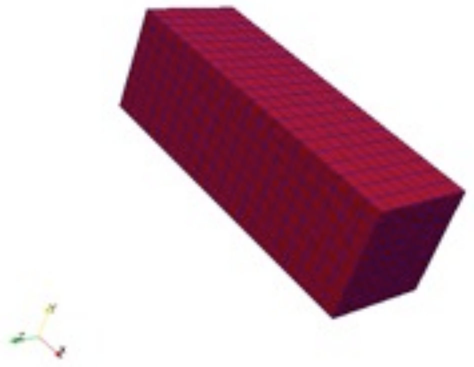
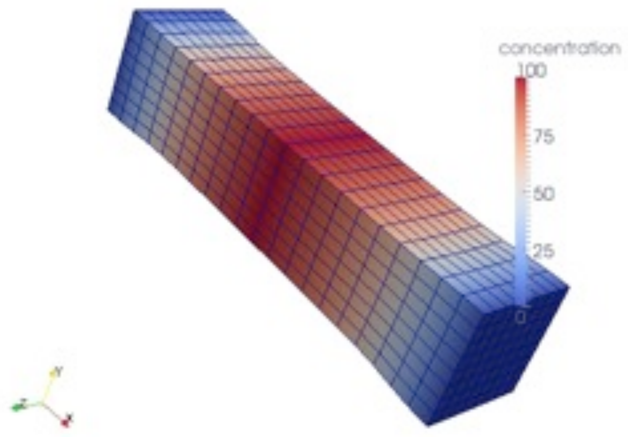
Coupled Problems in Nonlinear Solid Mechanics: Non-Fickian Diffusion

Deal.II Workshop

August 23 - 25 2010
Heidelberg





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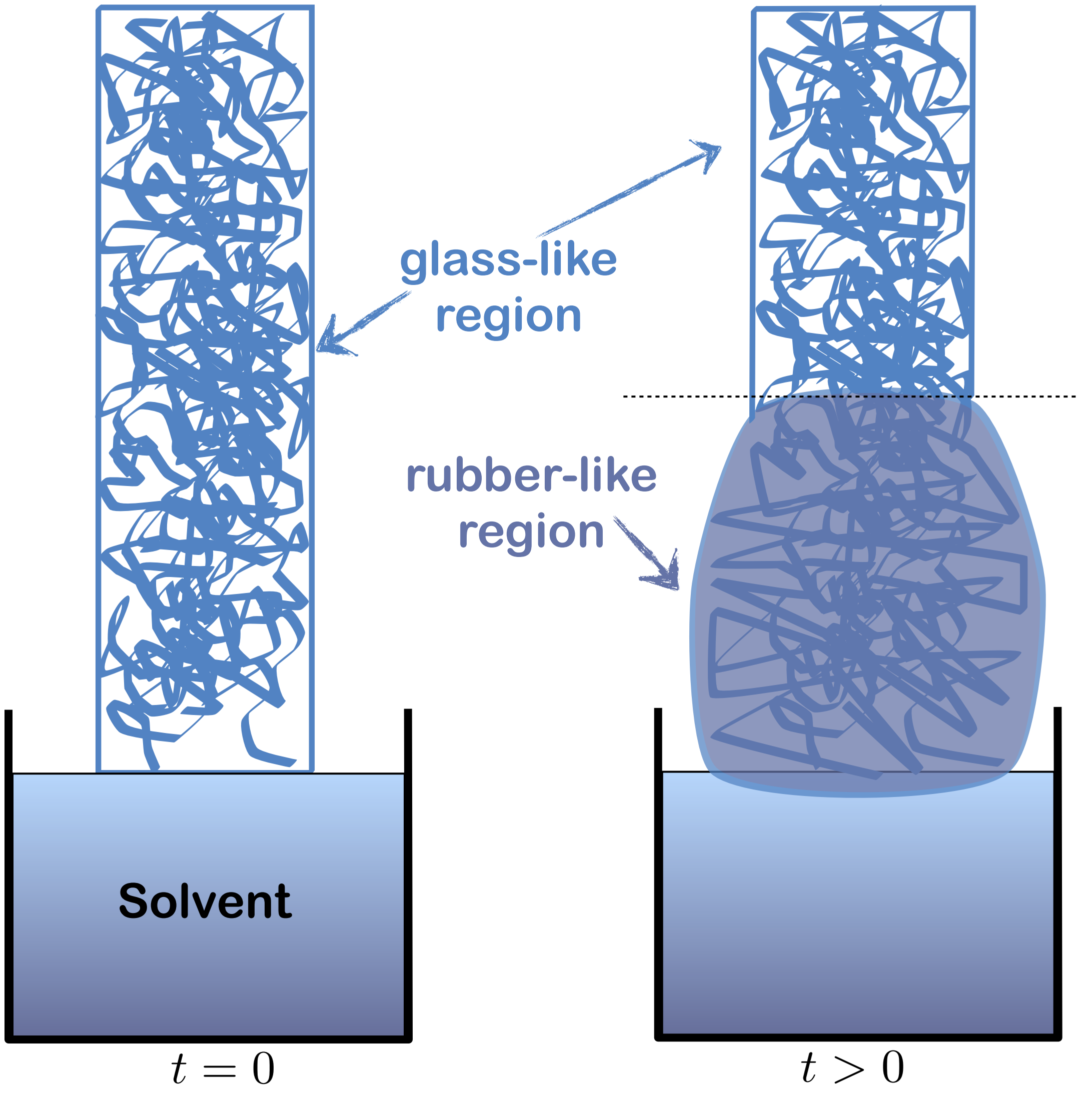
Motivation: Case II diffusion

- Case II diffusion (CII) occurs during diffusion of low molecular weight solvent in polymeric solid
- Solid is originally in a glass-like state
- Solvent wave progresses through polymer at fixed rate (constant velocity)
- Solvent causes polymer change to a rubber-like material
- Highly-coupled non-linear phenomenon
  - Relaxation time of polymer depends on concentration and swelling
  - Solvent exerts a pressure on polymer and visa-vera (swelling and concentration dependent)
  - Diffusivity depends on swelling and concentration
  - Polymer needs finite amount time to rearrange to accommodate solvent limiting diffusion rate
  - Large swelling in rubber-like region
  - Polymer near-incompressible
- See DE KEE ET AL (2005) and VESELY (2008) for reviews



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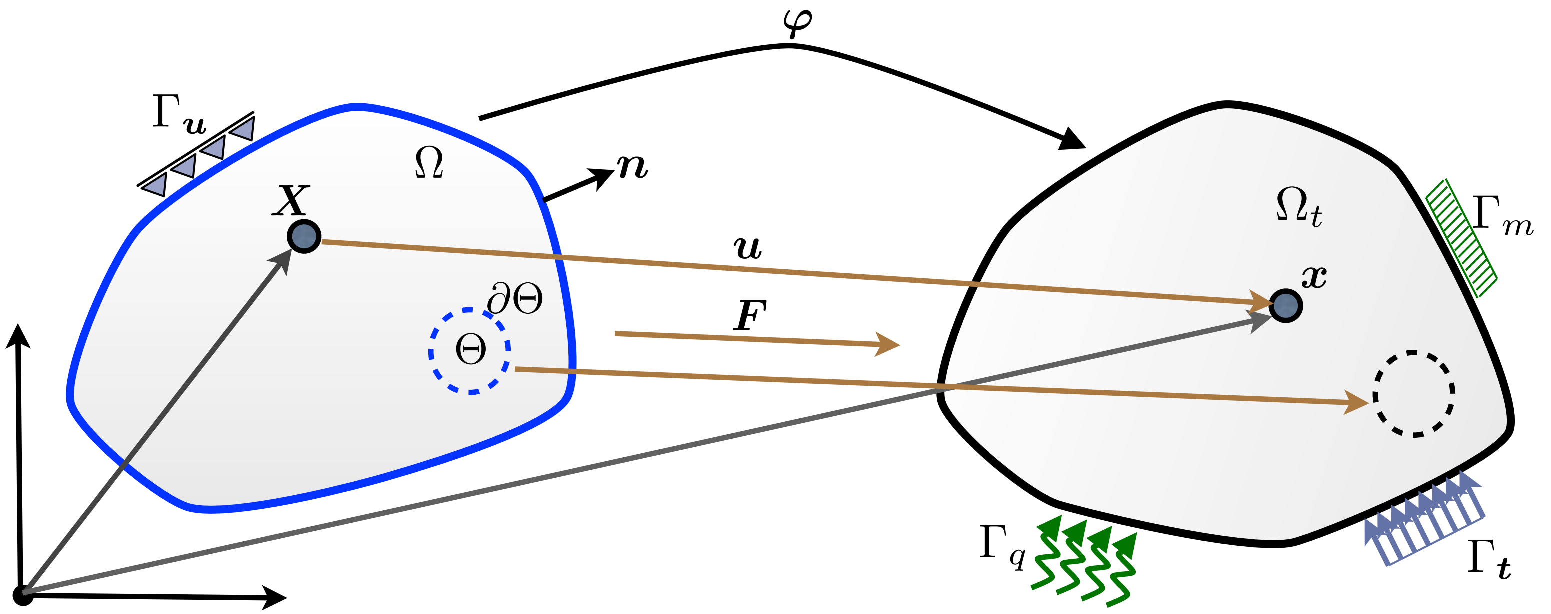
Overview

- Applications based presentation
  - Case II a prototype for highly non-linear coupled problems
- Describe the governing equations
  - Focus on internal variable formulation of viscoelasticity
  - Integration algorithms for internal inelastic variables
- Review models for case II diffusion
  - Strongly coupled diffusion-deformation
- Solution strategies using finite elements
- Consider a reduced model
  - Focus on spatial adaptivity with internal variables in deal.II
- Example problem

Work in progress (does not actually all work yet): comments and suggestions greatly appreciated. Actually, a lot of the questions I ask in the talk have been answered and better strategies proposed. Thanks

Governing equations



$$\Gamma = \Gamma_{\boldsymbol{u}} \cup \Gamma_{\boldsymbol{t}}$$
$$\Gamma_{\boldsymbol{u}} \cap \Gamma_{\boldsymbol{t}} = \emptyset$$
$$\Gamma = \Gamma_m \cup \Gamma_q$$
$$\Gamma_m \cap \Gamma_q = \emptyset$$
$$\bar{\Omega} = \overline{\Omega \cup \Gamma}$$

Kinematics

$$\boldsymbol{\varepsilon}(\boldsymbol{u}) = \frac{1}{2}\left[\nabla \boldsymbol{u} + [\nabla \boldsymbol{u}]^T\right]$$
$$\boldsymbol{F} = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}}$$
$$j = \det(\boldsymbol{F})$$

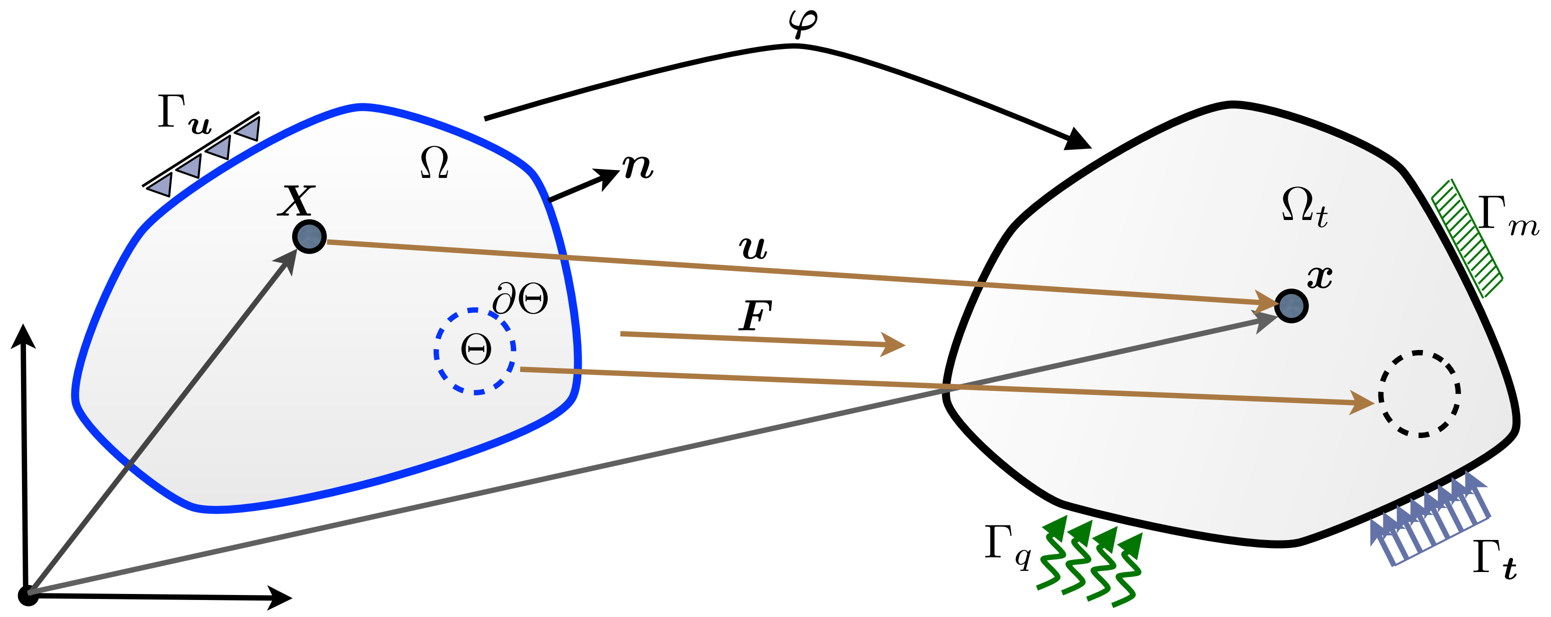
Equilibrium

$$\operatorname{div} \boldsymbol{\sigma} = \boldsymbol{0} \quad \text{in } \Omega$$
$$\boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{on } \Gamma_{\boldsymbol{u}}$$
$$\boldsymbol{t} := \boldsymbol{\sigma} \cdot \boldsymbol{n} = \bar{\boldsymbol{t}} \quad \text{on } \Gamma_{\boldsymbol{t}}$$

Conservation of solvent mass

$$\dot{m} = -\operatorname{div} \boldsymbol{h} \quad \text{in } \Omega \times [0, T]$$
$$m = \bar{m} \quad \text{on } \Gamma_m$$
$$q := -\boldsymbol{h} \cdot \boldsymbol{n} = \bar{q} \quad \text{on } \Gamma_q$$

Constitutive relations



Free energy

$$\psi = \psi(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}, m)$$

inelastic (viscous) strain

Stress

$$\boldsymbol{\sigma} = \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}}$$

Solvent flux

ideal mixtures:

$$\boldsymbol{h} = -\boldsymbol{D}(m) \cdot \nabla m$$

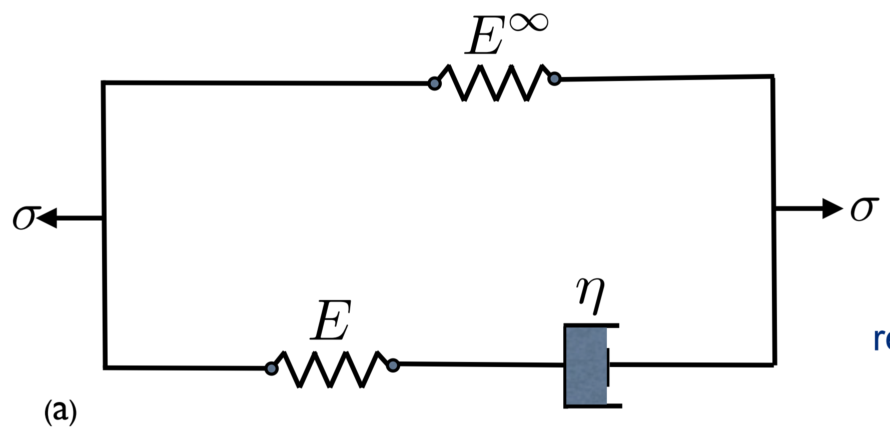
non-ideal mixtures:

$$\boldsymbol{h} = -\boldsymbol{D}(m)m \cdot \nabla\mu(m, j)$$

chemical potential

Constitutive relations: viscoelasticity

- Polymeric solid response is well described as a viscoelastic solid
- Adopt a model due to SIMO & HUGHES (1998)
  - Inelastic strain treated as an internal variable
- Consider the one-dimensional standard linear solid:



inelastic (viscous) strain

$$\sigma = E_{\infty}\varepsilon + \sigma^{v}$$

$$\sigma^{v} = \eta\dot{\alpha} = E\left[\varepsilon - \alpha\right]$$

$$\sigma = \underbrace{E_0}_{E_{\infty}+E}\ \varepsilon - E\alpha$$

viscosity

$$\tau = \frac{\eta}{E}$$

relaxation time

$$\text{Evolution of } \alpha \begin{cases} \dot{\alpha} + \dfrac{\alpha}{\tau} = \dfrac{\varepsilon}{\tau} \\ \lim\limits_{t\to-\infty} \alpha(t) = 0 \end{cases}$$

Viscoelasticity

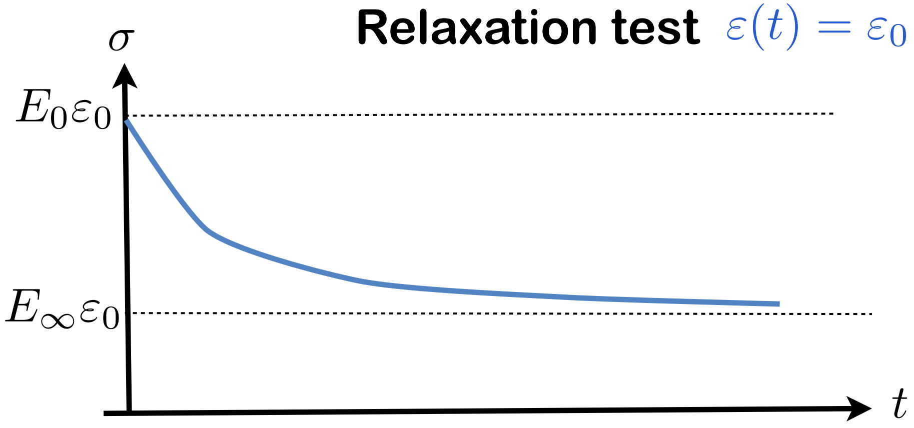
Convolution representation

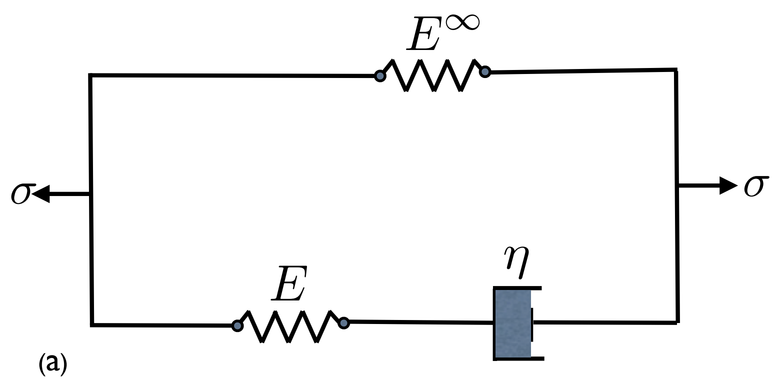
$$\sigma(t) = \int_{-\infty}^{t} G(t-s)\dot{\varepsilon}(s)\ \mathrm{d}s$$

$$G(t) = E_\infty + E\exp\left(\frac{-t}{\tau}\right)$$

relaxation function

Relaxation test $\varepsilon(t) = \varepsilon_0$





Thermodynamics

$$\psi(\varepsilon,\alpha) := \tfrac{1}{2}E_\infty\varepsilon^2 + \tfrac{1}{2}E\left[\varepsilon-\alpha\right]^2$$

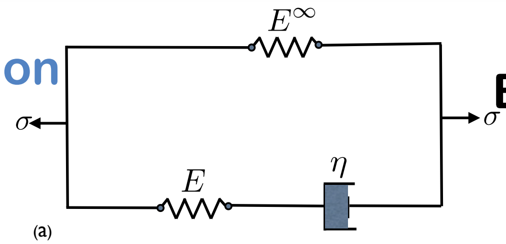
$$\mathcal{D} = \sigma^v\dot{\alpha} = \eta\dot{\alpha}^2 \geq 0$$ dissipation

$$\sigma^v = -\frac{\partial\psi(\varepsilon,\alpha)}{\partial\alpha}$$ viscous stress

$$\sigma = \frac{\partial\psi(\varepsilon,\alpha)}{\partial\varepsilon}$$ stress

Viscoelasticity

Alternative representation



viscous stress

$$q := E\alpha$$

$$\sigma = E_0 \varepsilon - q$$

$$\begin{cases} \gamma := \dfrac{E}{E_0} \\ \gamma_\infty := \dfrac{E_\infty}{E_0} \end{cases}$$

$$W^0(\varepsilon) := \tfrac{1}{2}\varepsilon E_0 \varepsilon$$

initial stored-energy function

elastic stress

$$\sigma = \frac{\partial W^0(\varepsilon)}{\partial \varepsilon} - q$$

viscous stress evolution

$$\dot{q} + \frac{q}{\tau} = \frac{\gamma}{\tau}\frac{\partial W^0(\varepsilon)}{\partial \varepsilon}$$

$$\lim_{t \to -\infty} q(t) = 0$$

Extension to $\mathbb{R}^3$

deviatoric / volumetric split

$$\boldsymbol{\varepsilon} = \boldsymbol{e} + \tfrac{1}{3}\Theta\mathbf{1}$$

$$\boldsymbol{e} := \operatorname{dev}\boldsymbol{\varepsilon} \quad \text{and} \quad \Theta := \operatorname{tr}\boldsymbol{\varepsilon}$$

$$W^0(\boldsymbol{\varepsilon}) = \bar{W}^0(\boldsymbol{e}) + U^0(\Theta)$$

$$\boldsymbol{\sigma}^0 := \frac{\partial W^0(\boldsymbol{\varepsilon})}{\partial \boldsymbol{\varepsilon}} = \operatorname{dev}\left(\frac{\partial \bar{W}^0}{\partial \boldsymbol{e}}\right) + U^{0\prime}\mathbf{1}$$

$$\boldsymbol{\sigma}(t) = \boldsymbol{\sigma}^0(t) - \boldsymbol{q}$$

$$\dot{\boldsymbol{q}} + \frac{\boldsymbol{q}}{\tau} = \frac{\gamma}{\tau}\operatorname{dev}\left(\frac{\partial W^0(\boldsymbol{e})}{\partial \boldsymbol{e}}\right)$$

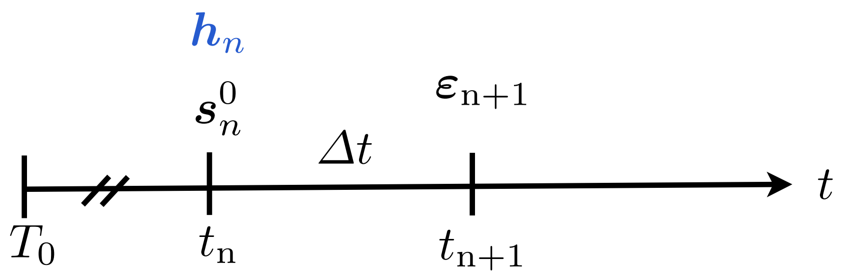
$$\lim_{t \to -\infty} \boldsymbol{q}(t) = 0$$

$$\boldsymbol{\sigma}(t) = U^{0\prime}\mathbf{1} + \int_{-\infty}^{t} g(t-s)\frac{\mathrm{d}}{\mathrm{d}s}\left[\operatorname{dev}\left(\frac{\partial \bar{W}^0(\boldsymbol{e}(s))}{\partial \boldsymbol{e}}\right)\right] \mathrm{d}s$$

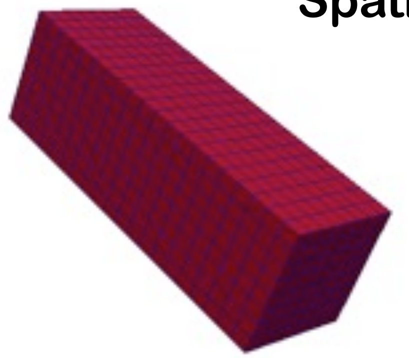
$$g(t) := \gamma_\infty + \gamma_i \exp\left(\frac{-t}{\tau}\right)$$

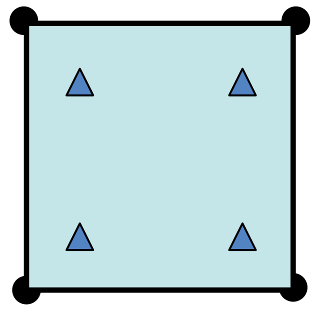
Integration algorithm for viscoelasticity

Temporal discretisation



Spatial discretisation





- Strain driven formulation
- Transform convolution representation for internal variables via two-step recurrence relationship
  - (approach restricted to relaxation functions consisting of linear combinations of functions in time that possess semi-group property)

$$\boldsymbol{e}_{n+1} = \operatorname{dev}(\boldsymbol{\varepsilon}_{n+1})$$

$$\boldsymbol{s}^0_{n+1} = \operatorname{dev}\left(\frac{\partial \bar{W}^0(\boldsymbol{e}_{n+1})}{\partial \boldsymbol{e}}\right)$$

$$\boldsymbol{h}_{n+1} = \exp\left(\frac{-\Delta t_n}{\tau}\right)\boldsymbol{h}_n + \exp\left(\frac{-\Delta t_n}{2\tau}\right)\left[\boldsymbol{s}^0_{n+1} - \boldsymbol{s}^0_n\right]$$

$$\boldsymbol{\sigma}_{n+1} = U^{0'}(\Theta_{n+1})\mathbf{1} + \gamma_\infty \boldsymbol{s}^0_{n+1} + \gamma \boldsymbol{h}_{n+1}$$

•data at level quadrature point
•no continuity relations
•State not determined from the nodal variables alone

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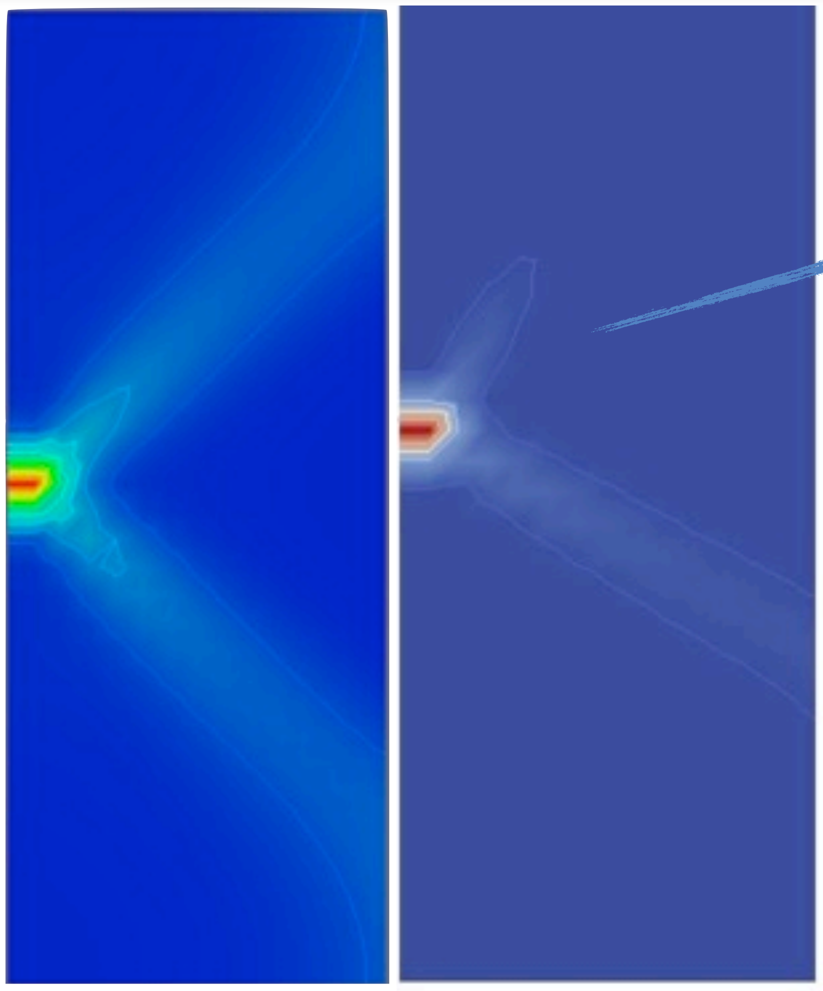
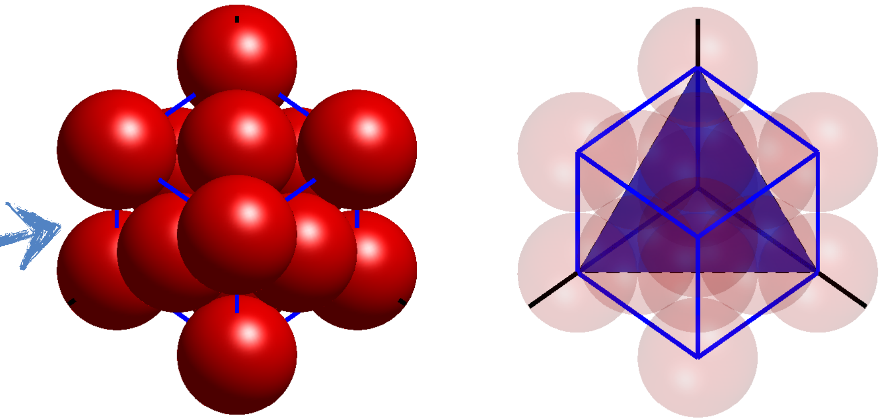
Internal variable formulations



$v_1 = 0$ $v_1 = 15$



Algorithms for crystal plasticity
McB, Reddy, Richardson

Internal variables:

- Additional state variables
- Evolve subject to an evolution equation that is possibly dependent on the primary nodal variables
- Possess no continuity requirements
- Generally treated directly in strong form at the level of the quadrature point

Another example: Plasticity

Rate independent continuum or crystal plasticity

- Plastic strain (multiplier) generally treated as an internal variable
- More complex as the evolution of the plastic strain is subject to KTT constraints
- Damage, etc.

Models for Case II diffusion

Hyperbolic diffusion

- Classical diffusion relations are parabolic
  - CII concentration propagates as a wave at a fixed velocity: hyperbolic behaviour
- Following CATTANEO (1948) and VERNOTTE (1958) for Fourier's law of heat conduction:

$$\dot{m} = -\operatorname{div} \boldsymbol{h}$$

$$\dot{\boldsymbol{h}} + \beta \boldsymbol{h} = -\beta D \nabla_{\boldsymbol{x}} m$$

assuming constant diffusivity

$$\underbrace{\operatorname{div} \dot{\boldsymbol{h}}}_{\ddot{m}} + \beta \underbrace{\operatorname{div} \boldsymbol{h}}_{\dot{m}} = \beta D \nabla^2 m$$

$$\dot{m} + \frac{1}{\beta} \ddot{m} = D \nabla^2 m \longleftarrow \text{hyperbolic diffusion}$$

- Propagation of heat as thermal wave (second sound) in fluids:

  PESHKOV (1944, 1946) and PELLAM (1948)

  and gases:

  ACKERMANN & OVERTON (1966), JACKSON ET AL (1970), NARAYANAMURTI & DYNES (1972)
- Also see framework of AIFANTIS (1980)
- Case II diffusion see KALOSPIROS ET AL (1991)

and the GENERIC formulation of EL AFIF & GRMELA (2002)

Models for Case II diffusion

Strongly coupled non-Fickian models

- Non-Fickian diffusion coupled to a viscoelastic solid
    - Wu & Peppas (1993), Govindjee & Simo (1993), Vijalapura & Govindjee (2003, 2005)
- Models of Govindjee et al are far more well developed and advanced

Equilibrium and Solvent mass balance

$$\mathrm{Div}\,(\boldsymbol{F}\cdot\boldsymbol{S}) = \boldsymbol{0}$$

$$\dot{M} = \mathrm{Div}\,(\boldsymbol{D}(M, J, \underset{\nwarrow}{R}))\, M\boldsymbol{C}^{-1}\cdot\nabla_{\boldsymbol{X}}\mu$$

concentration reacted sites

$$\left(\boldsymbol{c} := \boldsymbol{F}^T\boldsymbol{F}\right)$$

PKII stress $\boldsymbol{S} = Jp\boldsymbol{C}^{-1} + \boldsymbol{S}_{\mathrm{dev}}$

$$\boldsymbol{S}_{\mathrm{dev}} = \boldsymbol{S}^{\infty}_{\mathrm{dev}} + 2\rho_0 j^{\frac{2}{3}}\,\mathrm{dev}\,\boldsymbol{Q}$$

elastic stress $\boldsymbol{S}^{\infty}_{\mathrm{dev}} = 2\rho_0\dfrac{\partial\psi^E}{\partial\boldsymbol{C}}$

pressure $p = p^{\infty}(j) + p_s(j, M) + q(j, M)$

$$\dot{q} + \frac{q}{\tau(j, M)} = \gamma_1\dot{p}^{\infty}$$

$$\dot{\boldsymbol{Q}} + \frac{\boldsymbol{Q}}{\tau(j, M)} = \gamma_2\overline{\left[\frac{\partial\psi^E}{\partial\boldsymbol{C}}\right]}^{\,\boldsymbol{\cdot}}$$

- Finite deformation setting
- Solid modelled Neo-Hookean viscoelastic (incompressible)
- Highly coupled and non-linear
- Perfect mixing not assumed: extension of Flory-Huggins model to transient regime

Proposed models

Introduce the following features into two reduced models for case II diffusion:

Non-linear coupled diffusion and deformation

- Key features of the GOVINDJEE ET AL model but restricted to small strains
- Prototype for coupled mixed formulations
- Work in progress

1

Non-linear coupled hyperbolic diffusion deformation

- As 1 but adopt a hyperbolic diffusion model
- Treat reflection of concentration waves
- Future work

2

- Spatial adaptivity
  - Solvent propagates through medium as a wave
  - Exploit existing methodologies for hyperbolic problems
  - Need to consider the projection of inelastic internal variables
- Space-time finite elements
  - Extend spatial adaptivity features of deal.II to temporal adaptivity use finite element in space and time
- Optimal solvers and automatic differentiation routines (Sacado in Trilonos)
- Parallel implementation
- Finite strain formulation

Good problem for MeshWorker and NoX in Trilinos

Reduced model 1

Governing DAEs

$$\operatorname{div} \boldsymbol{\sigma}(\boldsymbol{u}, \boldsymbol{\alpha}, m) = \boldsymbol{0} \quad \text{in } \Omega \times [0, T]$$

$$\dot{m} = -\operatorname{div} \boldsymbol{h}(\boldsymbol{u}, m) \quad \text{in } \Omega \times [0, T]$$

Boundary and initial conditions

$$\boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{on } \Gamma_{\boldsymbol{u}}$$

$$\boldsymbol{t} := \boldsymbol{\sigma} \cdot \boldsymbol{n} = \bar{\boldsymbol{t}} \quad \text{on } \Gamma_{\boldsymbol{t}}$$

$$m = \bar{m} \quad \text{on } \Gamma_m$$

$$q = -\boldsymbol{h} \cdot \boldsymbol{n} = \bar{h} \quad \text{on } \Gamma_q$$

$$m(\boldsymbol{x}, t = 0) = m_0(\boldsymbol{x})$$

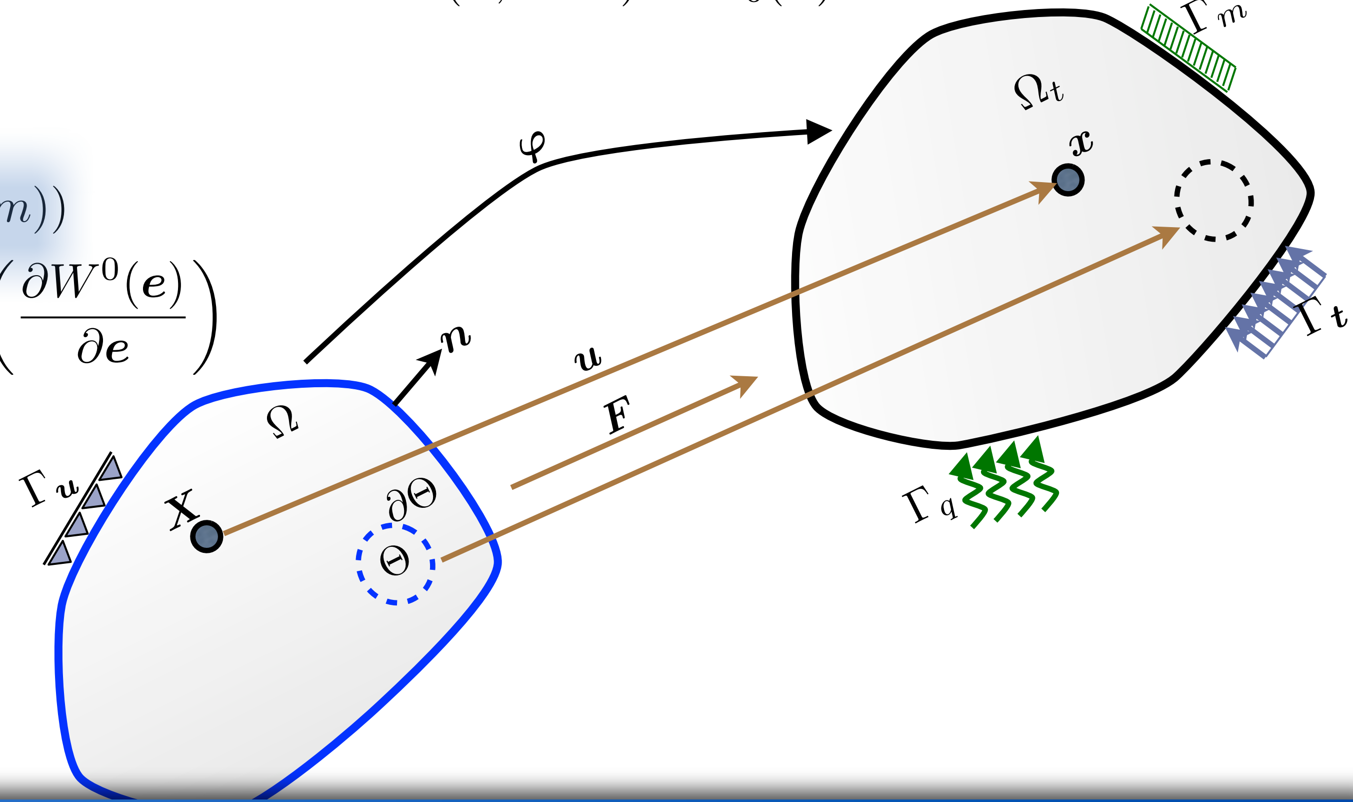
Constitutive relations

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{u}, \boldsymbol{q}, m)$$

$$\boldsymbol{h} = -D(m)\nabla m$$

$$(\boldsymbol{h} = -D(m)m\nabla\mu(J, m))$$

$$\dot{\boldsymbol{q}} + \frac{\boldsymbol{q}}{\tau(m)} = \frac{\gamma}{\tau(m)} \operatorname{dev}\left(\frac{\partial W^0(\boldsymbol{e})}{\partial \boldsymbol{e}}\right)$$



Reduced model 1

Weak form equilibrium equation

$$(\operatorname{div}\boldsymbol{\sigma}, \boldsymbol{v})_\Omega = 0 \qquad \forall \boldsymbol{v} \in H_0^1(\Omega)^{n_{\text{dim}}}$$
$$(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}(\boldsymbol{v}))_\Omega = (\bar{\boldsymbol{t}}, \boldsymbol{v})_{\Gamma_t}$$

Temporal discretisation

$$[0,T] \approx [0, t^1, \dots, t^{\mathrm{n}}, t^{\mathrm{n}+1}, \dots, T]$$
$$\Delta t = t^{\mathrm{n}+1} - t^{\mathrm{n}}$$

Conservation of solvent mass

$$\frac{m^{\mathrm{n}+1} - m^{\mathrm{n}}}{\Delta t} = -\left[\theta \operatorname{div}\boldsymbol{h}^{\mathrm{n}+1} + [1-\theta]\operatorname{div}\boldsymbol{h}^{\mathrm{n}}\right] \qquad \theta \in [0,1]$$
$$m^{\mathrm{n}+1} + \theta \Delta t \operatorname{div}\boldsymbol{h}^{\mathrm{n}+1} = m^{\mathrm{n}} - [1-\theta]\,\Delta t \operatorname{div}\boldsymbol{h}^{\mathrm{n}}$$

Weak form

$$\left(m^{\mathrm{n}+1}, v^{\mathrm{n}+1}\right)_\Omega + \theta\Delta t\left(\operatorname{div}\boldsymbol{h}^{\mathrm{n}+1}, v^{\mathrm{n}+1}\right)_\Omega = \left(m^{\mathrm{n}}, v^{\mathrm{n}+1}\right)_\Omega - [1-\theta]\,\Delta t\left(\operatorname{div}\boldsymbol{h}^{\mathrm{n}}, v^{\mathrm{n}+1}\right)_\Omega \qquad \forall v \in H_0^1(\Omega)$$
$$\left(m^{\mathrm{n}+1}, v^{\mathrm{n}+1}\right)_\Omega - \theta\Delta t\left(\boldsymbol{h}^{\mathrm{n}+1}, \nabla v^{\mathrm{n}+1}\right)_\Omega = \left(m^{\mathrm{n}}, v^{\mathrm{n}+1}\right)_\Omega + [1-\theta]\,\Delta t\left(\boldsymbol{h}^{\mathrm{n}}, \nabla v^{\mathrm{n}+1}\right)_\Omega + \theta\Delta t\left(q^{\mathrm{n}+1}, v^{\mathrm{n}+1}\right)_{\Gamma_q} + [1-\theta]\,\Delta t\left(q^{\mathrm{n}}, v^{\mathrm{n}+1}\right)_{\Gamma_q}$$

- •Following Step-23 we discretise in time first and then space: Rothe's method
- •Allow for spatial adaptivity

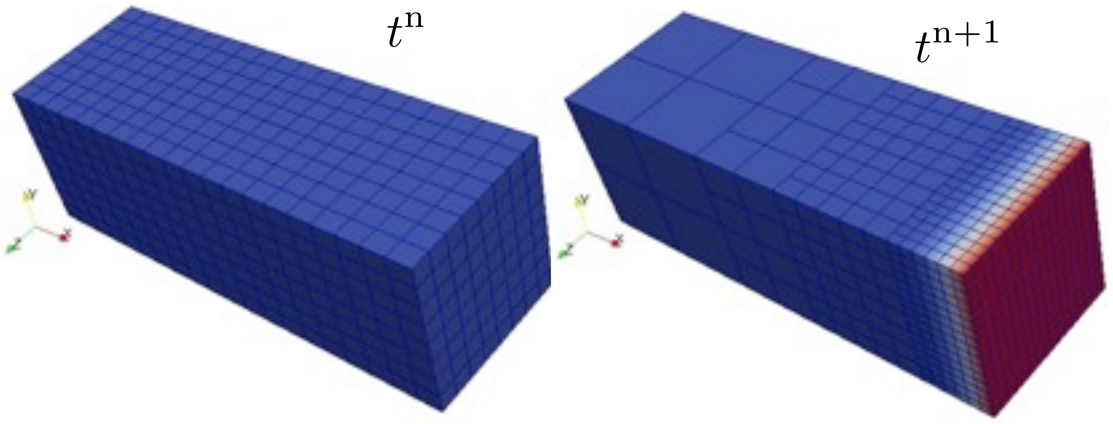
Reduced model 1

Displacement

$$\boldsymbol{u}(\boldsymbol{x}) \approx \boldsymbol{u}_h(\boldsymbol{x}) = \sum_{i=1}^{n_{\mathrm{dof}}} \boldsymbol{\Phi}_i^{\boldsymbol{u}}(\boldsymbol{x}) U_i$$

$$\boldsymbol{v}(\boldsymbol{x}) \approx \boldsymbol{v}_h(\boldsymbol{x}) = \sum_{i=1}^{n_{\mathrm{dof}}} \boldsymbol{\Phi}_i^{\boldsymbol{u}}(\boldsymbol{x}) \bar{U}_i$$

$$\boldsymbol{\varepsilon}(\boldsymbol{v}) \approx \boldsymbol{\varepsilon}(\boldsymbol{v}_h) = \sum_{i=1}^{n_{\mathrm{dof}}} \nabla^{\mathrm{sym}} \left(\boldsymbol{\Phi}_i^{\boldsymbol{u}}(\boldsymbol{x})\right) \bar{U}_i$$



$$\left(m^{\mathrm{n}}, v^{\mathrm{n+1}}\right)_\Omega \approx \sum_{i=1}^{n_{\mathrm{dof}}} M_i^{\mathrm{n}} \sum_{j=1}^{n_{\mathrm{dof}}} \left(\Phi_i^{m,(\mathrm{n})}, \Phi_j^{m,(\mathrm{n+1})}\right)_\Omega \bar{M}_j^{\mathrm{n+1}}$$

Concentration

$$m^{\mathrm{n+1}}(\boldsymbol{x}) \approx m_h^{\mathrm{n+1}}(\boldsymbol{x}) = \sum_{i=1}^{n_{\mathrm{dof}}} \Phi_i^{m,(\mathrm{n+1})}(\boldsymbol{x}) M_i^{\mathrm{n+1}}$$

$$m^{\mathrm{n}}(\boldsymbol{x}) \approx m_h^{\mathrm{n}}(\boldsymbol{x}) = \sum_{i=1}^{n_{\mathrm{dof}}} \Phi_i^{m,(\mathrm{n})}(\boldsymbol{x}) M_i^{\mathrm{n}}$$

$$\nabla v^{\mathrm{n+1}}(\boldsymbol{x}) \approx \nabla m_h^{\mathrm{n+1}}(\boldsymbol{x}) = \sum_{i=1}^{n_{\mathrm{dof}}} \nabla \left(\Phi_i^{m,(\mathrm{n+1})}(\boldsymbol{x})\right) \bar{M}_i^{\mathrm{n+1}}$$

- Shape functions are defined on different meshes.
  1. Perform the integration on the finest common mesh (Step 28)
  2. Project solution at *n* to *n+1* (Steps 31-33)

Reduced model 1

Fully-discrete residual equations

$$
\begin{aligned}
\boldsymbol{R}(\boldsymbol{U},\boldsymbol{M}) &:= [\boldsymbol{R}^{\boldsymbol{u}}\ \boldsymbol{R}^{m}]^T \\
\boldsymbol{R}^{\boldsymbol{u}} &:= (\boldsymbol{\sigma}_h, \boldsymbol{\varepsilon}(\boldsymbol{v}_h))_\Omega - (\bar{\boldsymbol{t}}_h, \boldsymbol{v}_h)_{\Gamma_{\boldsymbol{t}}} \\
\boldsymbol{R}^{m} &:= \left(m_h^{\mathrm{n}+1}, v_h^{\mathrm{n}+1}\right)_\Omega - \left(m_h^{\mathrm{n}}, v_h^{\mathrm{n}+1}\right)_\Omega \\
&\quad - \theta \Delta t \left(\boldsymbol{h}_h^{\mathrm{n}+1}, \nabla v_h^{\mathrm{n}+1}\right)_\Omega - [1-\theta]\,\Delta t \left(\boldsymbol{h}_h^{\mathrm{n}}, \nabla v_h^{\mathrm{n}+1}\right)_\Omega \\
&\quad - \theta \Delta t \left(q_h^{\mathrm{n}+1}, v_h^{\mathrm{n}+1}\right)_{\Gamma_q} - [1-\theta]\,\Delta t \left(q_h^{\mathrm{n}}, v_h^{\mathrm{n}+1}\right)_{\Gamma_q}
\end{aligned}
$$

$$\boldsymbol{R}_{\mathrm{i}+1} = \boldsymbol{0}$$

$$\boldsymbol{R}_{\mathrm{i}} + \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{U}}\delta \boldsymbol{U} + \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{M}}\delta \boldsymbol{M} = \boldsymbol{0}$$

$$\begin{bmatrix} \dfrac{\partial \boldsymbol{R}^{\boldsymbol{u}}}{\partial \boldsymbol{U}} & \dfrac{\partial \boldsymbol{R}^{\boldsymbol{u}}}{\partial \boldsymbol{M}} \\ \dfrac{\partial \boldsymbol{R}^{m}}{\partial \boldsymbol{U}} & \dfrac{\partial \boldsymbol{R}^{m}}{\partial \boldsymbol{M}} \end{bmatrix} \begin{bmatrix} \delta \boldsymbol{U} \\ \delta \boldsymbol{M} \end{bmatrix} = \begin{bmatrix} -\boldsymbol{R}^{\boldsymbol{u}}_i \\ -\boldsymbol{R}^{m}_i \end{bmatrix}$$

•Non-symmetric, potentially highly non-linear even for the reduced problem. Full finite deformation problem is horrendously non-linear! (see Govindjee et al.)

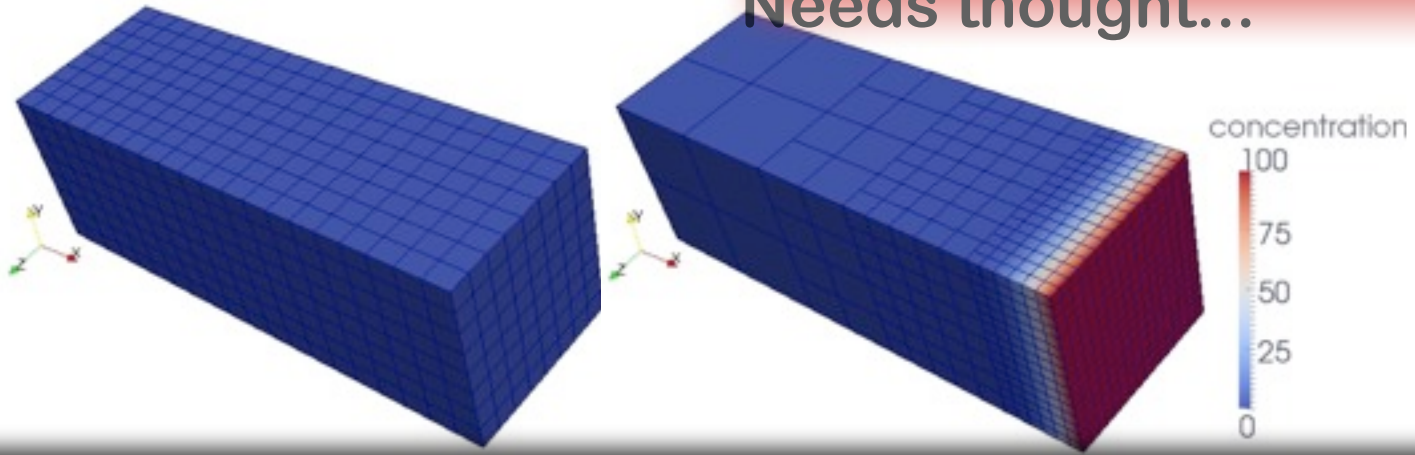
- Currently solve using a monolithic Newton scheme to solve
  - ToDo: Investigate the use of split schemes
- Currently using an approximation to tangent
  - ToDo: Investigate the use of automatic differentiation tools in Sacado (Trilinos)

(Or several other suggestions made so far)

Mesh adaptivity with internal variables

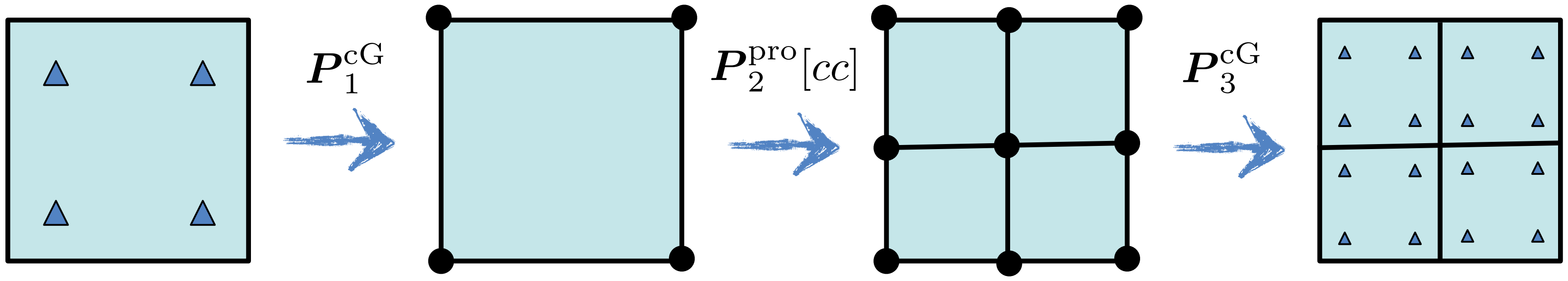
- Spatial adaptivity with nodal unknowns is mature within DEAL.II
  - Hanging nodes with continuity imposed via linear constraints
  - Fully parallelised implementation
- Spatial adaptivity with inelastic internal variables less well developed
  - Projection of quadrature point data between refinement levels
  - Storage of cell related data cumbersome and restricts parallel implementation

Discussed during workshop. Needs thought...



Mesh adaptivity with internal variables

1 Refinement



$\boldsymbol{y}' \in \mathbb{R}^{n_{\mathrm{qp}}}$

$\boldsymbol{y}[cc] \in \mathbb{R}^{n_{\mathrm{qp}}}$

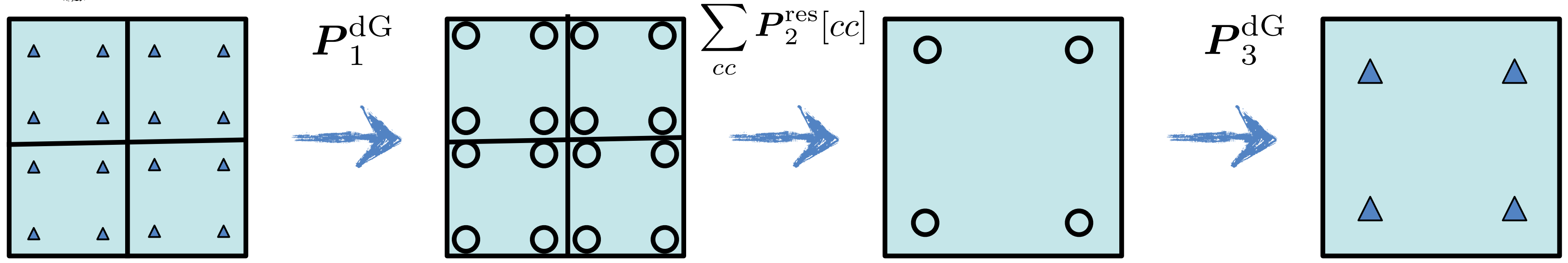
$$\boldsymbol{P}^{\mathrm{ref}}[cc] = \boldsymbol{P}_3^{\mathrm{cG}} * \boldsymbol{P}_2^{\mathrm{pro}}[cc] * \boldsymbol{P}_1^{\mathrm{cG}}$$
$$\boldsymbol{y}[cc] = \boldsymbol{P}^{\mathrm{ref}}[cc] * \boldsymbol{y}'$$

```
FE_Q<deal_II_dimension> fe_projection_cg(u_degree);

FETools::compute_projection_from_quadrature_points_matrix
(fe_projection_cg,...,P_1_cg);
FETools::compute_interpolation_to_quadrature_points_matrix
(fe_projection_cg,..., P_3_cg);
for (unsigned int cc = 0 ; cc < n_children ; cc++) {
     FullMatrix<double> P_2_i_prolongation =
     fe_projection_cg.get_prolongation_matrix(cc);
     P_refine[cc] = P3_P2_pro_P1;
}
```

•All projection matrices are computed once and for all on the reference cell
•Method valid for all components of internal variables

Mesh adaptivity with internal variables

2 Coarsening



$\boldsymbol{y}'[cc] \in \mathbb{R}^{n_{\text{qp}}}$

$$\boldsymbol{P}^{\text{coarse}}[cc] = \boldsymbol{P}_3^{\text{dG}} * \boldsymbol{P}_2^{\text{res}}[cc] * \boldsymbol{P}_1^{\text{dG}}$$

$$\boldsymbol{y} = \sum_{cc} \boldsymbol{P}^{\text{coarse}}[cc] * \boldsymbol{y}'[cc]$$

$\boldsymbol{y} \in \mathbb{R}^{n_{\text{qp}}}$

```
FE_DGQ<deal_II_dimension> fe_projection_dg(u_degree);

FETools::compute_projection_from_quadrature_points_matrix
(fe_projection_dg,...,P_1_dg);
FETools::compute_interpolation_to_quadrature_points_matrix
(fe_projection_dg,..., P_3_dg);
for (unsigned int cc = 0 ; cc < n_children ; cc++) {
     FullMatrix<double> P_2_i_restriction =
     fe_projection_dg.get_restriction_matrix(cc);
     P_coarsen[cc] = P3_P2_res_P1;
}
```

- All projection matrices are computed once and for all on the reference cell
- Note: the summation
- Method valid for all components of internal variables: i.e. works for scalars, vectors and symmetric second order tensors

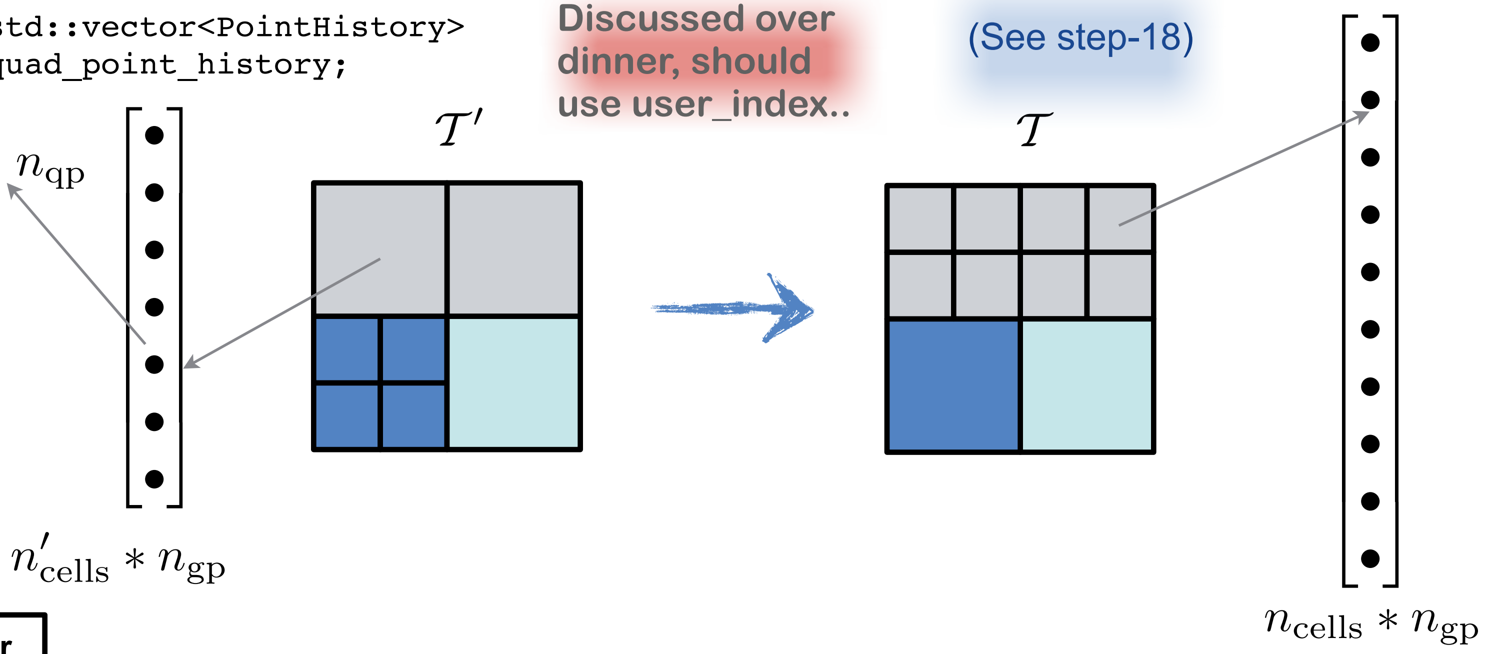
Mesh adaptivity with internal variables

```
std::vector<PointHistory>
quad_point_history;
```

Discussed over dinner, should use user_index..

(See step-18)

PointHistory
InternalVariables
+PointHistory (internal_variables) +getInternalVariables



n_{qp}
$\mathcal{T}'$
$\mathcal{T}$
$n'_{\text{cells}} * n_{\text{gp}}$
$n_{\text{cells}} * n_{\text{gp}}$

RefinementListener

↑

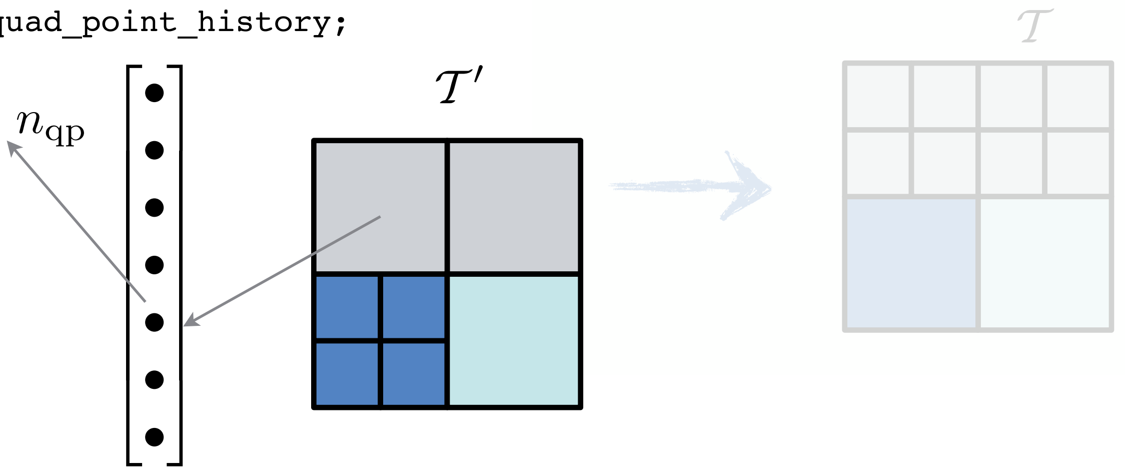
RefinementManager
quad_point_history quad_point_history_tmp refine / coarsen projections
+pre_refinement_notification (Triangulation&) +post_refinement_notification (Triangulation&)

```
GridRefinement::refine_and_coarsen_fixed_number (triangulation,...)
refinement_manager.limit_refinement_levels(triangulation);

BlockVector<double>  x_X = X;

SolutionTransfer<deal_II_dimension, BlockVector<double> >
        solution_transfer(dof_handler);
triangulation.prepare_coarsening_and_refinement();
solution_transfer.prepare_for_coarsening_and_refinement(x_X);
triangulation.execute_coarsening_and_refinement ();
setup_system();
solution_transfer.interpolate (x_X, X);
update_state(true);
```

Mesh adaptivity with internal variables

```
std::vector<PointHistory>
quad_point_history;
```

PointHistory
InternalVariables
+PointHistory (internal_variables)   +getInternalVariables



RefinementListener

RefinementManager
quad_point_history   quad_point_history_tmp   refine / coarsen projections
+pre_refinement_notification (Triangulation&)   +post_refinement_notification (Triangulation&)

- Copy `quad_point_history` to `quad_point_history_tmp`
- `quad_point_history.clear()`
- Redirect the `cell->user_pointer()` to `quad_point_history_tmp`
- Record the cells to be refined, coarsened and to remain

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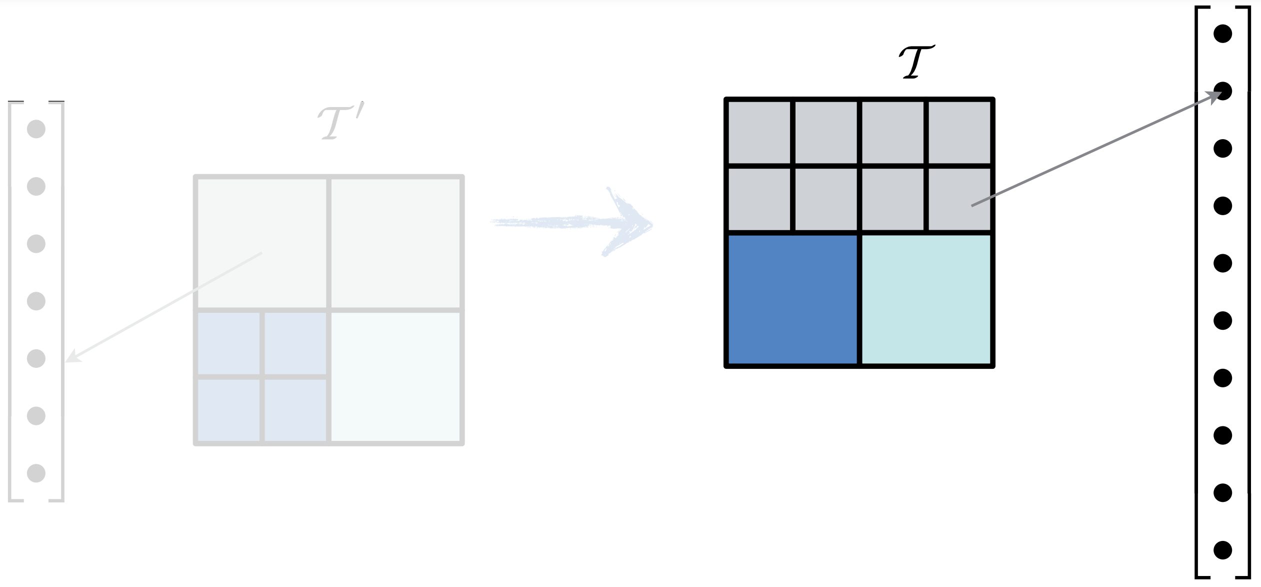
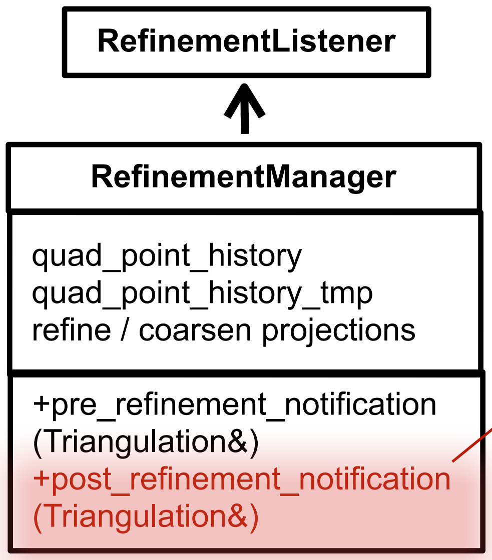
Mesh adaptivity with internal variables



Discussed over dinner, should use user_index..



quad_point_history
quad_point_history_tmp
refine / coarsen projections

+pre_refinement_notification (Triangulation&)
+post_refinement_notification (Triangulation&)

- Cells to remain:
  - Copy cell data from `quad_point_history_tmp` to `quad_point_history`
  - Redirect `cell->user_pointer`
- Cells to coarsen:
  - project data from children to parents
  - Add parent data to `quad_point_history`
  - Redirect `parent->user_pointer`
- Cells to refine:
  - project data from parents to children
  - Add children's data to `quad_point_history`
  - Redirect `children->user_pointer`

Mesh adaptivity with internal variables

Issues

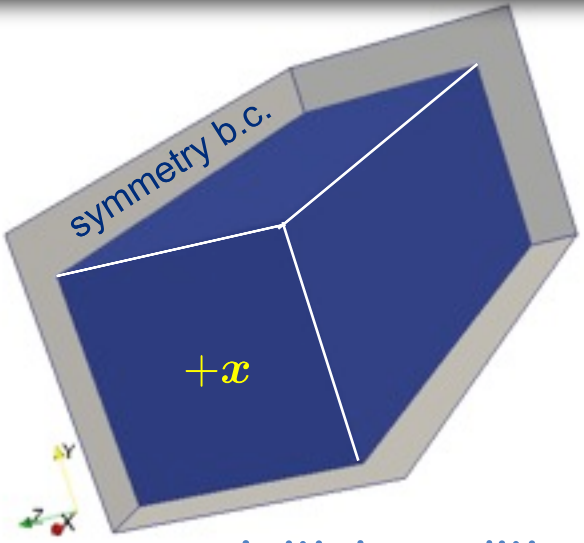
- Children do not know their parents :(
  - Complicates the coarsening routine as one can't simply ask those children flagged for coarsening for their parent
- The need to store the cell data in a std::vector causes headaches
  - The data should be associated more tightly with a cell and management abstracted from the user
  - Abstract class CellData that the user can overload
  - Member data of this class include the projections to perform coarsening and refinement
  - Simple to handle memory as the CellData is coupled to cell?
  - Parallelisation friendly?
- The cell user_pointer is used by deal.II code itself. Ideally a user should be "me" or "you" and not deal.II

Already discussed during workshop

Example problem

Constitutive laws

$$W^0(\boldsymbol{\varepsilon}) = \bar{W}^0(\boldsymbol{e}) + U^0(\Theta)$$
$$= \mu \boldsymbol{e} : \boldsymbol{e} + \tfrac{1}{2}\left[\lambda + \tfrac{2}{3}\mu\right]\Theta^2$$
$$\nu = \tfrac{1}{3} \quad \text{and} \quad \mu = 1000$$
$$D(c) = \begin{cases} \frac{1}{10} & \text{if } m > 50 \\ \frac{1}{1000} & \text{otherwise} \end{cases}$$
$$\tau(m) = \begin{cases} \frac{1}{10} & \text{if } m > 50 \\ 10000 & \text{otherwise} \end{cases}$$



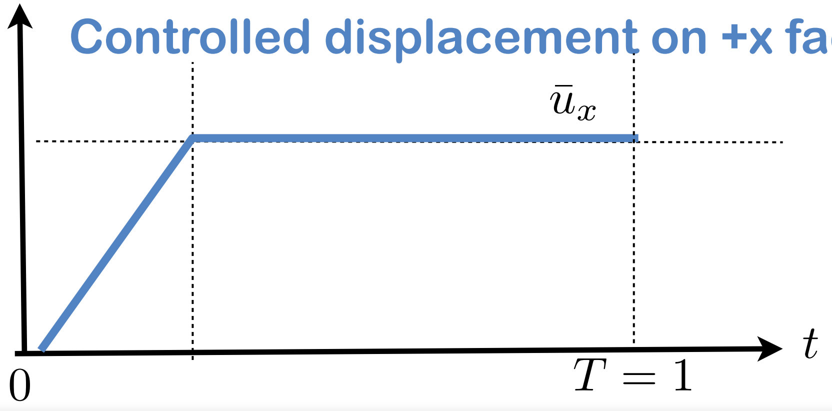
- 400 equal time-steps
  - ToDo temporal adaptivity
- Refine and coarsen a set fraction 0.1 at every time step
  - Need better refinement measure
- Kelly error indicator on concentration KELLY ET AL (1983)
- $Q_1 - Q_1$ elements
- SparseDirectUMFPACK!

Initial conditions and concentration shock boundary condition

$$m(\boldsymbol{x}, t=0) = 0$$
$$m(+\boldsymbol{x}, t=0) = 100$$

- Coupling is still only one-way: need to account for influence of the solvent on the swelling of the polymer
- Diffusivity and relaxation times are not functions of the deformation
- Polymeric solid still compressible

Controlled displacement on +x face



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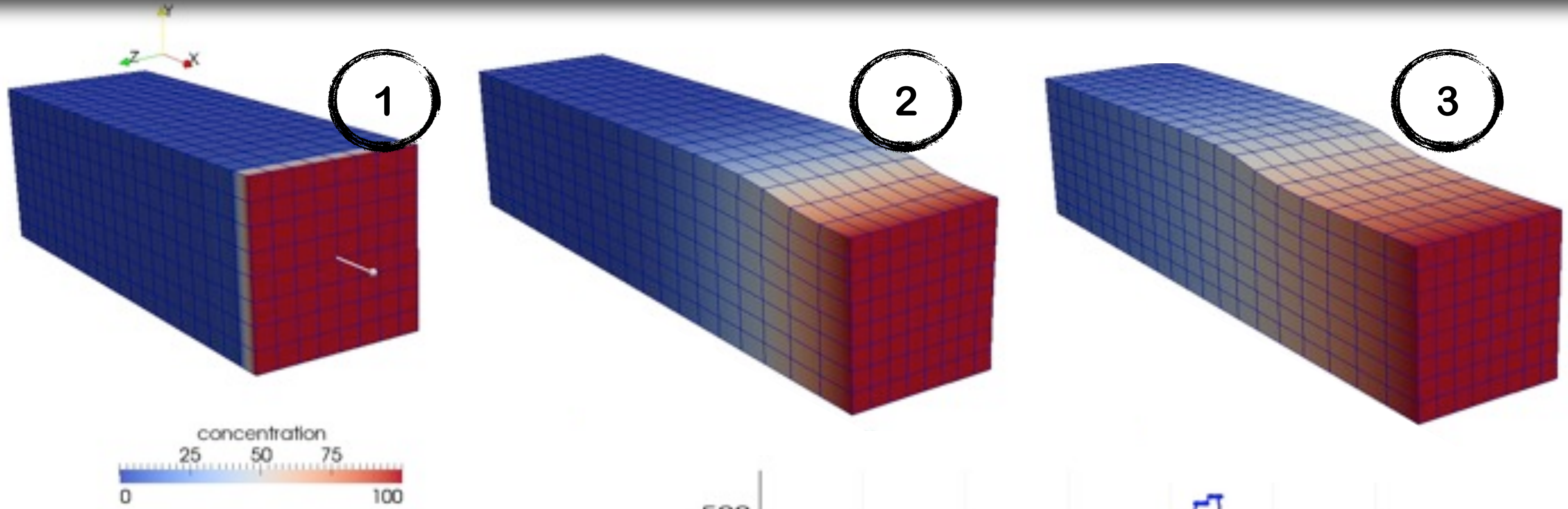
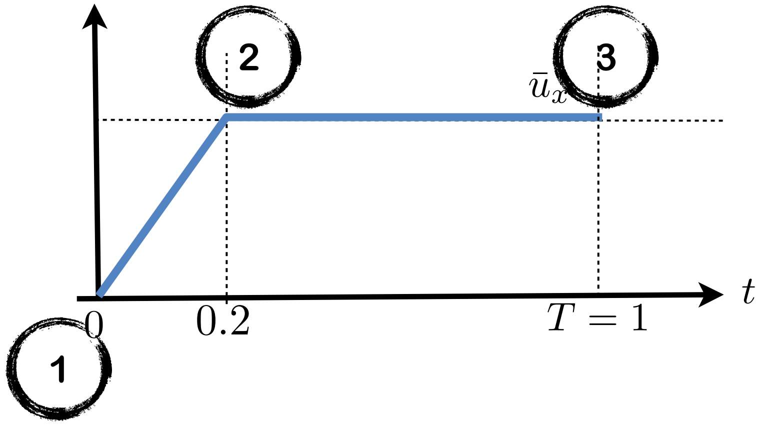
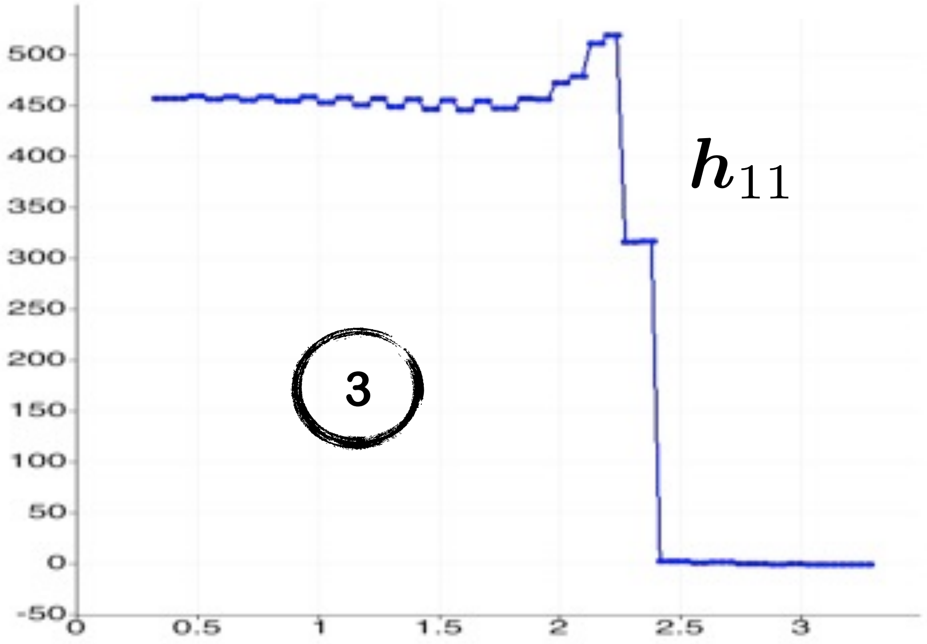
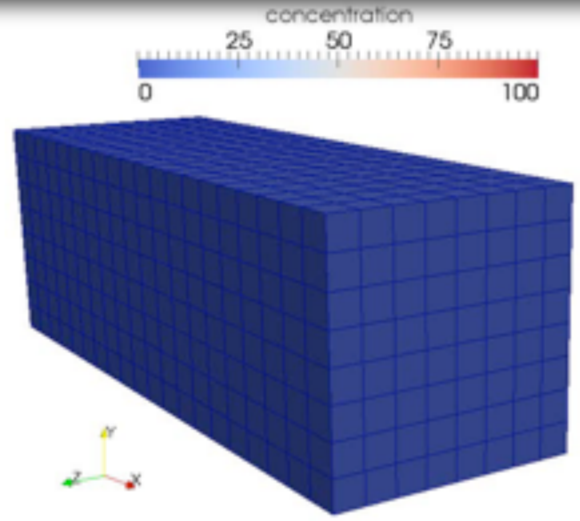
Example problem

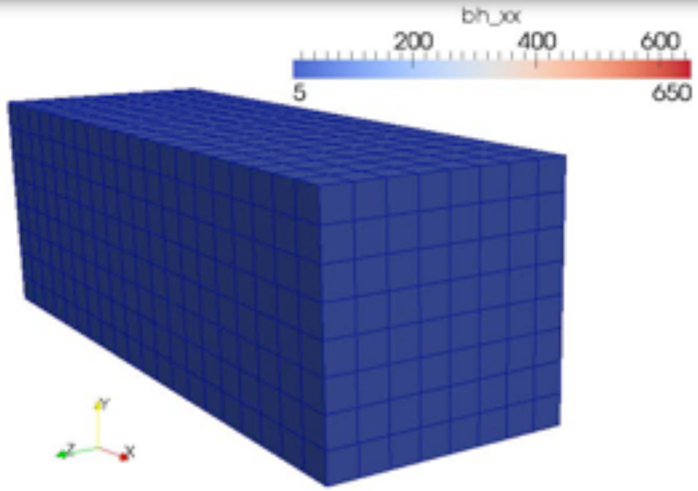


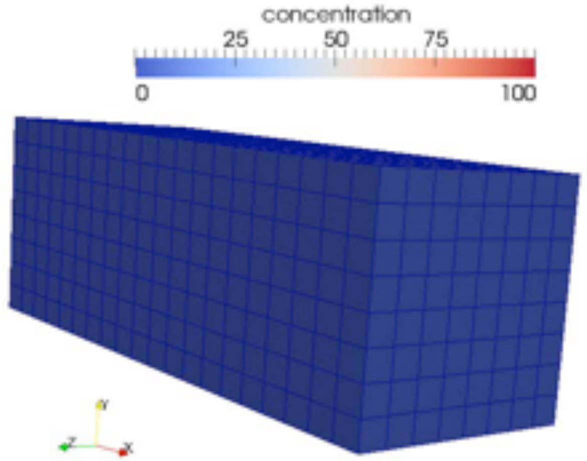


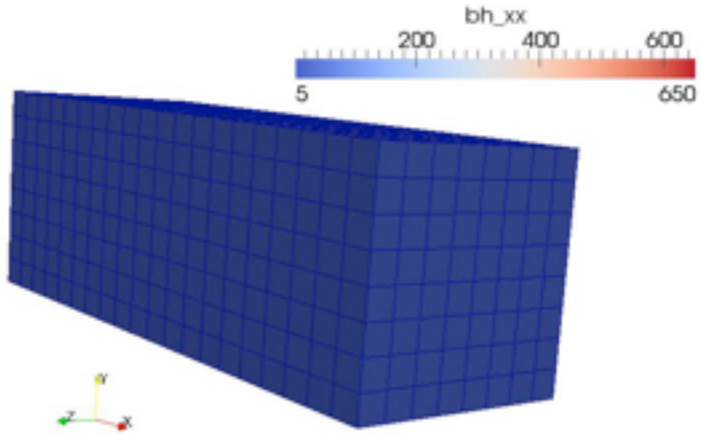


Example problem









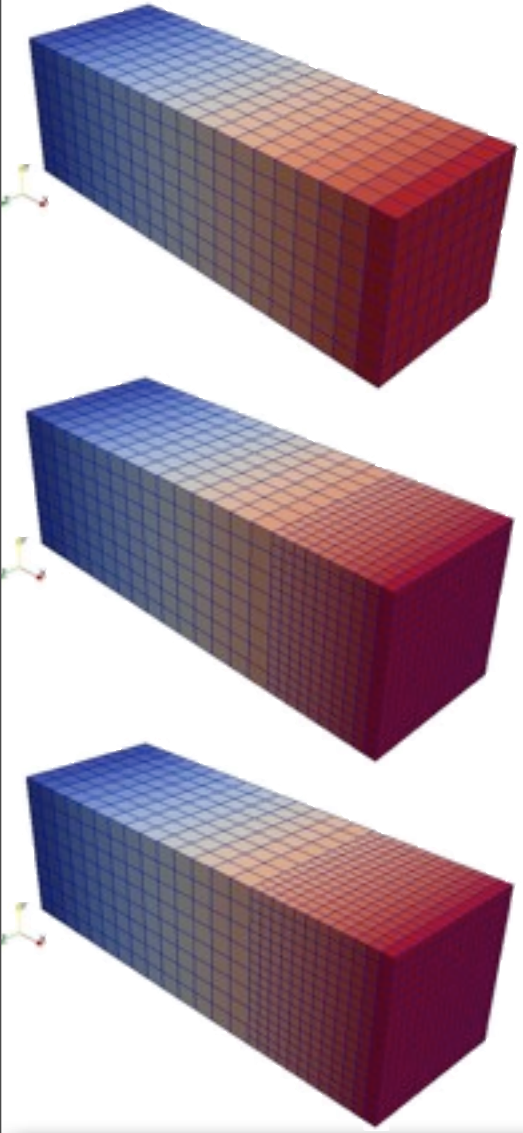
Refinement only...

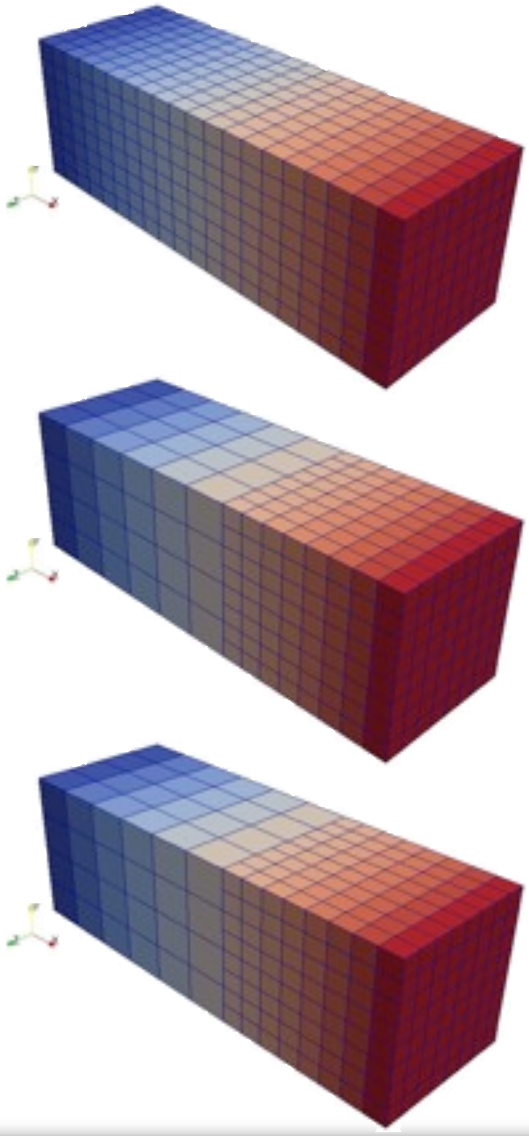
Example problem: the value of test cases. Add the x-coordinate as an internal variable...

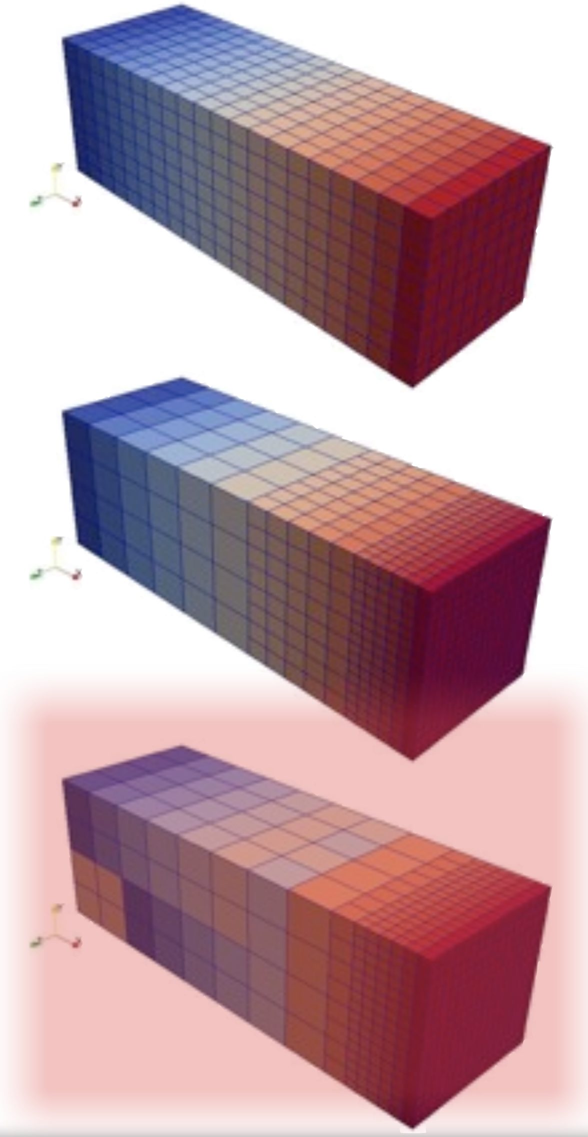
Refine

Coarsen

Refine and coarsen







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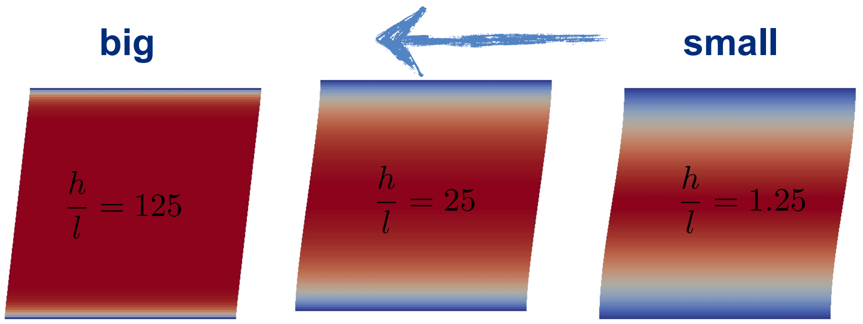
Conclusions

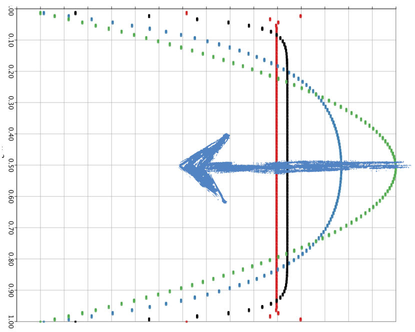
- Spatial adaptivity with internal variables is viable within current structure of deal.II
- Internal variable formulations are widely used in solid mechanics but few (no) solid mechanics codes offer the flexibility and capability of deal.II
- Extend the user base of deal.II if one could facilitate such formulations
  - Strategy to give internal variable data a similar status to nodal variables
  - refinement and projection of internal variables
  - parallel implementation

Discussed in deal.II future ideas

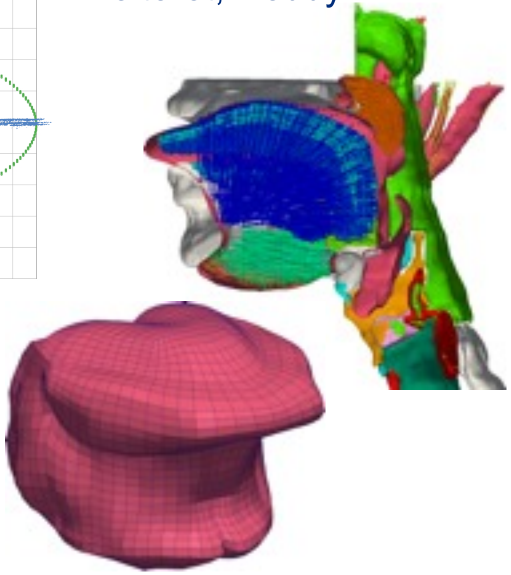
Work in progress: comments and suggestions greatly appreciated

A word of thanks





Sleep Apnoea
Pelteret, Reddy

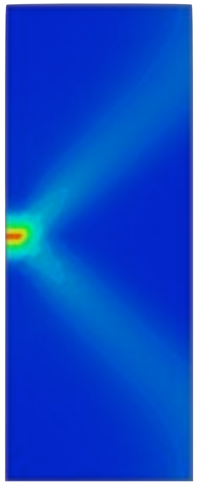


Non-local crystal plasticity
McB, Reddy, Richardson, Gurtin

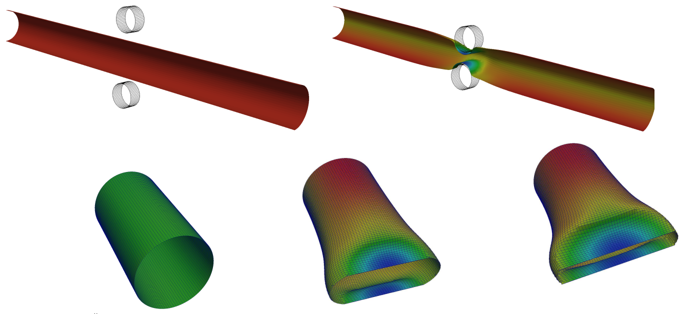
Deal.II at the University of Cape Town,

- Geographically distant and (very) small local support community
- Adopted deal.II as in-house code in 2008
- Small group of ~20 students in DEM, FEM, CFD, particle methods
- Completed or in-progress using deal.II:
  - 4 MSc and 4 PhD
- User group that meets regularly
- **Support and code greatly appreciated! Made projects possible and is a fantastic learning tool**

Algorithms for crystal plasticity
McB, Reddy, Richardson



Shell formulations with applications in biomechanics
Bartle, Reddy, McB



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Thanks. Comments, suggestions and questions please

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