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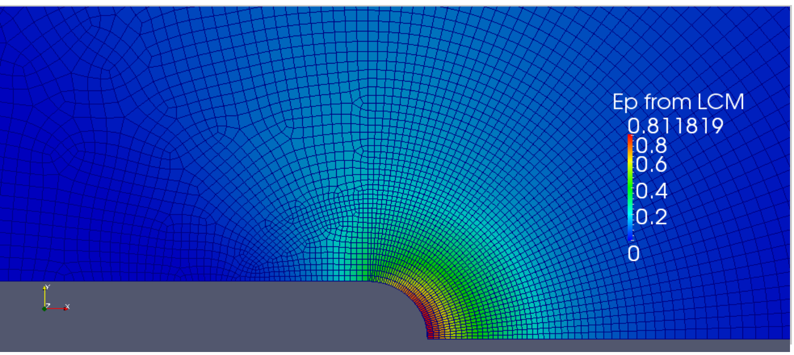

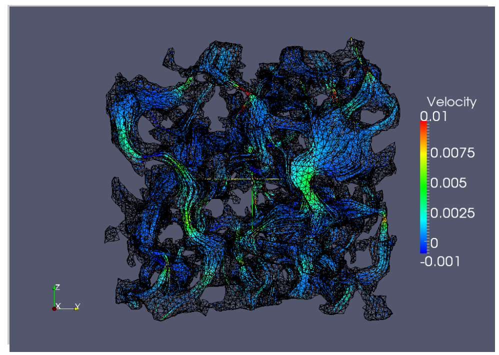

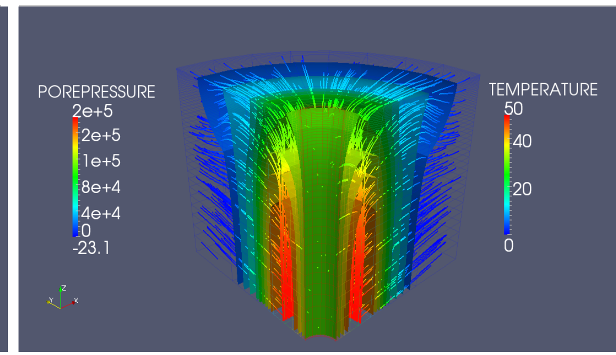

Concurrent Multi-physics Capacities in Laboratory of Computational Mechanics

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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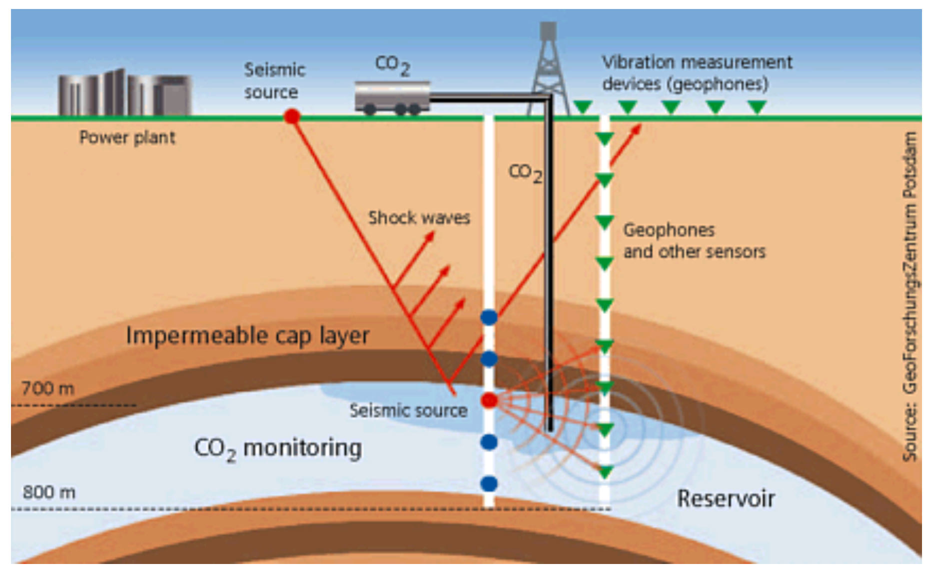
Motivations

- ❑ Hydrogen Transport
  - ❑ Understand interaction between hydrogen gas and host material, in particular hydrogen enhanced fracture, embrittlement.
  - ❑ Critical for hydrogen economy, especially for developing code and standards, life-cycle design..etc.

- ❑ Poromechanics
  - ❑ Understand interaction between mechanical and hydraulic coupling mechanism of solid-fluid mixture.
  - ❑ Keys for CO2 sequestration, oil recovery, geotechnical earthquake engineering, bone replacement, soft tissue modeling…etc.



Overview of Multiphysics Problems in Laboratory of Computational Mechanics

- Monolithic, implicit multiphysics capabilities currently available in LCM:
  1. Finite deformation thermo-mechanics (diffusion+ deformation)
  2. Finite deformation fully coupled hydrogen transport (advection-diffusion + deformation)
  3. Finite deformation poromechanics (diffusion + deformation)
  4. Finite deformation thermoporoplasticity (2 diffusion + deformation)
- Purpose:
  - Analyze and faithfully replicate physical processes which occur simultaneously interacting with each others.
- Challenge:
  - Additional physics requires additional equation + DOFs which may or may not have the same mathematical properties of the displacement field (e.g inf-sup condition).

Hydrogen Transport

Stabilized hydrogen diffusion-deformation K-field problem for low diffusive materials

Balance of Linear Momentum

$$\nabla^{\boldsymbol{X}} \cdot \boldsymbol{P}(\boldsymbol{F}, \overline{\boldsymbol{z}}, C_T) = \boldsymbol{0}$$

Concentration Sensitive Yield Function

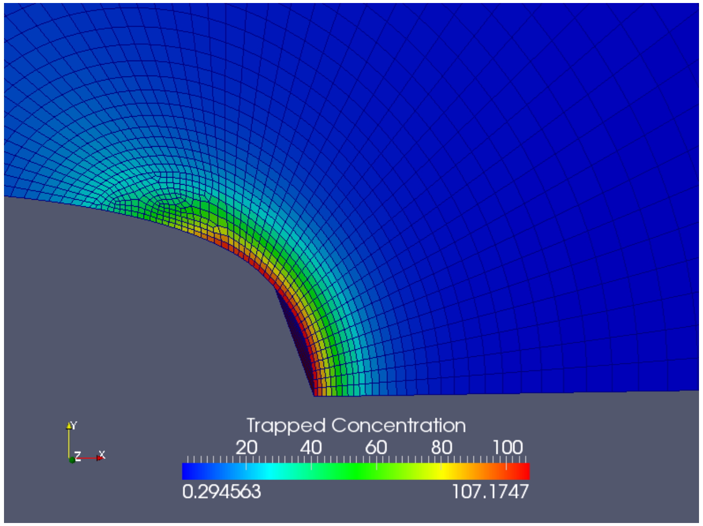
$$f(\boldsymbol{\tau}, \overline{\boldsymbol{z}}, C_T) = ||\text{dev}[\boldsymbol{\tau}]|| - \sqrt{\frac{2}{3}}[\sigma_Y(C_T) + K\alpha \leq 0$$

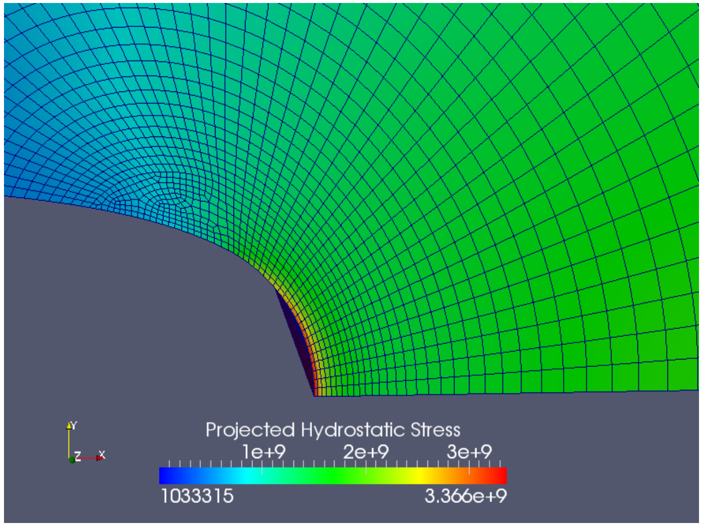
Hydrogen Transport Theorem

$$D^* \dot{C}_L - \nabla^{\boldsymbol{X}} \cdot \boldsymbol{D_L} \nabla^{\boldsymbol{X}} C_L + \nabla^{\boldsymbol{X}} \cdot \frac{V_H}{RT} C_L \boldsymbol{D_L} \nabla^{\boldsymbol{X}} S_H + \theta_T \frac{dN_T}{d\epsilon_p} \dot{\epsilon}_p = 0$$

L2 Projection of Hydrostatic Stress

$$\int_{\mathcal{B}} N_a(\sigma_h - N_b \sigma_b)\, dV = 0$$





Challenges on Implementation of Hydrogen Transport Problem

1. Numerical instability may occur if (1) time step is too small and/or (2) diffusivity is too small (i.e. stainless steel) and (3) boundary layer due to the advection term is thinner than the side length of the finite element.

2. Hydrogen transport problem is highly nonlinear, thus require a consistent linearization to implicitly solve for solutions (i.e., NUMEROUS manual, mechanical derivations EACH time the problem is amended).

3. Volmetric Locking, which may occur under perfectly plastic response / isochoric deformation..etc.

Example

Say we want to find the linearized D* (i.e., the first order
term in the Taylor expansion). D* depends on the trapped solvent, temperature, lattice concentration—but trapped solvent also depends on equivalent plastic strain and hence, displacement, yield stress…etc.

How do we derive consistent linearization with respect to all the dependent variables ?

Notice that we need to restart the entire process if we make any changes….

$$D^* - \textit{effective diffusion constant}$$

$$D^* = \frac{N_T N_L}{K_T C_L^2}\left[\frac{1}{(1+\frac{N_L}{K_T C_L})^2}\right]$$

$$C_T = \frac{N_T}{1+\frac{N_L}{K_T C_L}}$$

$$\theta_T = \frac{1}{1+\frac{N_L}{K_T C_L}}$$

$$C_T = \theta_T N_T$$

$$D_L = D_0 e^{-Q/RT}$$

$$N_L = N_A/V_M$$

$$K_T = e^{W_B/RT}$$

$$N_T = 10^{(A-Be^{-C\epsilon_p})}$$

$$\sigma_e = \sigma_0 + H\epsilon_p^m$$

$D_0 = 2.0 \times 10^{-6}\ m^2/s$ – *pre-exponential factor*

$Q = 6900 J/mol$ – *diffusion activation enthalpy*

$R = 8.314\ J/(molK)$ – *ideal gas constant*

$T = 300\ K$ – *room temperature*

$D_L = 1.27 \times 10^{-8}\ m^2/s\ (300K)$ – *diffusion coefficient*

$N_A = 6.0232 \times 10^{23}\ atoms/mol$ – *Avogadro's number*

$V_M = 7.166 \times 10^{-6}\ m^3/mol$ – *molar volume of Fe*

$N_L = 1.40 \times 10^5$ *solvent lattice* mol/m^3

$W_B = 60 \times 10^3\ J/mol$ – *trap binding energy*

$K_T = 2.801 \times 10^{10}$ – *equilibrium constant*

$V_H = 2.0 \times 10^{-6}\ m^3/mol\ (\sim 300K)$ – *partial molar volume*

$\Delta H_s = 28.6 \times 10^3\ J/mol$ – *enthalpy of solution*

$p_{H_2} = 1\ atm$ – *hydrogen pressure*

$C_{L,0} = 2.0 \times 10^{26} e^{-\Delta H_s/RT}\sqrt{p_{H_2}}\ atoms/m^3$

$C_{L,0} = 3.47 \times 10^{-3}\ mol/m^3$ – *initial concentration*

$N_T = 10^{(23.3-2.33e^{-4.0\epsilon_p})}/N_A$ – *trapped solvent* mol/m^3

$N_{T,0} = 1.549 \times 10^{-3}$ – *trapped solvent* mol/m^3

$\theta_{T,0} = 0.9986$

$C_{T,0} = 1.547 \times 10^{-3}\ mol/m^3$ – *initial concentration*

$C_{total,0} = C_{L,0} + C_{T,0} = 5.017 \times 10^{-3}\ mol/m^3$

$$\frac{\partial N_T}{\partial \epsilon_p} = 10^{(A-Be^{-C\epsilon_p})} ln(10) BCe^{-C\epsilon_p}/N_A - \textit{trapped solvent } mol/m^3$$

Implementation of Hydrogen Diffusion-Mechanics Problem with automatic differentiation

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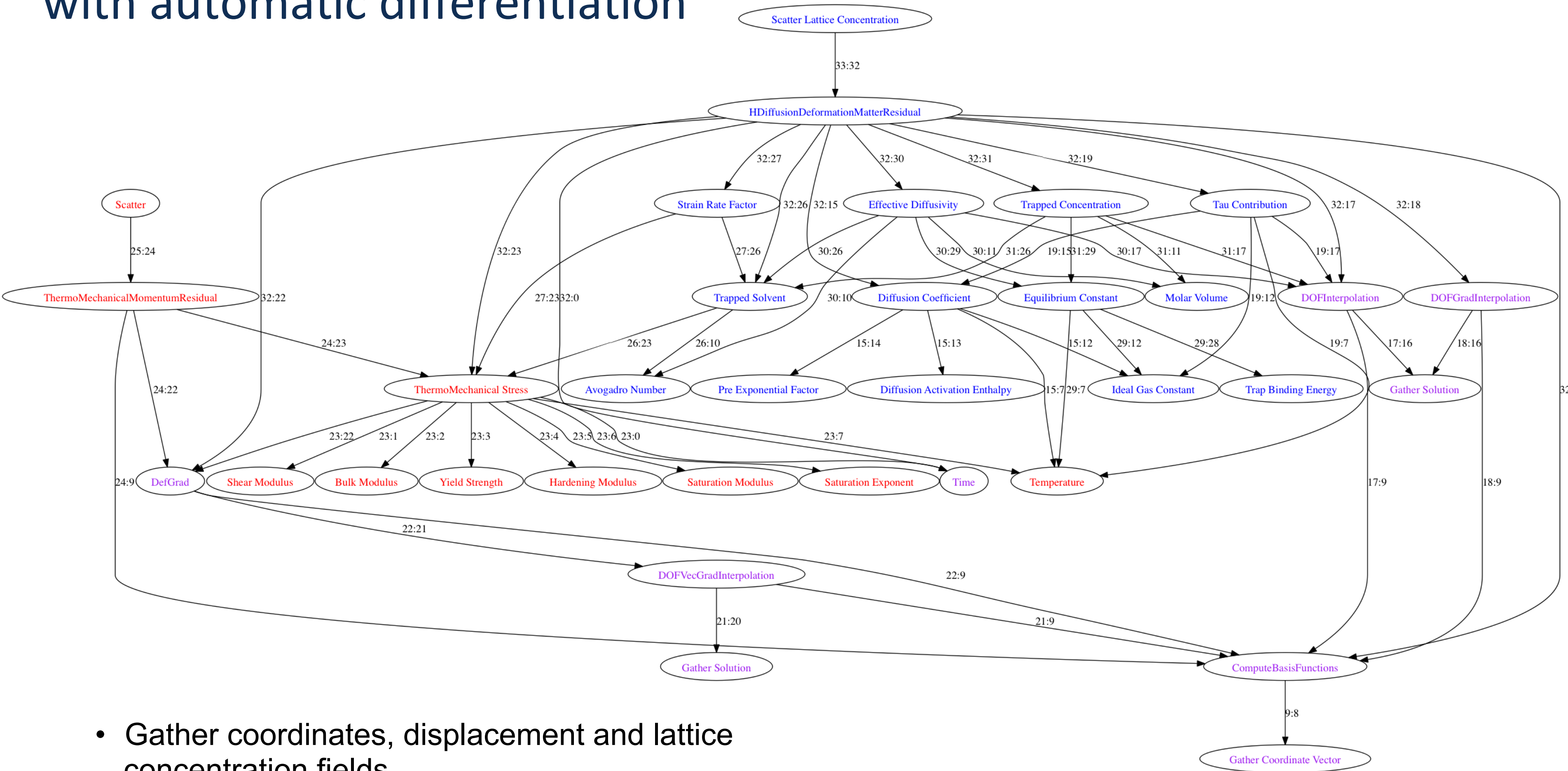


- Gather coordinates, displacement and lattice concentration fields
- Interpolate fields and gradients to integration points
- Chain together Evaluators to compute Momentum and Conservation of Hydrogen Residuals
- Scatter back to the global system of equations

Blue = Hydrogen Transport

Red = Solid Mechanics (J2 Plasticity)

Purple = coupled terms

Combined F-bar formulation

Isochoric-volumetric split

$$\boldsymbol{F} = \boldsymbol{F}_{\text{vol}} \cdot \boldsymbol{F}_{\text{iso}}$$

Replacing volumetric split with assumed term

$$\overline{\boldsymbol{F}} = \bar{J}^{1/3} \boldsymbol{F}_{\text{iso}} = \bar{J}^{1/3} J^{-1/3} \boldsymbol{F}$$

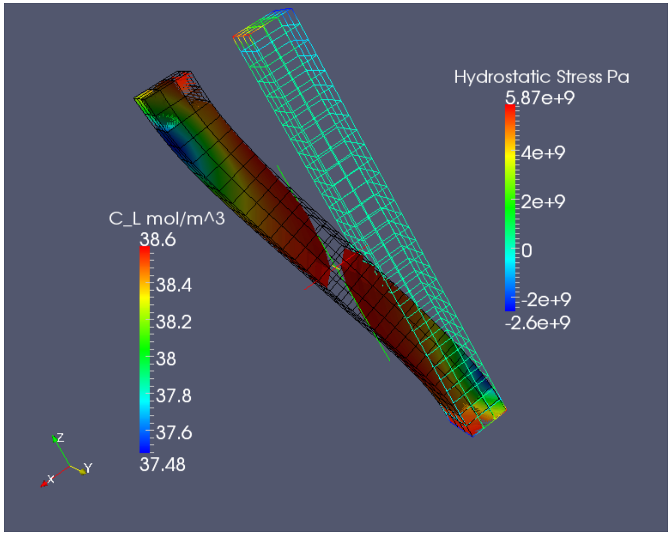
Classical Combined F-bar approach

$$\widetilde{\boldsymbol{F}} = \alpha \boldsymbol{F} - (1-\alpha) \overline{\boldsymbol{F}}.$$

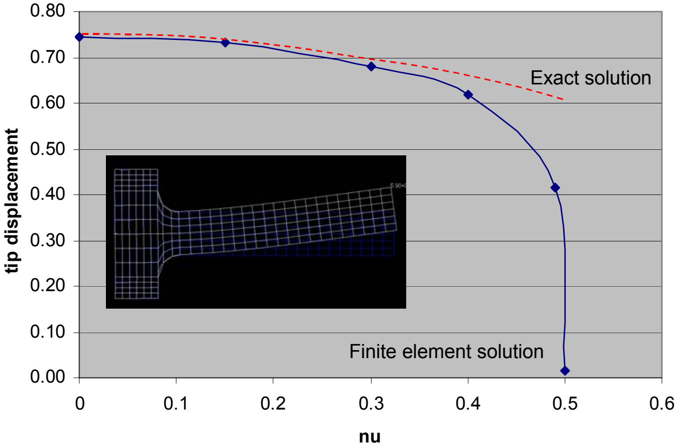
Current Approach via Lie algebra

$$J = J^e J^p J^C \quad ; \quad J^C = 1 + \lambda (C - C_o)$$

$$\widetilde{J}(X) = \exp\left(\frac{1-\alpha}{\mathrm{V}_{\mathcal{B}^e}} \int_{\mathcal{B}^e} \log J(X) \, \mathrm{dV} + \alpha \log J(X) \right)$$



Concentration prediction affected by locking



Volumetric Locking

Stabilization at small time limit

Hydrogen Transport Theorem

$$D^* \dot{C}_L - \nabla^{\boldsymbol{X}} \cdot \boldsymbol{D_L} \nabla^{\boldsymbol{X}} C_L + \nabla^{\boldsymbol{X}} \cdot \frac{V_H}{RT} C_L \boldsymbol{D_L} \nabla^{\boldsymbol{X}} S_H + \theta_T \frac{dN_T}{d\epsilon_p} \dot{\epsilon}_p = 0$$

transient term — Hydrogen diffusion term — Advection coupling term — Plastic strain nonlinear coupling term

- Spurious oscillations may occur when
  - D^* is large, which means local rate of change dominates
  - The mesh size h is large (relative to the advection and diffusion length scale)
  - The time step is small (relative to the advection and diffusion time scale).
  - Notice that Peclet number measures whether advection of diffusion is more important, but did not tell much about the transient term!

- Examples of stabilization scheme
  - Petrov-Galerkin/streamline upwind method (Hughes, 1978, Johnson, 1984)
  - Space-time finite incremental calculus method (Onate and Manzan 2000)
  - SUPG with adaptive stabilization parameters (Tezduyar 2003)
  - Spurious oscillations at layers diminishing method (Volker and Schmeyer, 2008).
  - Artificial diffusivity (Onate and Manzan, 2000).

Stabilization for hydrogen convection-diffusion problem

- For transient problem, stability criteria must be satisfied for the pair of time step and element size *h* used in simulations. γ is the parameter for backward Euler time integrator (Harari, 2004).

$$\frac{h^2 D^*}{6\gamma D_L \Delta t} < 1$$

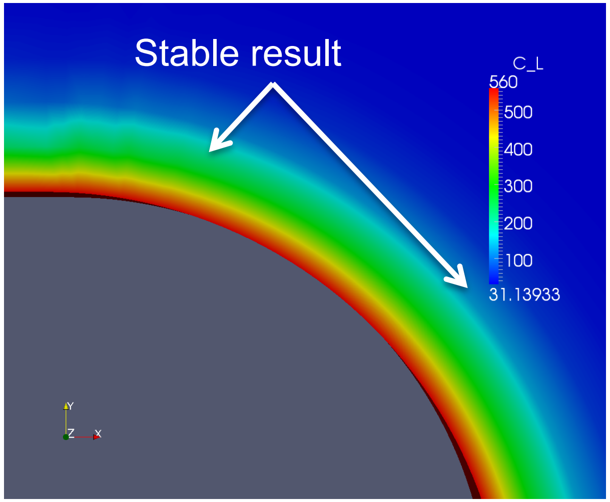
- Meanwhile, stability of the steady solution can be predicted by the Peclet number. If Pe is less than 1 and D^*/D_L is reasonably close to h^2/dt

$$Pe = \frac{V_H}{RT} | \nabla^{\boldsymbol{X}} S_H | h < 1$$

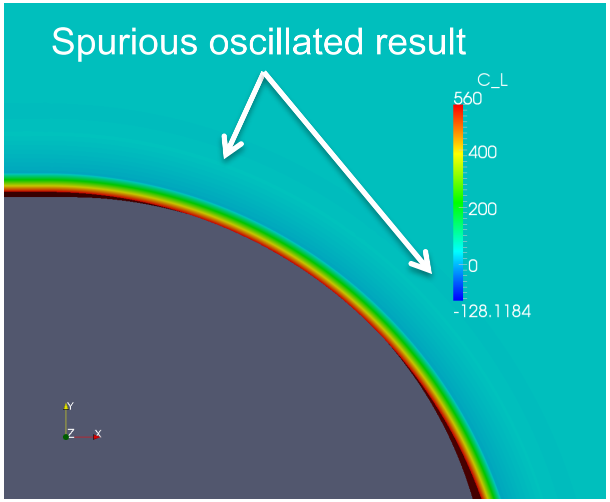
- add stabilization term to penalize the deficiency

$$R_{stab} = \int_\Omega [\tau(\eta^h - \frac{1}{V_\Omega}\int_\Omega \eta^h d\Omega)(\dot{C}_L^h - \frac{1}{V_\Omega}\int_\Omega \dot{C}_L^h d\Omega)]\, d\Omega$$

$$R_{stab} = \int_\Omega \tau \, \nabla^{\boldsymbol{X}} \eta^h \, \nabla^{\boldsymbol{X}} \dot{C}_L^h \, d\Omega$$

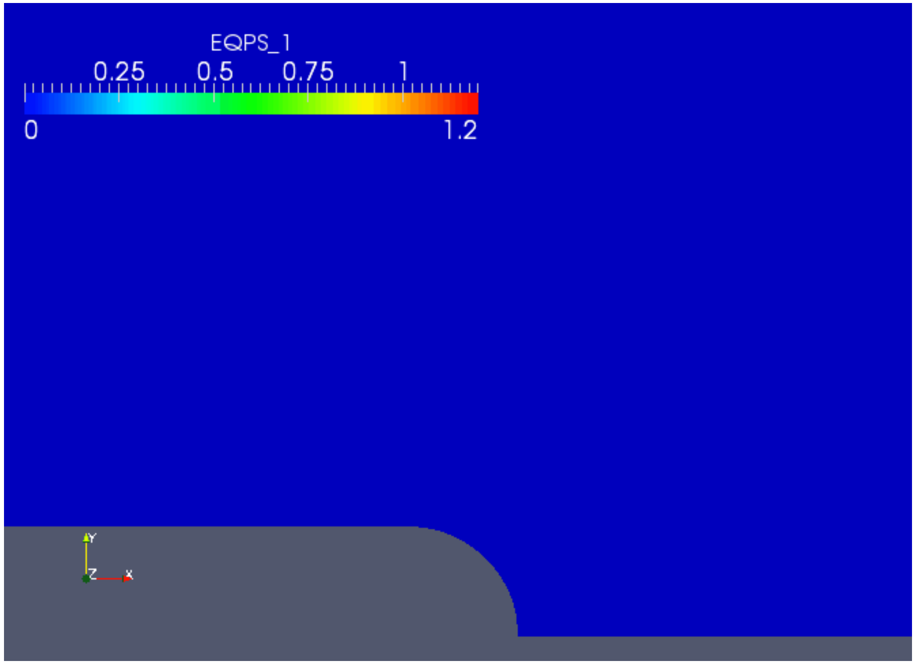


Stabilized Implicit Gakerlin Formulation

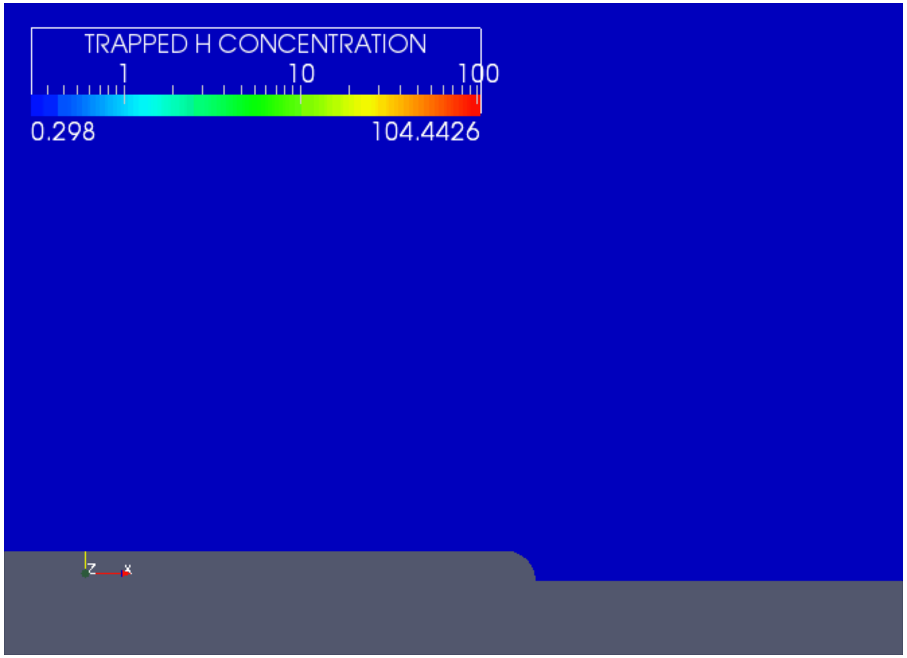


Standard Implicit Galerkin Formulation

K-field blunt tip problem



Equivalent Plastic Strain

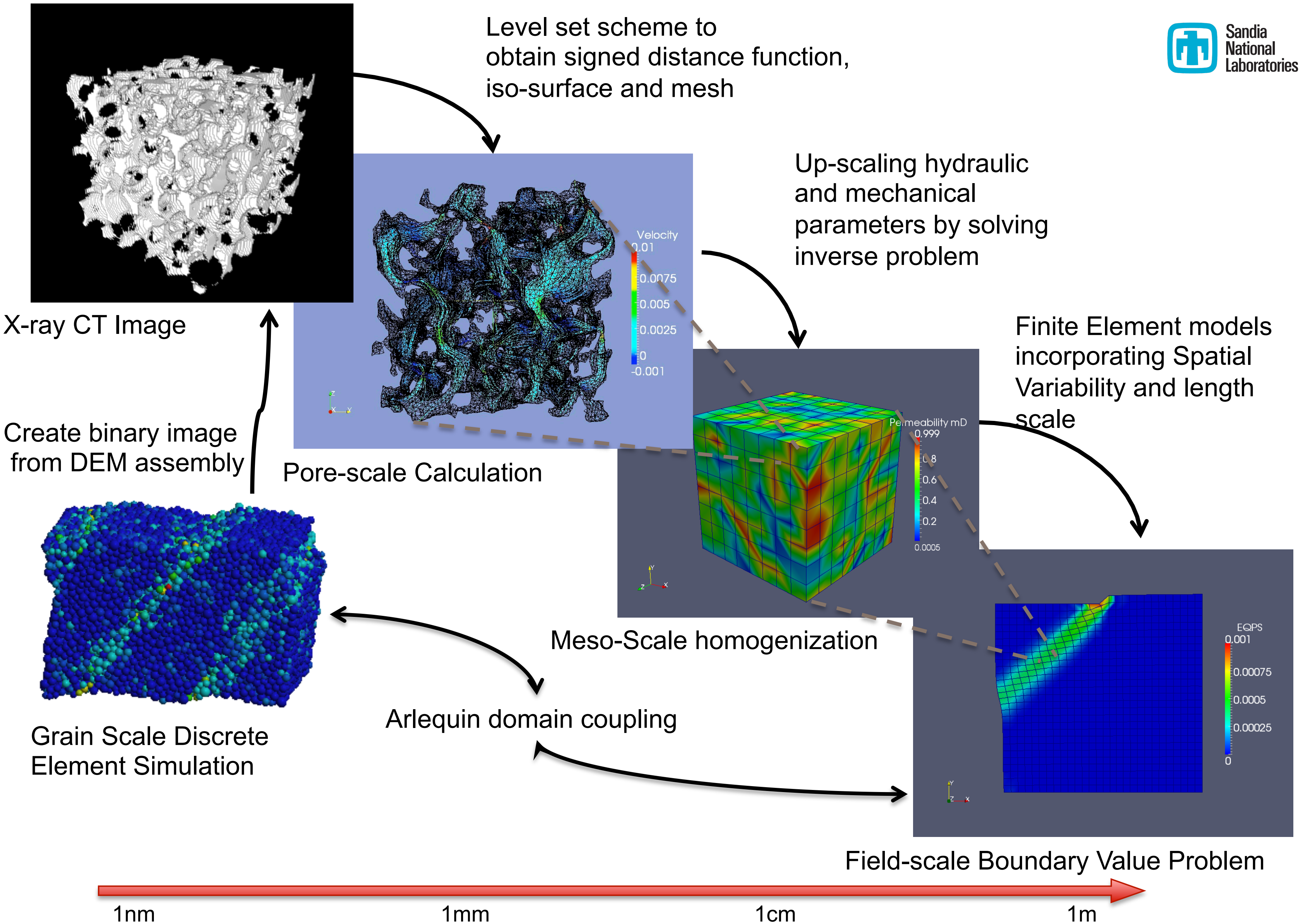


Trapped Hydrogen Concentration

Conclusion

- We have implemented a fully implicit hydrogen transport model in the Laboratory of Computational Mechanics package with the following desirable features
  - Open-source, open for collaborations.
  - Capacity to conduct fully coupled, fully implicit simulations with stabilization scheme.
  - Automatic differentiation, which makes it fast and easy to make amendment to existing model and eliminate chance of making error in derivation
  - Stabilization scheme available to handle material with extremely low diffusivity, thin boundary layer…etc.
  - A L2 projection scheme to obtain a C^0-continuous stress gradient term that enables the advection term to be correctly modeled without introducing errors during the extrapolation process.

Poromechanics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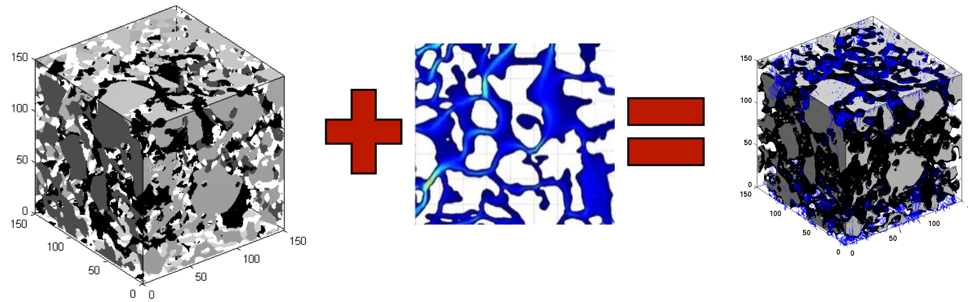
X-ray CT Image
Level set scheme to obtain signed distance function, iso-surface and mesh
Velocity
0.01
0.0075
0.005
0.0025
0
-0.001
Pore-scale Calculation
Up-scaling hydraulic and mechanical parameters by solving inverse problem
Permeability mD
0.999
0.8
0.6
0.4
0.2
0.0005
Meso-Scale homogenization
Finite Element models incorporating Spatial Variability and length scale
EQPS
0.001
0.00075
0.0005
0.00025
0
Field-scale Boundary Value Problem
Create binary image from DEM assembly
Grain Scale Discrete Element Simulation
Arlequin domain coupling
1nm
1mm
1cm
1m

U-P Formulation of Poromechanics Problem

Balance of Linear Momentum

$$\nabla^{\boldsymbol{X}} \cdot \boldsymbol{P} + J(\rho^s + \rho^f)\boldsymbol{G} = \boldsymbol{0}$$



Solid skeleton Solid skeleton

POROUS MEDIA

Effective Stress Concept

$$\boldsymbol{P}(\boldsymbol{F}, \boldsymbol{z}, p^f) = \boldsymbol{P'}(\boldsymbol{F}, \boldsymbol{z}) - J\left(1 - \frac{K}{K_s}\right)p^f \boldsymbol{F}^{-T}$$

Balance of Mass

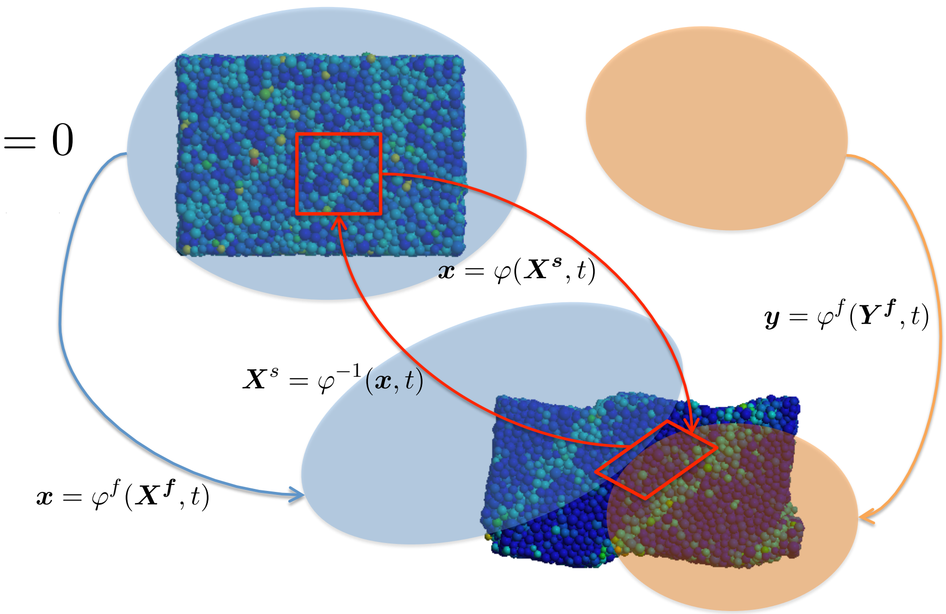
$$\frac{DB}{Dt}\left(\log J + \frac{p^f}{K_s}\right) + \frac{B}{J}\frac{DJ}{Dt} + \frac{1}{M}\frac{Dp^f}{Dt} + \nabla^{\boldsymbol{X}} \cdot \boldsymbol{Q} = 0$$

Darcy's Law

$$\frac{1}{\rho_f}\boldsymbol{W} = \boldsymbol{K} \cdot (-\nabla^{\boldsymbol{X}} p^f + \rho_f \boldsymbol{F}^{\mathrm{T}} \cdot \boldsymbol{G})$$

$$\boldsymbol{K} = J\boldsymbol{F}^{-1} \cdot \boldsymbol{k} \cdot \boldsymbol{F}^{-\mathrm{T}}$$

$$\boldsymbol{Q} = (1/\rho_f)\boldsymbol{W}$$



Challenges on Implementation of Poromechanics Problem

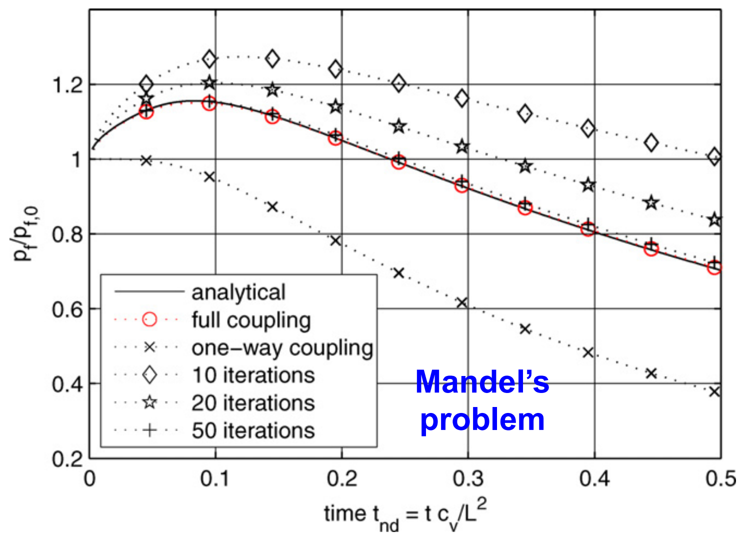
1. Preserve Mandel-Cryer effect (pore pressure changes non-monotonically in time upon subjected to mechanical loading).

2. Only a selection of finite element space satisfying inf-sup condition and equal-order finite element discretization does not.

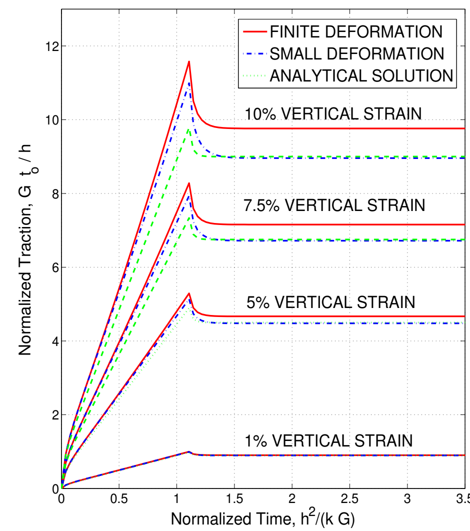
3. Volumetric Locking may occur under perfectly plastic response / isochoric deformation..etc.

4. Often requires addition field equations to capture essential physical processes (heat transport, chemo-mechanics…etc)

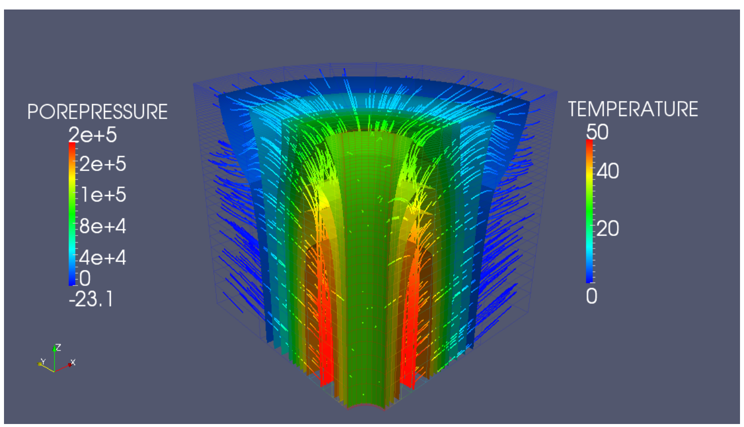
Key Features available in Poromechanics Models



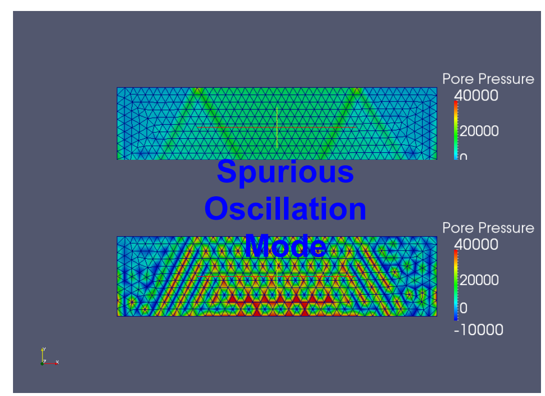
Monolithic Coupled Hydromechanics



Total Lagrangian Finite Strain Formulation



Thermomechanical effect of mixture



Stabilized Equal-order Discretization

Stabilization for Equal Order Mixed Finite Element

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Inf-sup Condition (not satisfied)

$$\sup_{\boldsymbol{u}_h \in V_{\boldsymbol{u}}{}^h, \boldsymbol{u}_h \neq \boldsymbol{0}} \frac{\int p_h \nabla^{\boldsymbol{x}} \cdot \boldsymbol{u}_h \, d\Omega}{||\boldsymbol{u}_h||_1} \geq \gamma ||p^h||_0, \forall p^h \in V_p^h$$

Weaker Inf-sup Condition (still satisfied)

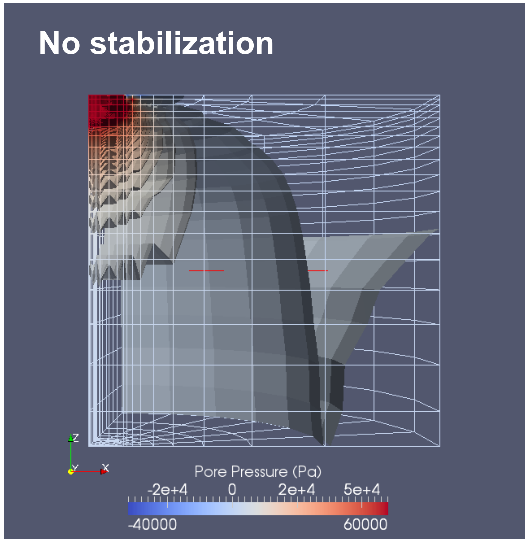
$$\sup_{\boldsymbol{u}_h \in V_{\boldsymbol{u}}{}^h, \boldsymbol{u}_h \neq \boldsymbol{0}} \frac{\int p_h \nabla^{\boldsymbol{x}} \cdot \boldsymbol{u}_h \, d\Omega}{||\boldsymbol{u}_h||_1} \geq \gamma_1 ||p^h||_0 - \gamma_2 h || \nabla^{\boldsymbol{x}} p^h ||_0, \forall p^h \in V_p^h$$

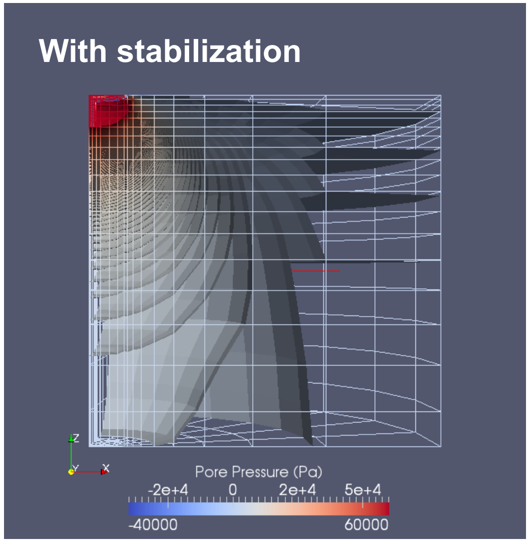
Pressure Projection Stabilization

- add stabilization term to penalize the deficiency in the displacement-pore pressure approximation pair.
- We use a adaptive scheme to turn on/off stabilization such that no excess diffusion is introduced.

$$R_{stab} = \int_\Omega [\tau(\eta^h - \frac{1}{V_\Omega} \int_\Omega \eta^h d\Omega)(p^h - \frac{1}{V_\Omega} \int_\Omega p^h d\Omega)] \, d\Omega$$

Stabilization parameter — Interpolated pore pressure field — Projected pore pressure field





Stabilized F-bar Poromechanics with Monolithic Coupling at finite strain

Balance Law

$$\nabla^{\boldsymbol{X}} \cdot \boldsymbol{P} + J(\rho^s + \rho^f)\boldsymbol{G} = \boldsymbol{0}$$

$$\frac{DB}{Dt}(\log J + \frac{p^f}{K_s}) + \frac{B}{J}\frac{DJ}{Dt} + \frac{1}{M}\frac{Dp^f}{Dt} + \nabla^{\boldsymbol{X}} \cdot \boldsymbol{Q} = 0$$

Regularization Energy

$$W^{pen}(p^f_\tau) = \frac{1}{2}\sum_{K \in \Omega} \int_K (p^f_\tau - \Pi p^f_\tau)\frac{\gamma}{M}(p^f_\tau - \Pi p^f_\tau) dV$$

$$W^{pen}(p^f_\tau) = \frac{1}{2}\sum_{K \in \Omega} h_K \int_K \nabla^{\boldsymbol{X}} p^f_\tau \cdot \beta \boldsymbol{K} \nabla^{\boldsymbol{X}} p^f_\tau dV$$

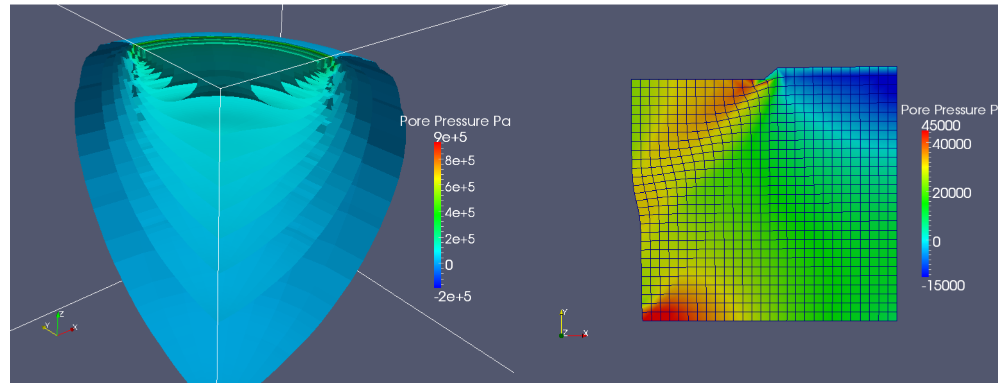
Harari's analysis

$$\gamma = (2 - 6\frac{\vartheta c \Delta t}{h^2})\Big(\frac{1}{2} + \frac{1}{2}\tanh(2 - 12\frac{\vartheta c \Delta t}{h^2})\Big)$$

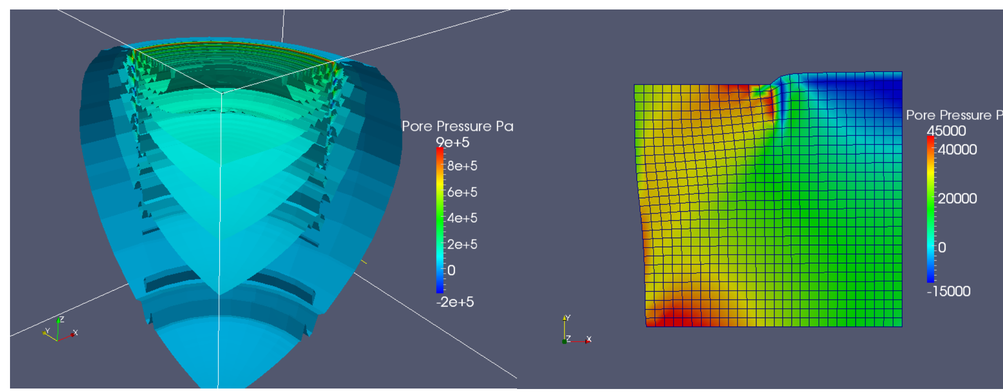
Weighted F-bar

$$\widetilde{\boldsymbol{F}} = \widetilde{J}^{1/3} J^{-1/3} \boldsymbol{F}$$

$$\widetilde{J}(X) = \exp\Big(\frac{1-\alpha}{V_{\mathcal{B}^e}} \int_{\mathcal{B}^e} \log J(X)\, dV + \alpha \log J(X)\Big)$$



Stabilized F-bar Mixed FEM



Standard Galerkin Method

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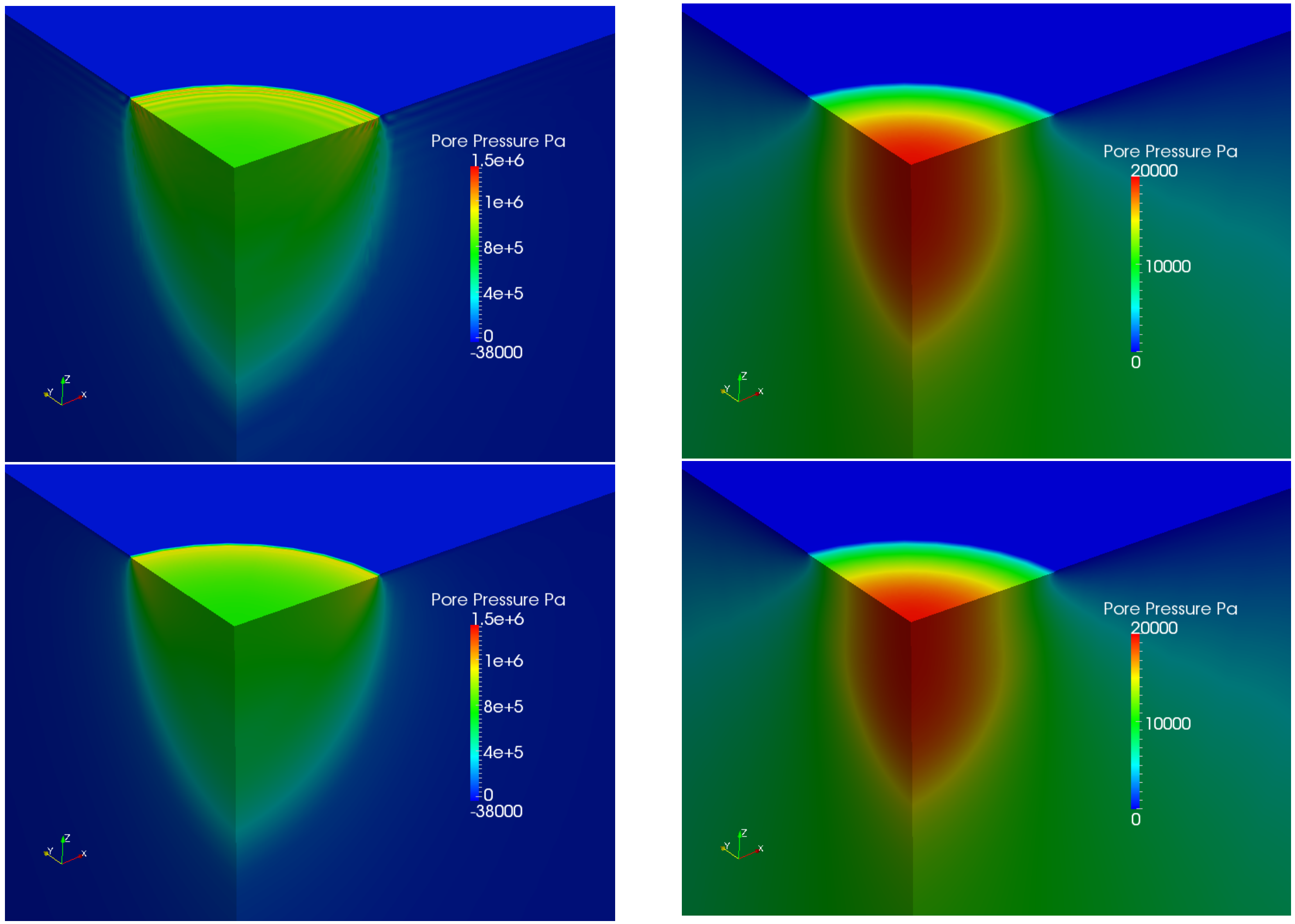
Footing placed on an elastoplastic porous medium

Without Stabilization

In low diffusivity case, the stabilization scheme is able to eliminate spurious oscillation.

With Stabilization

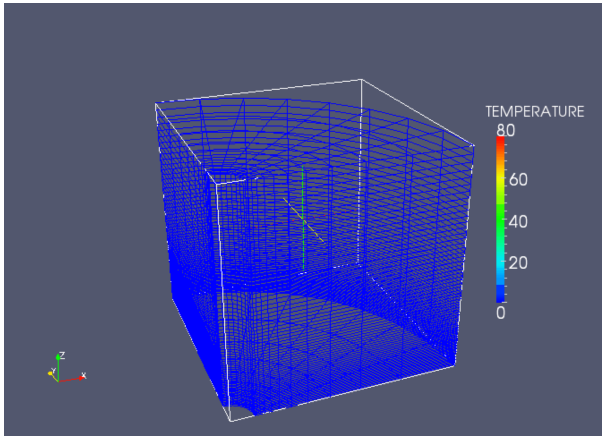
In high diffusivity case, the stabilization scheme does not introduce extra diffusivity that cause error.



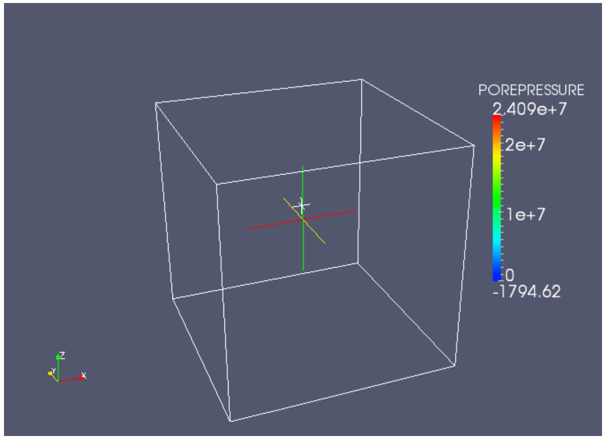
Low diffusivity case High diffusivity case

Heat pump problem

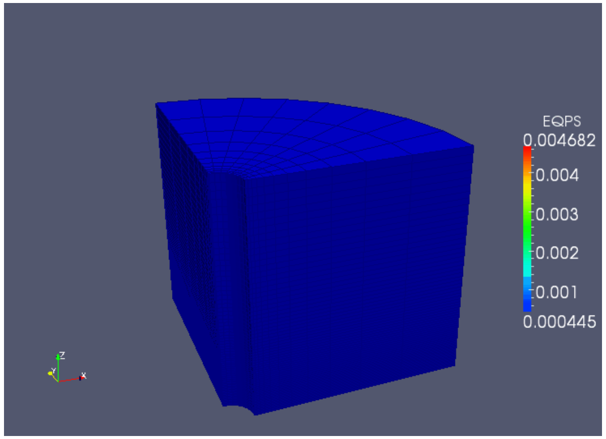
1. Hot liquid is injected into a elasto-plastic porous medium
2. Pore-fluid diffusion and heat diffusion occur at different rate
3. Porous medium expands even though no mechanical load is applied.



Temperature



Pore pressure



equivalent plastic strain

Conclusion

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- A fully coupled, finite deformation, stabilization poromechanics finite element model is implemented.
- This model preserve Mandel-Cryer effect, and is able to eliminate spurious oscillation due to the lack of inf-sup condition.
- Thermo-poro-plasticity model is extended and tested.
- Unsaturated flow and fully coupled thermo-poroelasiticty will be further tested via analytical solutions.

Bibliography

Sandia National Laboratories

- W.C. Sun, J.T. Ostien and A.G. Salinger, a stabilized enhanced deformation gradient finite element formulation for strongly coupled poromechanical simulations at finite strain, in preparation.
- J.W. Foulk III, W.C. Sun, G. Wagner, C. San Marchi, B. Somerday, the evolution of hydrogen concentration in 21 Cr-6Ni-9Mn austenitic stainless steel, in preparation.
- A. Mota, W.C. Sun, J.T. Ostien, J.W. Foulk III and K.N., Long, A variational transfer operator for mapping of internal variables, submitted *to Computer Methods in Applied Mechanics and Engineering*.
- W.C. Sun, Y.L. Young, Influence of soil heterogeneity on finite strain sedimentation-consolidation phenomena, submitted to *International Journal for Numerical and Analytical Methods in Geomechanics*.
- W.C. Sun, M.R. Kuhn, J.W. Rudnicki, Permeability in shear bands: a multiscale DEM-LBM analysis on shear band, submitted to *Acta geotechnica.*
- W.C. Sun, An unified method to predict diffuse and localized instabilities in sands, accepted, *Geomechanics and Geoengineering*.
- W.C. Sun, J.W. Rudnicki, J.E. Andrade and P. Eichhubl, Connecting microstructural attributes and permeability from 3-D tomographic images of in situ compaction bands using multi-scale computation, *Geophysical Research Letter*, doi : 10.1029/2011GL047683, 2011.
- W.C Sun, J.E. Andrade, J.W. Rudnicki, A multiscale method for characterization of porous microstructures and their impact on macroscopic effective permeability*, International Journal of Numerical Methods in Engineering*, Vol. 88, No.12, 1260-1279, 2011.
- R.I. Borja and W.C. Sun, Co-seismic sediment deformation during the 1989 Loma Prieta Earthquake, *Journal of Geophysical Research*, Vol.113, B08314,doi:10.1029/2007JB005265, 2008.
- R.I. Borja and W.C. Sun, Estimating inelastic sediment deformation from local site response simulations*, Acta Geotechnica*, Vol. 2, Number 3, 2007, pp.183-195.

Bibliography (Cont')

- W.C. Sun and J.E. Andrade, Capturing the effective permeability of field compaction band using hybrid lattice Boltzmann/Finite element simulations, Proceedings of 9th World Congress of Computational Mechanics/APCOM 2010, Sydney, Australia, 2010.
- W.C. Sun and J.E. Andrade, Surface Slumping of Submarine Slope And Its Relation To Material Instability, Proceedings of 16th US National Congress on Theoretical and Applied Mechanics, University Park, Pennsylvania, 2010.
- W.C. Sun and J.E. Andrade, Diffuse bifurcations of porous media under partially drained conditions, Proceedings of International Workshop on Multiscale and Multiphysics Processes in Geomechanics, Stanford, California, 2010.
- N. Lenoir, J.E. Andrade, W.C. Sun and J.W. Rudnicki, In situ permeability measurement inside compaction bands using X-ray CT and lattice Boltzmann calculations, Proceedings of 3th International Workshop on X-ray CT for geomaterials, New Orleans, Louisiana, 2010.
- J.E. Andrade, and W.C. Sun, Predictive framework for simulation of instabilities in sands, Jornadas Geotecnicas Colombianas, Bogota, Colombia, 2009.