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Finite-deformation diffusion of hydrogen in stainless steel alloys

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NNSA National Nuclear Security Administration

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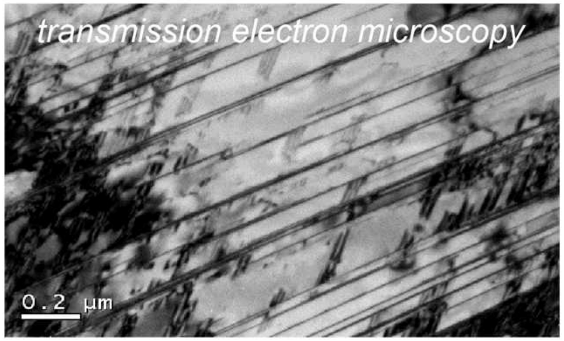
Introduction

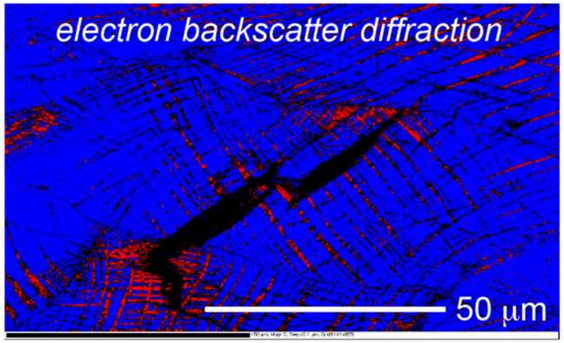
Academic Background

- Undergraduate: UT Austin (Class of 2013)
- Graduate: UC Berkeley (M.S. and Ph.D.)
  - Anticipated Graduation: ~05/2018
  - Research Advisor: Dr. Shaofan Li
  - Co-authored Publications:
    - A Peridynamics-SPH Coupling Approach to Simulate Soil Fragmentation Induced by Shock Waves (Feb. 2015)
    - A Hybrid Peridynamics-SPH Simulation of Soil Fragmentation by Blast Loads of Buried Explosive (in Press)

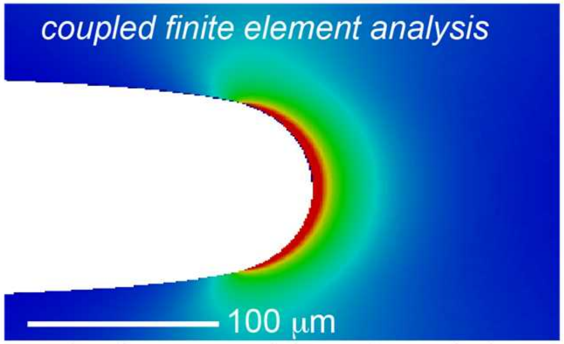
Motivation



deformation twins



phase transformations, fcc, bcc



plastic zone at blunted crack tip

Hydrogen Embrittlement

- Dissociated hydrogen molecules are introduced into a metal lattice through welding processes, environmental factors, etc..
- The embrittlement process can alter macroscopic material properties such as yield strength and ductility, which are driven by localized changes in the microstructure.
- Methods developed can be employed for phenomenological models of transport and trapping and continuum representations of microstructure.

Theoretical Background

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This path heavily leverages Sofronis/McMeeking (1989)* and Krom (1998).
Recent work by Leo and Anand (2013).

chemical potential

$$\mu_l = \mu_0 + RT\ln(\theta_l) - v_h\sigma_h$$

model for flux

$$\boldsymbol{j}_l = -\boldsymbol{m}_l c_l \nabla_{\boldsymbol{x}} \mu_l$$

$$\boldsymbol{F} = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} \qquad J = \det[\boldsymbol{F}]$$

$$\theta_l = c_l/n_l \qquad \theta_t = c_t/n_t$$

$$n_l = N_L/J \qquad n_t = N_T(\epsilon_p)/J$$

$$v_h = V_H J \qquad \tau_h = J\sigma_h$$

$$\boldsymbol{d}_l = RT\boldsymbol{m}_l$$

equilibrium of lattice/trap sites

$$\theta_t = \frac{1}{1 + \frac{1}{k_t\theta_l}}$$

$$\dot{c} = \dot{c}_l + \frac{\partial c_t}{\partial cl}\dot{c}_l + \frac{\partial c_t}{\partial n_t}\frac{\partial n_t}{\partial \epsilon_p}\dot{\epsilon}_p + \frac{\partial c_t}{\partial n_t}\frac{\partial n_t}{\partial J}\dot{J}$$

$$c_t = c_t(c_l, \epsilon_p, J)$$

conservation of hydrogen

$$\frac{d}{dt}\int_B c dv = -\int_{\partial B} \boldsymbol{j}\cdot\boldsymbol{n} da$$

$$C^* = c_l + \frac{n_t}{1 + \frac{n_l}{k_t c_l}} \qquad D^* = 1 + \frac{\partial c_t}{\partial c_l}$$

*P. Sofronis and R.M. McMeeking, J. Mech. Phys. Solids 37 (1989) 317

FEM Implementation

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conservation equation (reference configuration)

$$\frac{d}{dt}\int_{\mathcal{B}_0} C dV = -\int_{\partial B_0} J\boldsymbol{F}^{-1}\boldsymbol{j}\cdot\boldsymbol{N} dA$$

$$\Longrightarrow \int_{\mathcal{B}_0}\left(\dot{C} - \nabla_{\boldsymbol{X}}\cdot d_l\boldsymbol{C}^{-1}\nabla_{\boldsymbol{X}}C_L + \nabla_{\boldsymbol{X}}\cdot\frac{d_l V_H}{RT}\boldsymbol{C}^{-1}\nabla_{\boldsymbol{X}}\tau_h C_L\right)dV = 0$$

Multi-field variational formulation (Q1/P0 elements)

Variations in Displacement (η):

$$\int_{\mathcal{B}_0}\boldsymbol{P}\cdot\nabla_{\boldsymbol{X}}\boldsymbol{\eta} + \boldsymbol{B}\cdot\boldsymbol{\eta} dV - \int_{\partial\Gamma_0}\boldsymbol{t}\cdot\boldsymbol{\eta}\, dA = 0$$

Variations in Concentration (v):

$$\int_{\mathcal{B}_0}\left[\left(D^*\dot{C}_L + \theta_T\frac{dN_T}{d\epsilon_p}\dot{\epsilon}_p\right)v + d_l\boldsymbol{C}^{-1}\nabla_{\boldsymbol{X}}C_L\cdot\nabla_{\boldsymbol{X}}v - \frac{d_l C_L V_H}{RT}\boldsymbol{C}^{-1}\nabla_{\boldsymbol{X}}\hat{\tau}_h\cdot\nabla_{\boldsymbol{X}}v\right]dV + \int_{\partial\Gamma_0}J\boldsymbol{F}^{-1}\boldsymbol{j}_{app}\cdot\boldsymbol{N}v\, dA = 0$$

Variations in Pressure (ψ):

$$\int_{\mathcal{B}}\left(\tau_h - \hat{\tau}_h\right)\psi\, dV = 0$$

Example: 2D Block

Uniaxial extension of 2D block
With transient hydrogen diffusion:

Imposed Displacement $\boldsymbol{u} = \begin{bmatrix} AtX_1 \\ BtX_2 \\ 0 \end{bmatrix}$

Neo-hookean hyperelastic model $\boldsymbol{\sigma} = \frac{1}{2}\kappa\left[J_e - J_e^{-1}\right]\boldsymbol{I} + J_e^{-5/3}\mu dev[\boldsymbol{b}_e]$

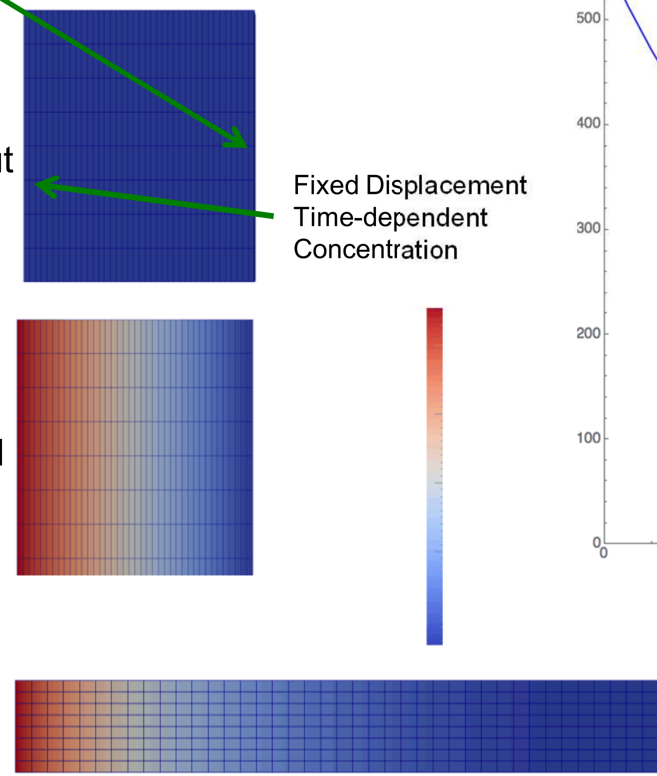
Time-dependent Displacement
Fixed Concentration

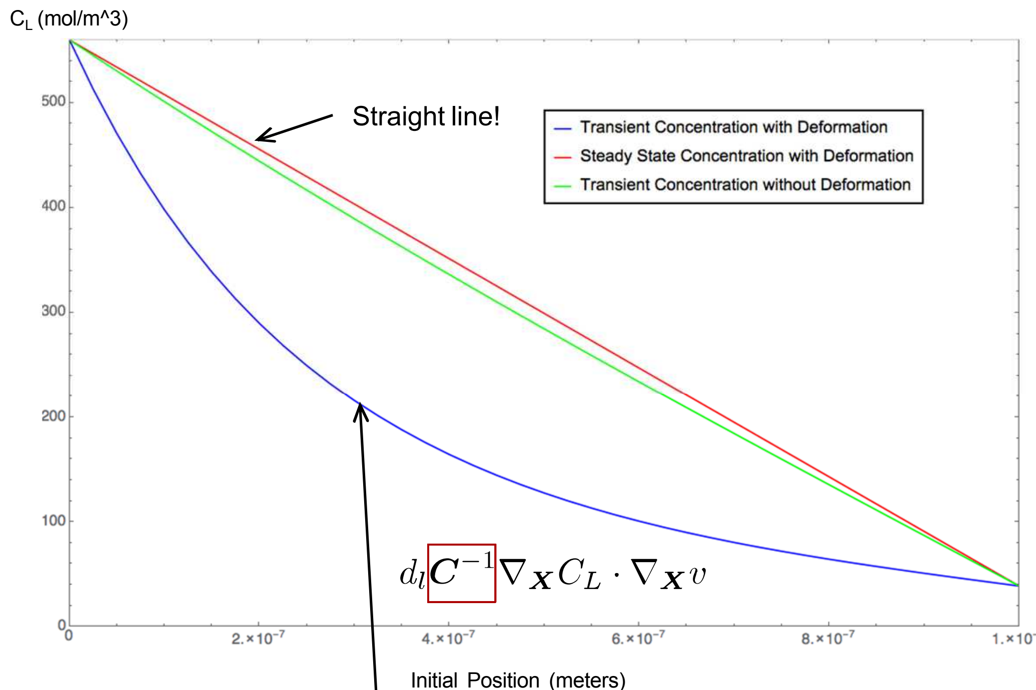
Initial Layout

Fixed Displacement
Time-dependent
Concentration

Undeformed

Deformed



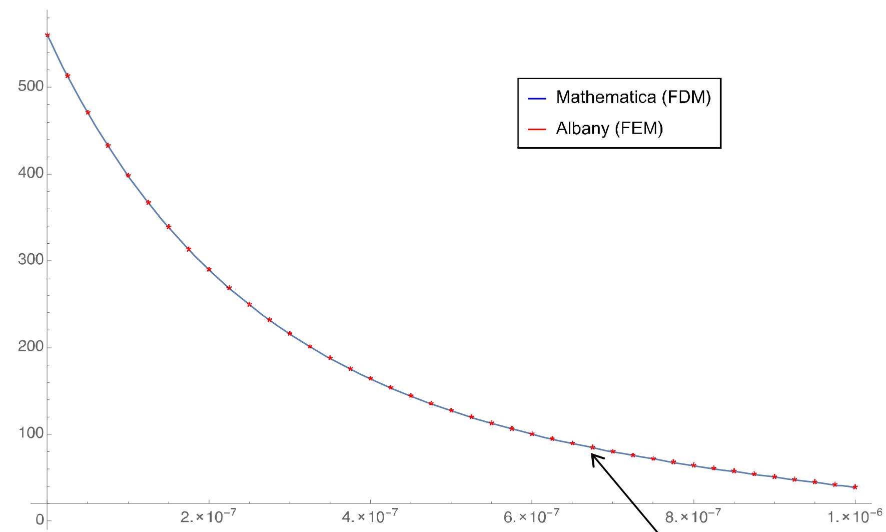


Pushback operation has distinct effect on the “Laplacian term” and hence, the concentration profile

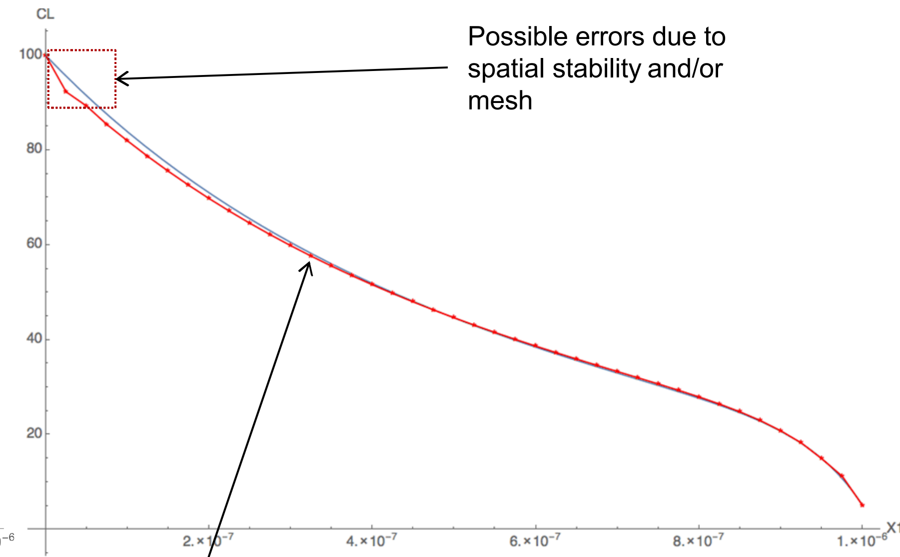
Example: 2D Block

Verification of solution: Goal is to implement tests to run in Albany

2D block diffusion without pressure gradient:



2D block diffusion with pressure gradient:



Possible errors due to spatial stability and/or mesh

Solutions match pretty well

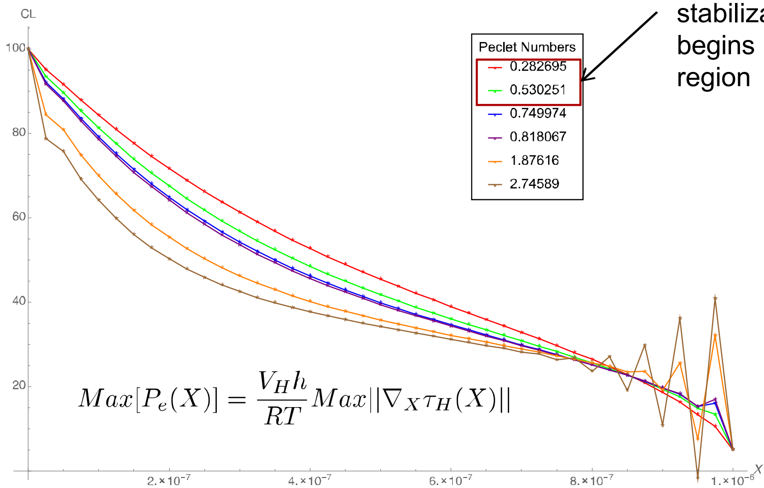
Example: 1D Stabilization Studies

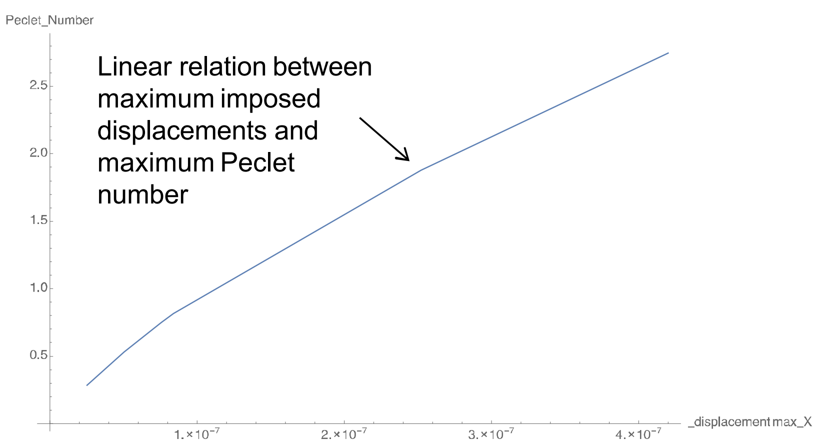
Spatial Stabilization and Spurious oscillation studies:

Imposed Displacements:

$$u(X) = C_0 + C_1 X + C_2 X^2 + C_3 X^3$$

Based on FEM (Albany):





Based on FDM (Mathematica):

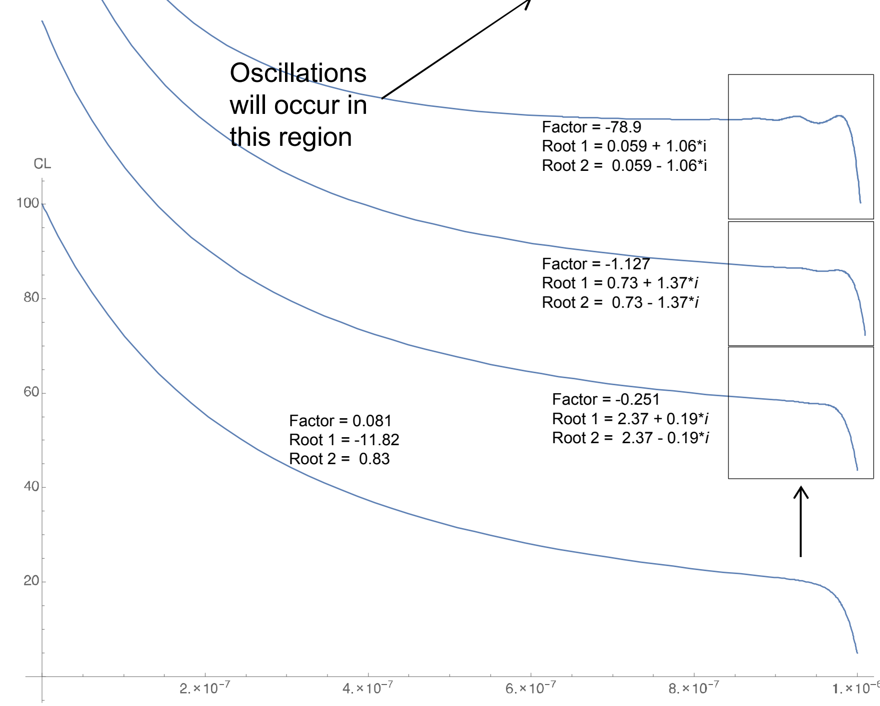
$$-\nabla_{\boldsymbol{X}} \cdot d_l \boldsymbol{C}^{-1} \nabla_{\boldsymbol{X}} C_L + \nabla_{\boldsymbol{X}} \cdot \frac{d_l V_H}{RT} \boldsymbol{C}^{-1} \nabla_{\boldsymbol{X}} \tau_h C_L = 0$$

$$\Longrightarrow \qquad \alpha C_{L,xx} + \beta C_{L,x} + \gamma C_L = 0$$

Plug FDM stencil into ODE:

$$\frac{1 \pm \sqrt{1 + 4\frac{\alpha^2 - \beta^2}{(\gamma + 2\alpha)^2}}}{\frac{2(\beta - \alpha)}{\gamma + 2\alpha}} = 0 \qquad \Longrightarrow \qquad \boxed{\frac{\alpha^2 - \beta^2}{(\gamma + 2\alpha)^2} \leq \frac{1}{4}}$$

Oscillations will occur in this region



Example: Simple channel fast pathway

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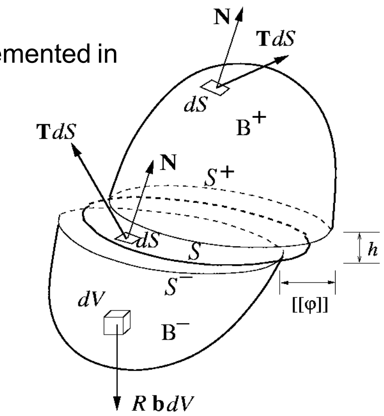
Implementation of Fast pathway (no deformation):

Jump is implemented in formulation

Cohesive Surface Element Formulation

$$C(\boldsymbol{X}) = \bar{C}(\boldsymbol{\phi}[\xi^1, \xi^2]) + \frac{[\![C]\!](\boldsymbol{\phi}[\xi^1, \xi^2])}{h}\xi^3$$



Diffusivity is a function of position when fast pathway is utilized

CSE thickness is needed to properly integrate the residual

CSE residual

$$\int_{\mathcal{B}^G} \nabla_{\boldsymbol{X}} v \boxed{D_L(\boldsymbol{X})} \nabla_{\boldsymbol{X}} C \, dV \approx \boxed{h} \sum_{j=1}^{N_{\text{int}}^M} \overline{W}(\xi_j^1, \xi_j^2) \left[v_a^+(\xi_j^1, \xi_j^2) \quad v_a^-(\xi_j^1, \xi_j^2) \right] \begin{bmatrix} \vec{B}^+(\xi_j^1, \xi_j^2) \\ \vec{B}^-(\xi_j^1, \xi_j^2) \end{bmatrix} D_L(\boldsymbol{X})$$

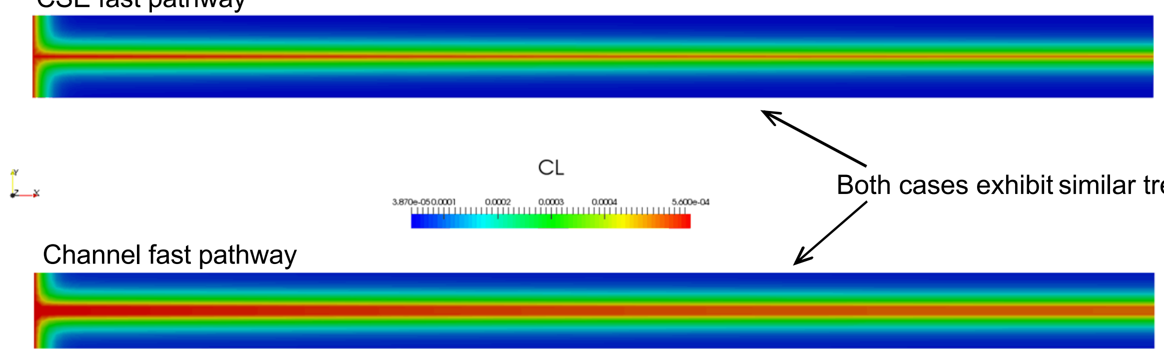
$$\left[\vec{B}^+(\xi_j^1, \xi_j^2) \quad \vec{B}^-(\xi_j^1, \xi_j^2) \right] \begin{bmatrix} C_a^+ \\ C_a^- \end{bmatrix}$$

$$(\ )$$

Increasing these terms will increase diffusion of the fast pathway

Comparison between channel and block

CSE fast pathway



Channel fast pathway

Both cases exhibit similar trends

Example: Polycrystals with fast pathway

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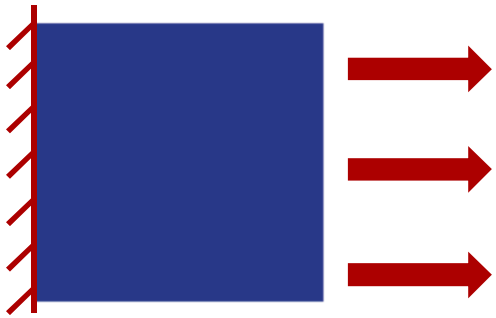
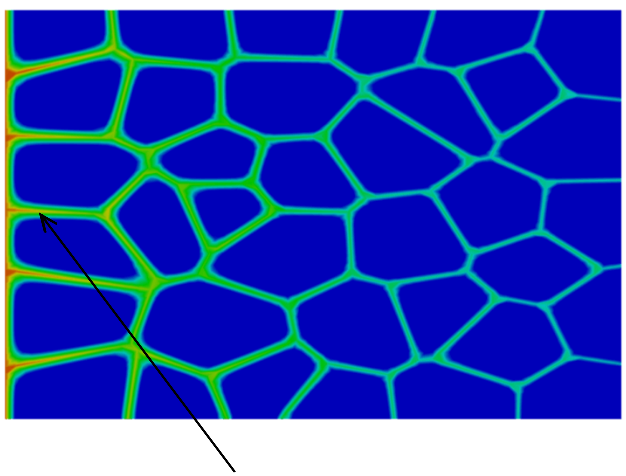
Grain interface diffusion coupled with mechanical loading:

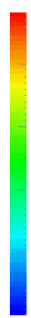


- Stretched in horizontal direction to a displacement of 2
- Fast pathway = 10^5*D_0

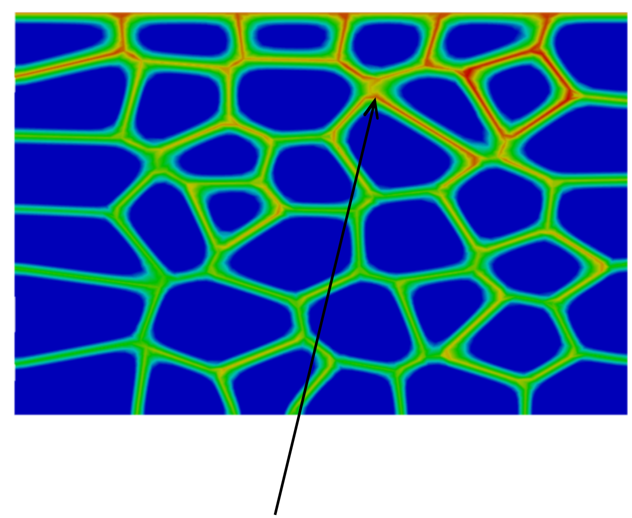
Horizontal diffusion (parallel to displacement)



Diffusion slows down.
Poisson effect will compress lattice along vertical direction.



Vertical diffusion (perpendicular to displacement)

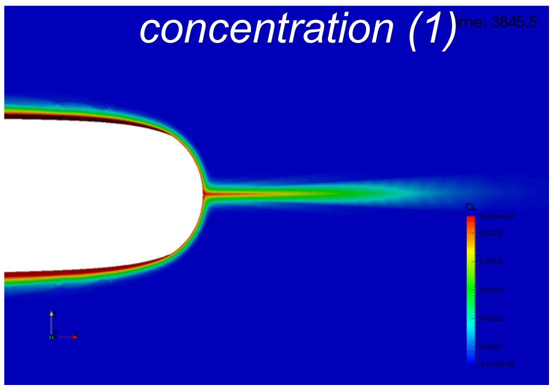


Diffusion speeds up as a result of the stretching of the lattice

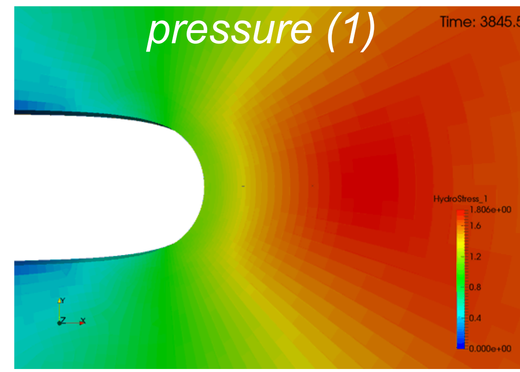
Example: Kfield simulation with embedded crack

Examining crack-tip diffusion:

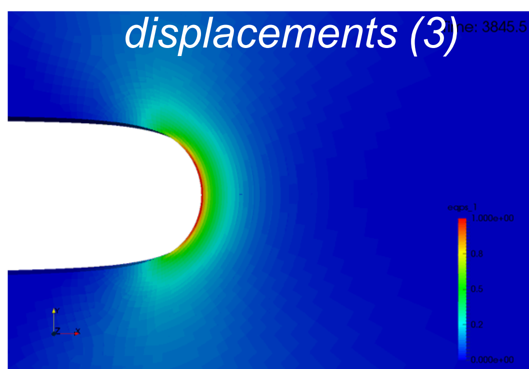
$$D^* \dot{C}_L$$



- Path: $10^5 D_0$
- K_{app}: 85 MPa m$^{1/2}$
- Time: 3850 s



$$\nabla_{\boldsymbol{X}} \cdot d_l \boldsymbol{C}^{-1} \nabla_{\boldsymbol{X}} C_L$$

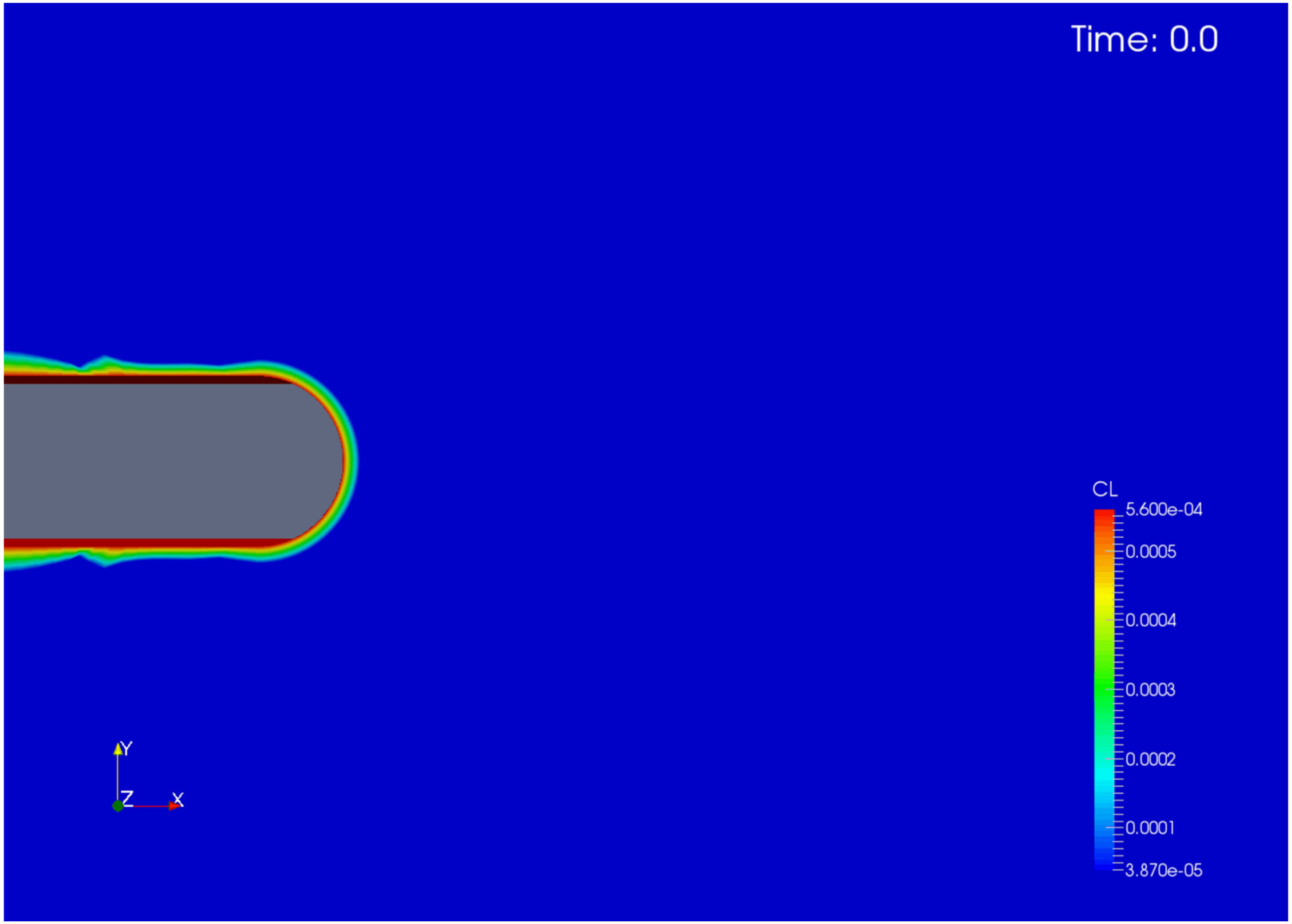


$$\nabla_{\boldsymbol{X}} \cdot \frac{d_l V_H}{RT} \boldsymbol{C}^{-1} \nabla_{\boldsymbol{X}} \tau_h C_L$$

$$+ \theta_T \frac{dN_T}{d\epsilon_p} \dot{\epsilon}_p$$

NOTE: 85 MPa m$^{1/2}$ is well below J_Q for 21Cr-6Ni-9Mn (220 MPa m$^{1/2}$)

Example: Kfield simulation with embedded crack (movie)



Summary

- Pushback operation significantly alters concentration profile (as seen in 2D block and polycrystal examples).
- The code can accommodate finite deformations and finite rotations when computing the concentrations.
- Spatial stabilization and the peclet number play a key role on the concentration profiles when using a coarse mesh, low diffusivities, or high pressure gradients.
- CSE provides efficient and accurate representation (relative to bulk elements) of a fast pathway.