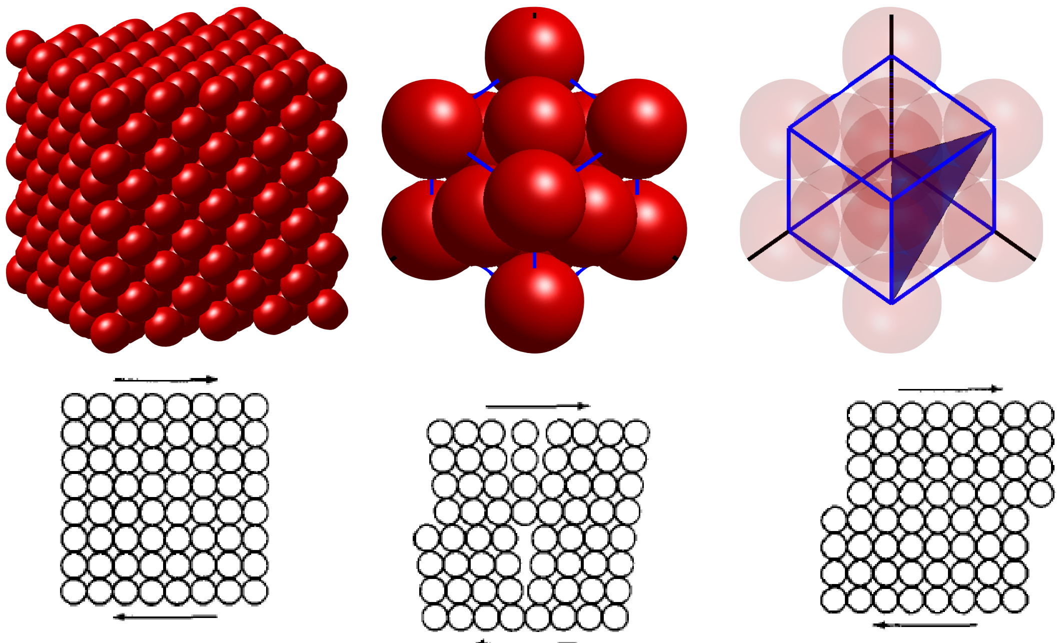
(f) $$\widehat{\boldsymbol{F}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1.25 & 0 & 0 \end{bmatrix}$$

$\|\boldsymbol{\tau}\|$

Single Crystal Plasticity



$\boxed{E = E^{\mathrm{e}} + E^{\mathrm{p}}}$

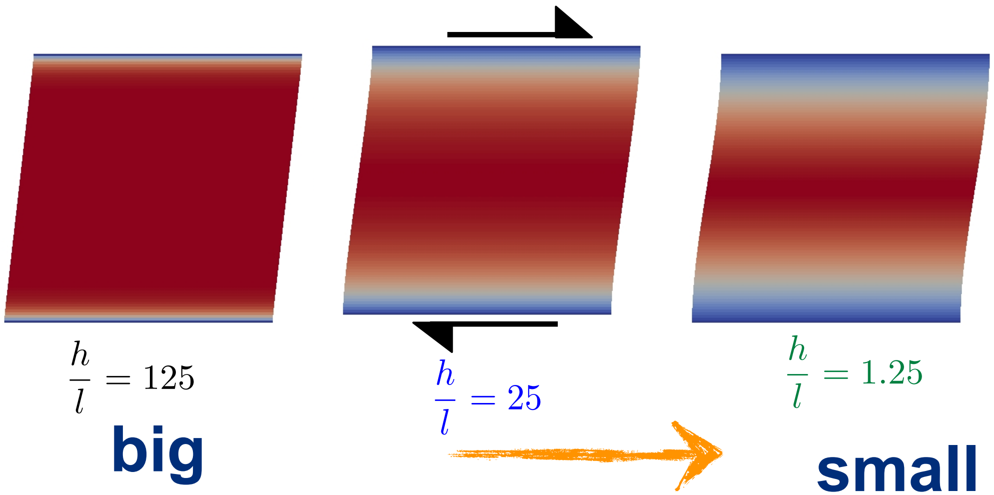


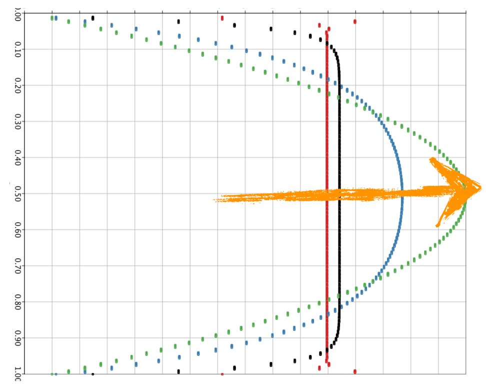
$$\tau^\alpha = \bar{\mathbf{s}}^\alpha \cdot \boldsymbol{\sigma}\bar{\mathbf{m}}^\alpha$$

- Richardson (2012), MSc
- Povall (2013), MSc
- Povall, McB, Reddy (2014), Comp Mat Sci

Gradient Single Crystal Plasticity

- Classical model of plasticity lack an inherent length scale:
  - cannot capture experimentally observed size effects: smaller is stronger

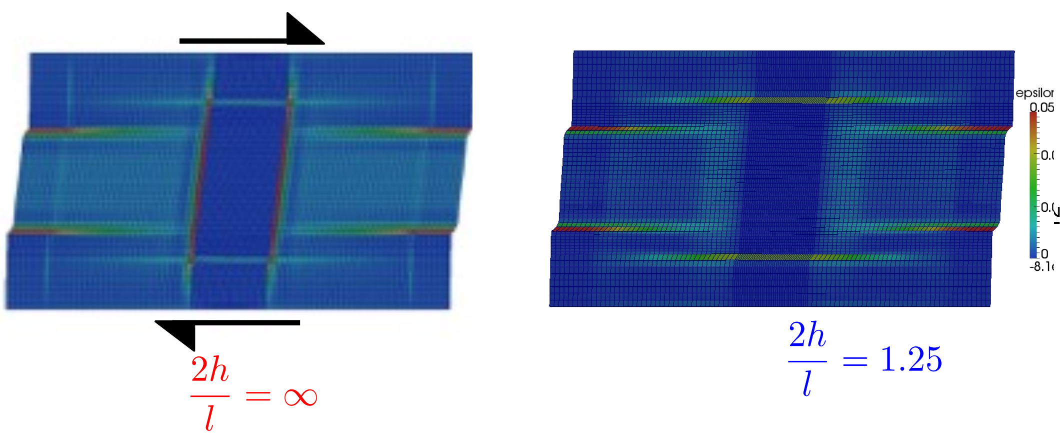


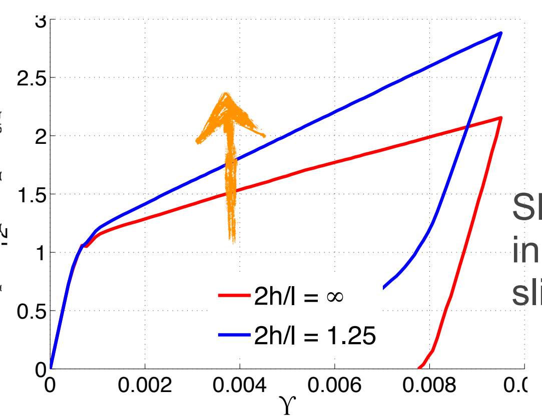


Constrained shear. Double slip system

1

Joint work with Daya Reddy and Morton Gurtin

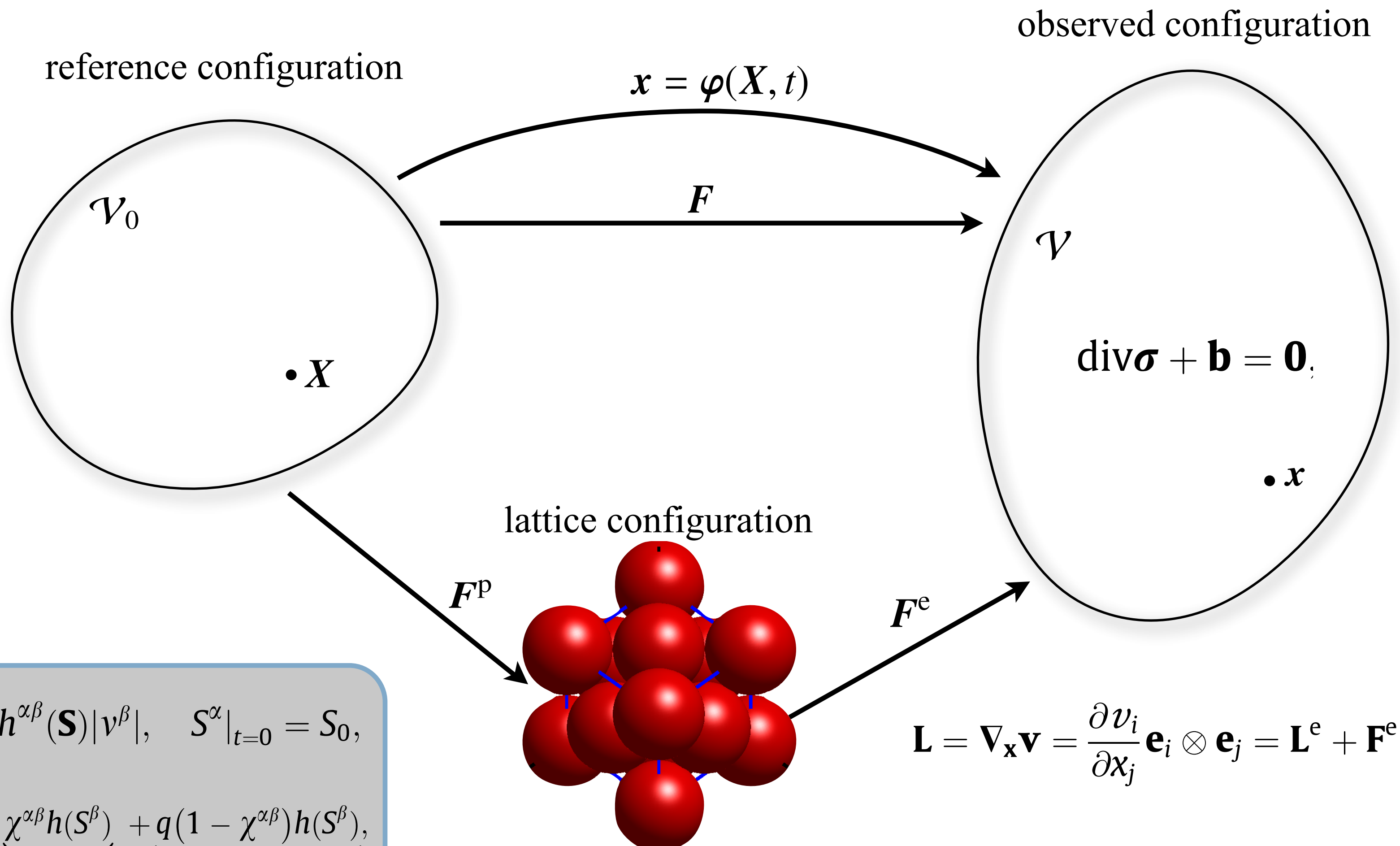




Shear with elastic inclusions. Double slip system

2

Single Crystal Plasticity: Hardening Relations



$$\mathbf{L} = \nabla_{\mathbf{x}}\mathbf{v} = \frac{\partial v_i}{\partial x_j}\mathbf{e}_i \otimes \mathbf{e}_j = \mathbf{L}^{\mathrm{e}} + \mathbf{F}^{\mathrm{e}}\mathbf{L}^{\mathrm{p}}\mathbf{F}^{\mathrm{e}-1},$$

$$\dot{S}^\alpha = \sum_\beta h^{\alpha\beta}(\mathbf{S})|\nu^\beta|, \quad S^\alpha|_{t=0} = S_0,$$

$$h^{\alpha\beta}(S^\beta) = \underbrace{\chi^{\alpha\beta}h(S^\beta)}_{\text{self hardening}} + \underbrace{q(1-\chi^{\alpha\beta})h(S^\beta)}_{\text{latent hardening}},$$

$$\mathbf{L}^{\mathrm{p}} = \sum_\alpha \nu^\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha.$$

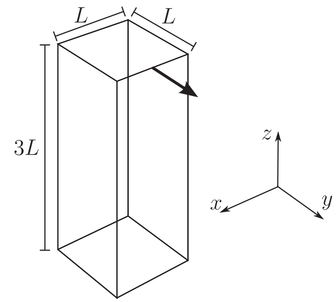
$$\phi^\alpha(\tau^\alpha, S^\alpha) = |\tau^\alpha| - S^\alpha \leqslant 0.$$

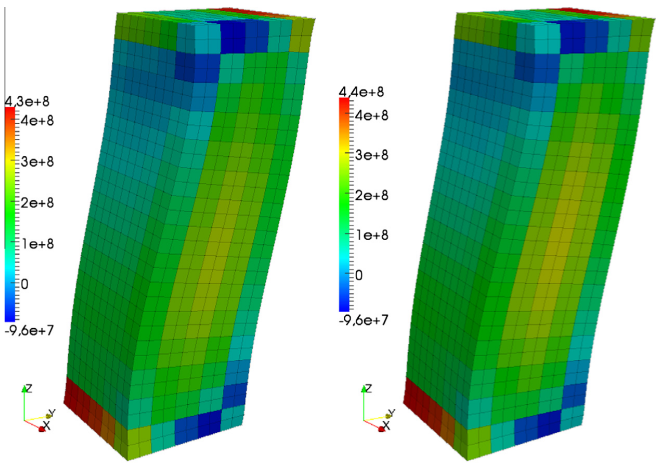
$$\lambda^\alpha \geqslant 0, \quad \phi^\alpha(\tau^\alpha, S^\alpha) \leqslant 0 \quad \text{and} \quad \lambda^\alpha\phi^\alpha(\tau^\alpha, S^\alpha) = 0.$$

Single Crystal Plasticity: Hardening Relations

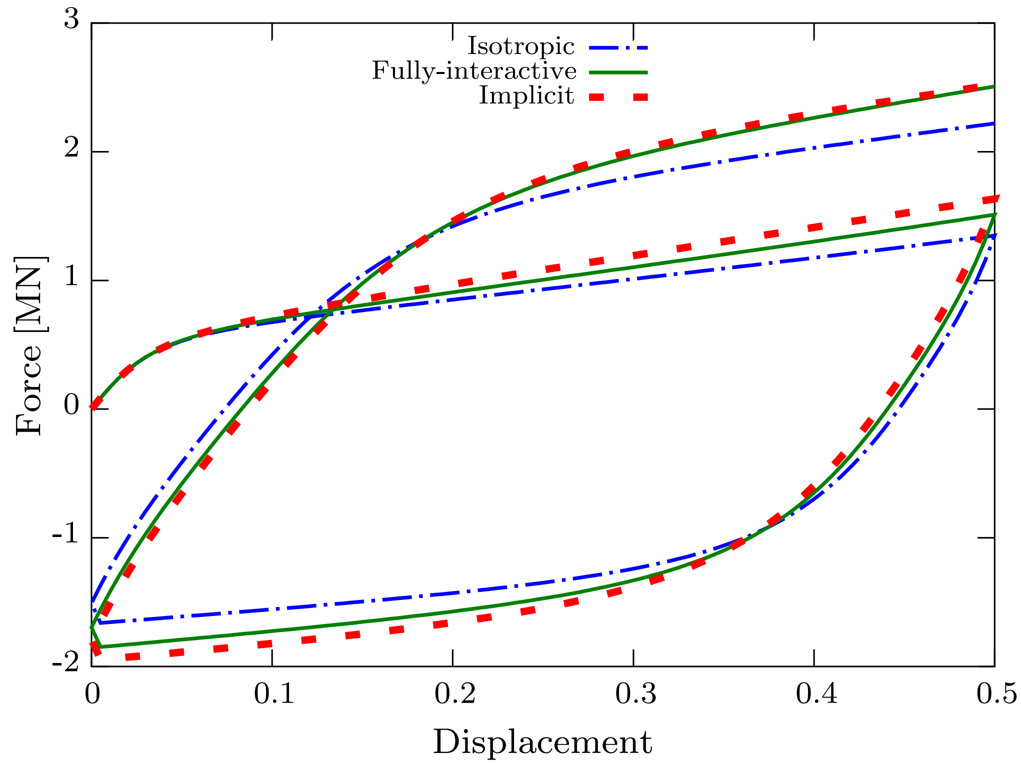
- Highly nonlinear problem
  - irreversible plasticity and nonlinear hardening
  - geometric and constitutive nonlinearities
  - incompressible plastic deformation
  - rate dependency to regularise the problem
- Solved using a predictor-corrector algorithm
  - inner Newton scheme at each quadrature point to compute slip and hardening (2x12 for FCC crystal)
  - exponential approximation for plastic deformation gradient evolution
  - fixed-point algorithm used for initial guess for implicit hardening
- Multithreaded using TBB
- Would be nice to extend to allow for adaptivity…projection qp data

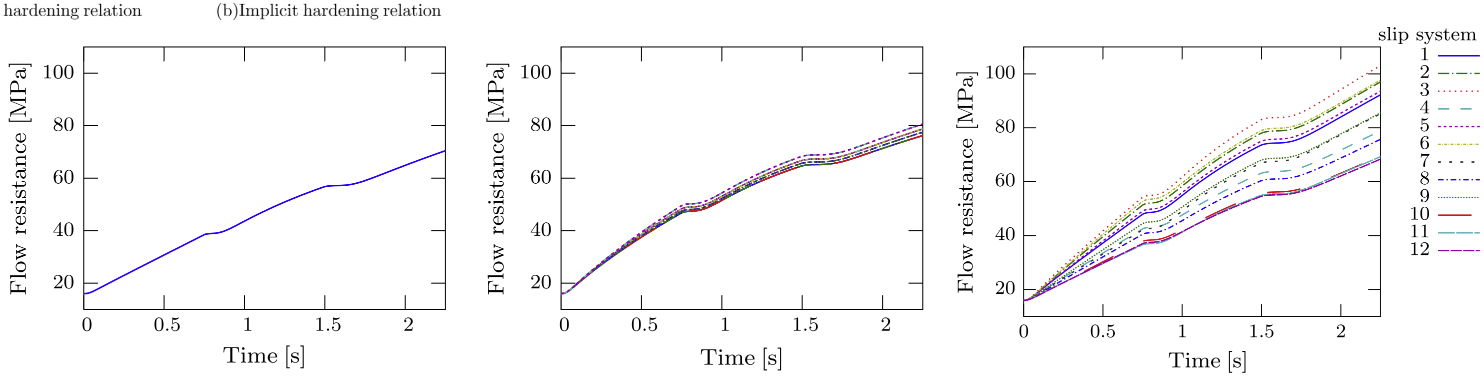
Single Crystal Plasticity: Hardening Relations





(a) Fully-interactive hardening relation (b)Implicit hardening relation

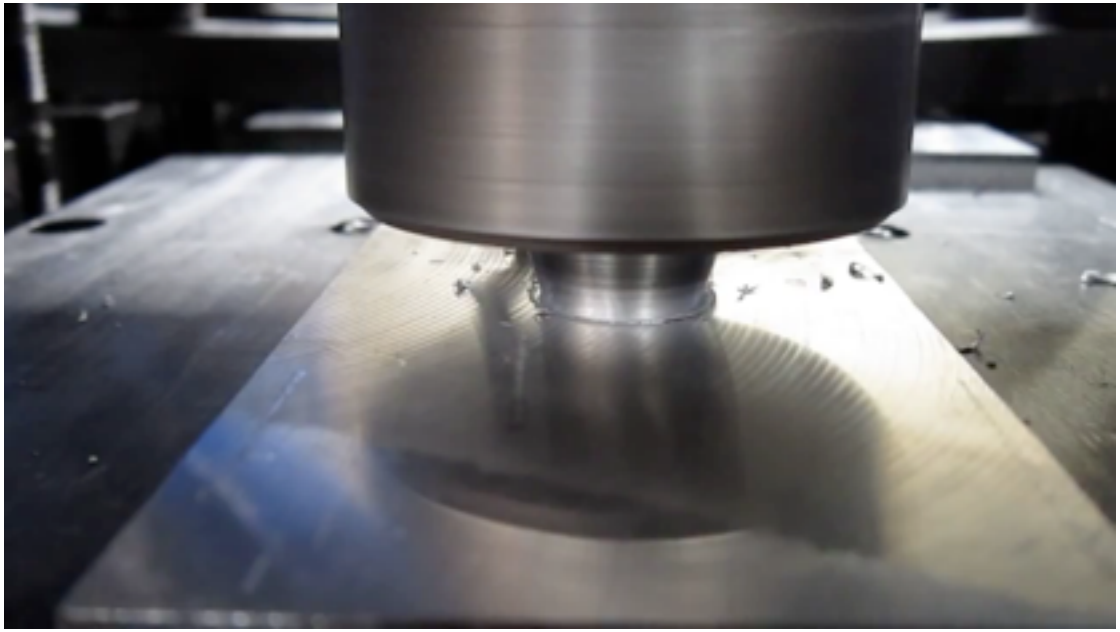




(a) Isotropic hardening relation (b) Implicit hardening relation (c) Fully-interactive hardening relation

FRICTION WELDING AND PROCESSING

- A family of solid state joining processes that rely on friction for heat generation
- A region of plasticised material is formed at the interface between the workpieces
- Forge force is maintained as the workpieces cool back down



❖ M Hamed (current) PhD (an attendee of the deal.II workshop in Cape Town)

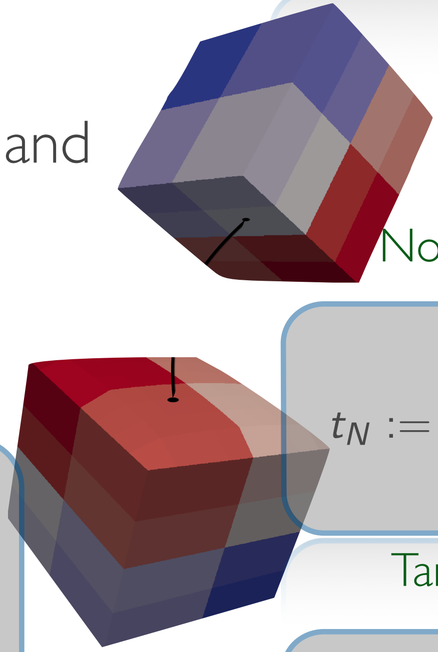
Mathematical Modelling of Friction Welding

- Coupled thermo-viscoplasticity
- Finite deformations:
  - Lagrangian-Eulerian-like nature to the process
- Thermomechanical multi-body friction and contact
- Microstructural texture evolution and grain growth

Balance linear momentum and energy

$$J \operatorname{div} \boldsymbol{\tau} + \rho \mathbf{b} = \rho \dot{\mathbf{v}}$$

$$\rho \dot{\psi} = J \boldsymbol{\tau} : \mathbf{d} - \operatorname{div} \mathbf{q} - \dot{\eta}\theta - \eta\dot{\theta}$$



Normal contact constraints

$$g(\mathbf{x}, \bar{\mathbf{y}}(\mathbf{x})) \leq 0$$

$$t_N := -\mathbf{n}(\bar{\mathbf{y}}(\mathbf{x})) \cdot \boldsymbol{\sigma}\, \mathbf{n}(\bar{\mathbf{y}}(\mathbf{x})) \geq 0$$

$$t_N\, g(\mathbf{x}, \bar{\mathbf{y}}(\mathbf{x})) = 0$$

Thermoplasticity

$$\boldsymbol{\tau} = pJ\mathbf{1} + \operatorname{dev}[\boldsymbol{\tau}]$$

$$\Phi = \|\operatorname{dev}[\boldsymbol{\tau}]\| - \sqrt{\frac{2}{3}}[K'(\alpha_n) + \hat{y}(\theta)] \leq 0$$

$$\lambda \geq 0 \quad , \quad \lambda\Phi = 0$$

Tangential contact constraints

$$h(\mathbf{x}, \bar{\mathbf{y}}(\mathbf{x})) := \|\mathbf{t}_T\| - \mu t_N \leq 0$$

$$\xi \geq 0$$

$$\xi h(\mathbf{x}, \bar{\mathbf{y}}(\mathbf{x})) = 0$$

Weak form and Implementation

Balance linear momentum and contact

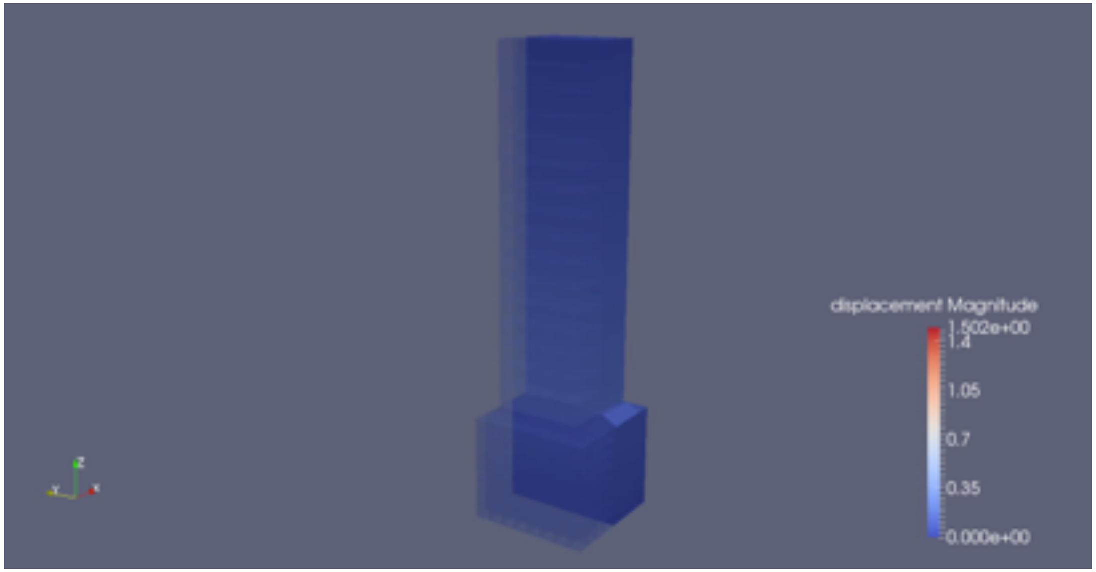
$$\int_\Omega \left\{ \operatorname{div} \overset{*}{\mathbf{u}} \bar{p} J + \nabla \overset{*}{\mathbf{u}} \cdot \operatorname{dev}[\boldsymbol{\tau}] \right\} \mathrm{d}\Omega - \left\{ \int_\Omega \overset{*}{\mathbf{u}} \cdot \mathbf{f} \mathrm{d}\Omega + \int_\Gamma \overset{*}{\mathbf{u}} \cdot \mathbf{t} \mathrm{d}\Gamma \right\} + \left\{ \int_\Gamma \overset{*}{g}\, t_N \mathrm{d}\Gamma \right\} = 0$$

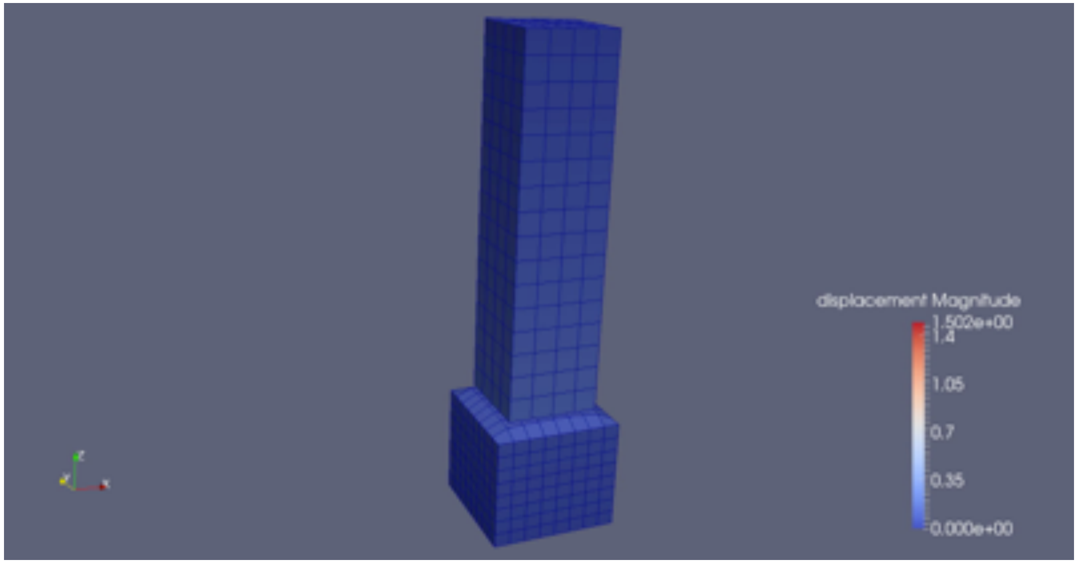
Balance energy

$$\int_\Omega \left\{ \overset{*}{\theta} \left[c\dot{\theta} - \mathcal{D}_{mech} + \bar{\mathcal{H}} \right] + \nabla \overset{*}{\theta} \cdot \mathbf{q} \right\} \mathrm{d}\Omega - \left\{ \int_\Omega \overset{*}{\theta} \bar{\mathcal{R}} \mathrm{d}\Omega + \int_\Gamma \overset{*}{\theta} \left[-\mathcal{S} \right] \mathrm{d}\Gamma \right\} = 0$$

- Distinct kinematics from constitute relations
- Parallel aware contact search
- Linearisation of the contact term requires the gradient of the Hessian….
  - work in progress

Contact with Plasticity and Heat Transfer





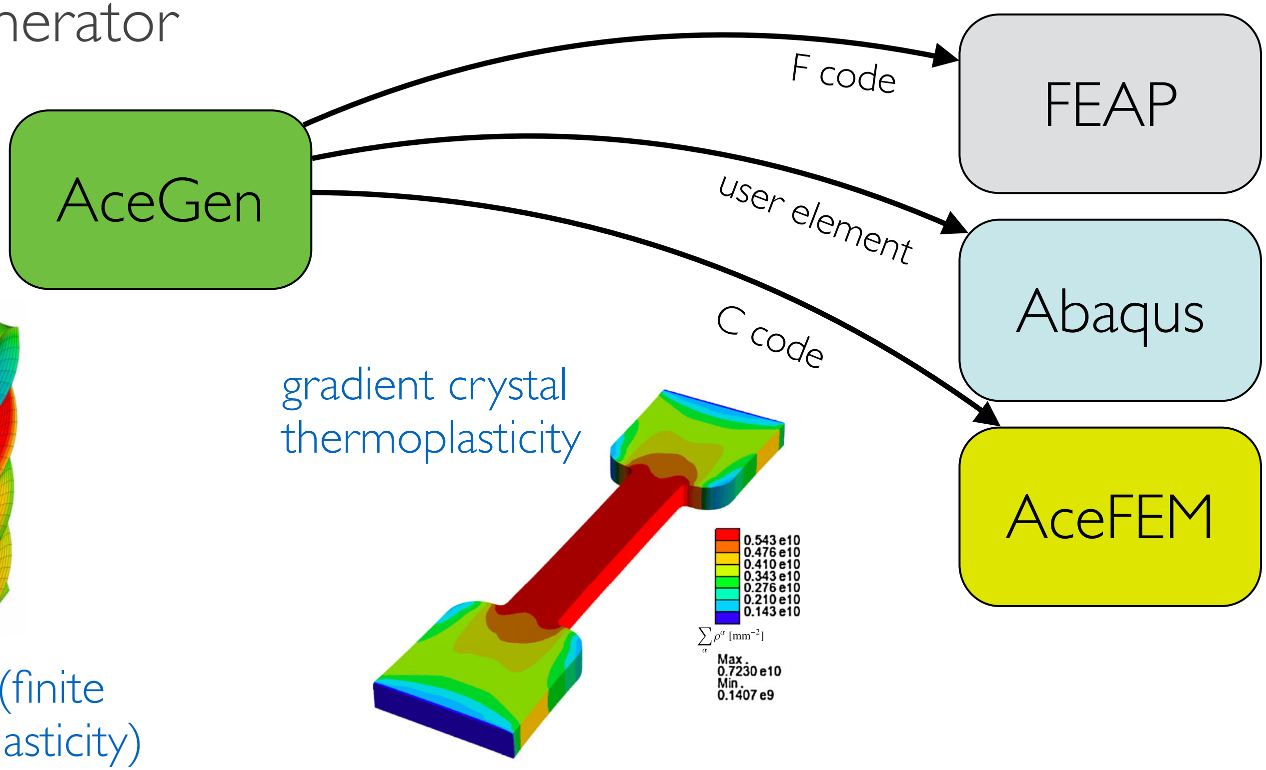
Some Observations

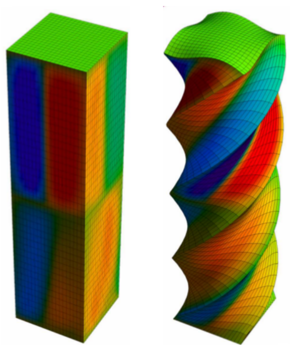
Vast majority of problems in nonlinear solid mechanics involve:

- complex material response:
  - elasticity, viscoelasticity, plasticity, coupled-problems etc
  - linearisation of the constitutive relations is arduous and error prone
  - an error in the residual often independent to another error in the tangent
  - handling of internal variables (stored at quadrature points, for example)
- relatively standard element choices
- robust nonlinear Newton scheme for monolithic equation system
  - fully-implicit or semi-implicit scheme
  - exact tangent often required
  - line-search, time-step or load control critical
- spatial adaptivity often critical
  - e.g. phase field models for fracture (see e.g. Heister, Wheeler, Wick (2015), CMAME)

Automatic Differentiation Tools

- Been involved in some projects recently that use Mathematica-based FE code generator





grain boundaries (finite gradient crystal plasticity)

❖ Gottschalk (2015) PhD (Hannover)

gradient crystal thermoplasticity

❖ McB, Bargmann, Reddy (2015), Comp Mech

- Similar functionality exists via Sacado (AD) coupled to NOX (Nonlinear solver) in Trilinos: detailed, focussed tutorial missing…I (we) would like to add one

Thank You

- special thanks to all developers and users of deal.II
- open-source libraries of this nature can have a huge impact on science development in emerging and developing countries