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eXtremeMAT: Preliminary Engineering Scale Simulations with a ROM Material

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Benjamin W Spencer, Laurent Capolungo

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Preliminary Engineering Scale Simulations with a ROM Material

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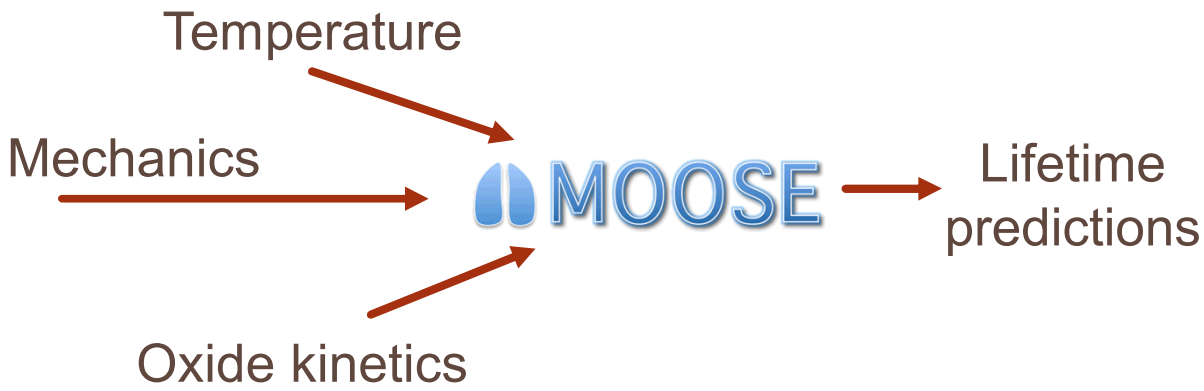
Mike Brady, Oak Ridge National Laboratory

Bottom Line Up Front

Task 2.5 Objective: Engineering scale simulations on the component scale using models informed by the different physics involved in oxidation

- Multiphysics problem for which the MOOSE framework is well suited
- Long-term goal of coupling the different physics required to model oxidation within an engineering scale simulation



- Preliminary work demonstrates the capability to solve mechanics simulations relevant to high temperature oxidation

Focus on Proof-of-Concept

Emphasis on demonstrating the capability of MOOSE to model the oxidation problem with simplified problems on the engineering component scale:

- Pressurized capsule under uniaxial tension
- Oxidized plate with prescribe oxide growth

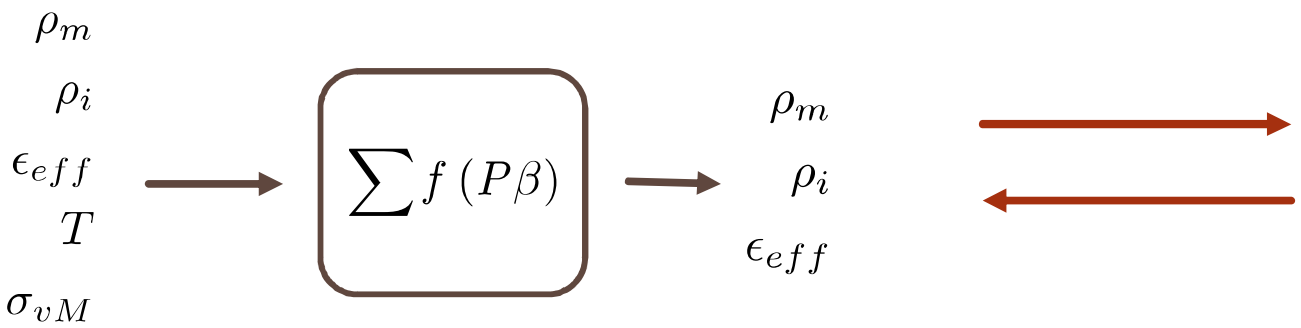
Goal to discuss how we can collaborate with the XMAT community to expand these preliminary modeling efforts:

- Brief overview of plans for next stage of engineering scale model and capability development

Pressurized Capsule

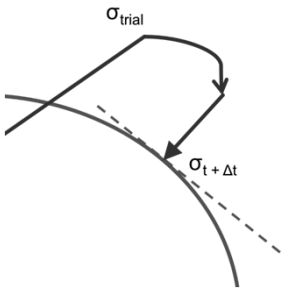
Demonstrates the use of a reduced order model, originally developed at LANL based on VPSC simulations and implemented as a constitutive model in MOOSE, to model a simplified pressurized capsule with uniaxial tension

LAROMANCE model



Calculates the effective plastic strain and dislocation densities from the previous stress, strain, dislocations, temperature state

MOOSE radial return algorithm



Iterates to return the stress state to the yield surface, using the LAROMANCE code as a constitutive model, to determine the required effective inelastic strain increment

LAROMANCE Model Development

The 'Los Alamos Reduced Order Models for Advanced Nonlinear Constitutive Equations' model is a polynomial regression with a weighted sum of terms:

$$\dot{\varepsilon}_{vm}(\bar{\rho}_{cell}, \bar{\rho}_w, \varepsilon_{vm}, \sigma_{vm}, T, \varphi) \sim \sum_{c,w,\varepsilon,\sigma,T,\varphi=0}^{degree} \alpha_{cw\varepsilon\sigma T\varphi} P_c(\bar{\rho}_{cell}) P_w(\bar{\rho}_w) P_\varepsilon(\varepsilon_{vm}) P_\sigma(\sigma_{vm}) P_T(T) P_\varphi(\varphi)$$

Outputs:

$\dot{\varepsilon}_{vm}, \dot{\bar{\rho}}_{cell}, \dot{\bar{\rho}}_w$

Inputs and outputs are transformed to reduce error accumulation

Inputs:

$\bar{\rho}_{cell}, \bar{\rho}_w, \varepsilon_{vm}, \sigma_{vm}, T, \varphi$

The coefficients capture the microstructural information that governs the strain response of the material and are material specific

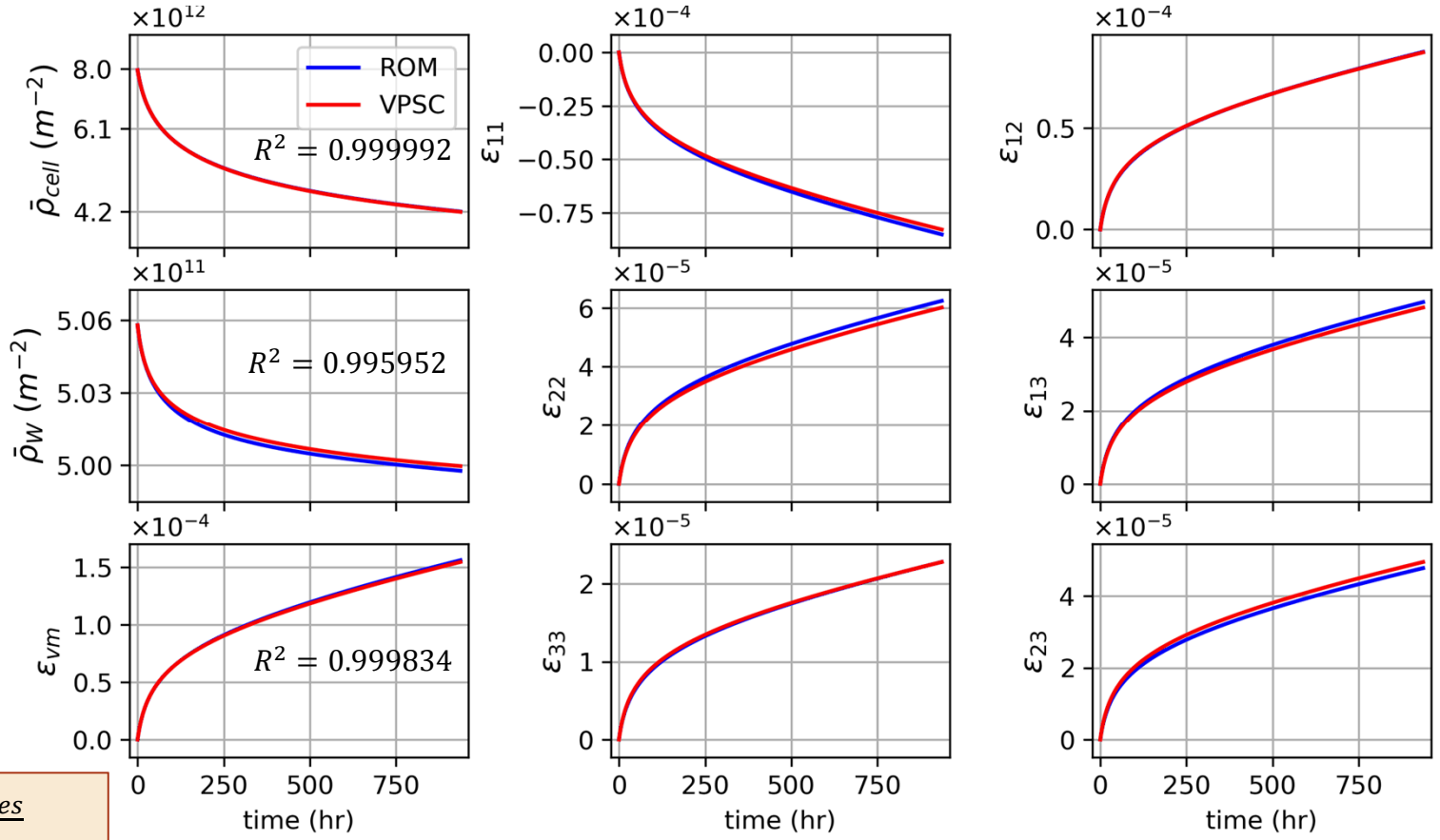
- Fit 3 x degree^6 coefficients

L. Capolungo

LAROMANCE Model Validation

Validated the LAROMANCE model against a VPSC simulation, comparing the predicted dislocation densities and strain

$$\sigma_{vm} = \sqrt{3J_2} = 10.45\ MPa$$
$$T_0 = 866.4K$$
$$\rho_{cell,0} = 7.951 \times 10^{12}\ m^{-2}$$
$$\rho_{w,0} = 5.058 \times 10^{11} m^{-2}$$



R^2 is measured for simulation of ε_{vm}: $R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$

$SS_{tot} = \sum(\varepsilon_{vm}^{VPSC} - \bar{\varepsilon}_{vm}^{VPSC})^2$; $SS_{res} = \sum(\varepsilon_{vm}^{ROM} - \varepsilon_{vm}^{VPSC})^2$

L. Capolungo

Verify Constitutive Functionality

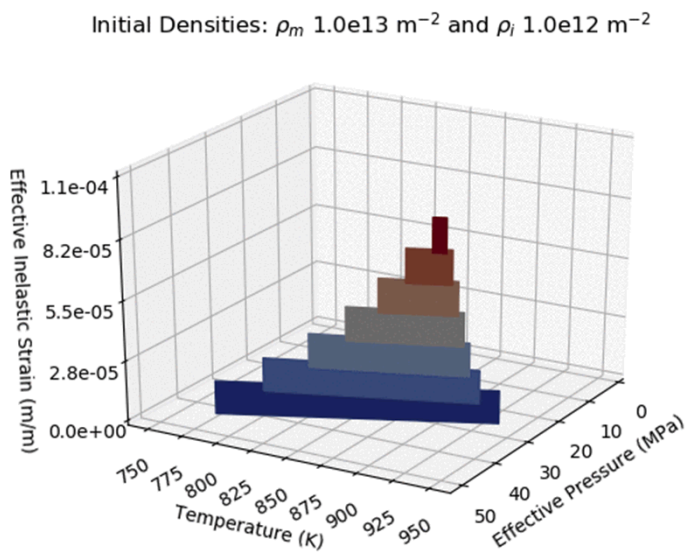
With the LAROMANCE constitutive model implemented in MOOSE, sampled the entire allowable input parameter space, evenly divided into six regions, to ensure the radial return implementation is reliable

Temperature (K)	Pressure (MPa)	Mobile Disl (m^{-2})	Immobile Disl (m^{-2})
950	50.0	1.0e13	1.0e12
910	40.9	9.0e12	8.6e11
870	30.0	8.0e12	7.2e11
830	20.0	7.0e12	5.8e11
790	10.0	6.0e12	4.4e11
750	2.0	5.0e12	3.0e11

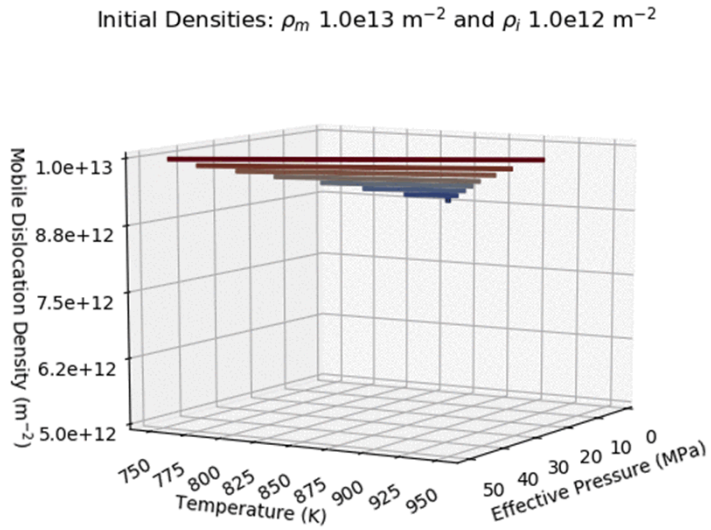
- Varied temperature and pressure individually while keeping mobile and immobile dislocations paired to simplify the parameter space
- Single Hex8 element, constant temperature and pressure

Verify Constitutive Functionality

With the LAROMANCE constitutive model implemented in MOOSE, sampled the entire allowable input parameter space, evenly divided into six regions

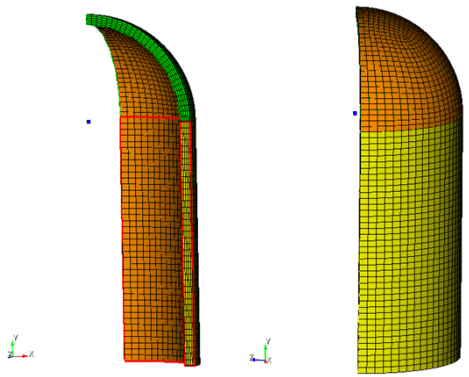


Higher effective strains calculated under in the higher temperature and pressure regions



More mobile dislocations are retained in the lower temperatures and pressures (fewer drivers for dislocation annihilation)

Capsule Geometry and Model



Use the LAROMANCE model in MOOSE for SS316H

- Developed for a previous cladding application

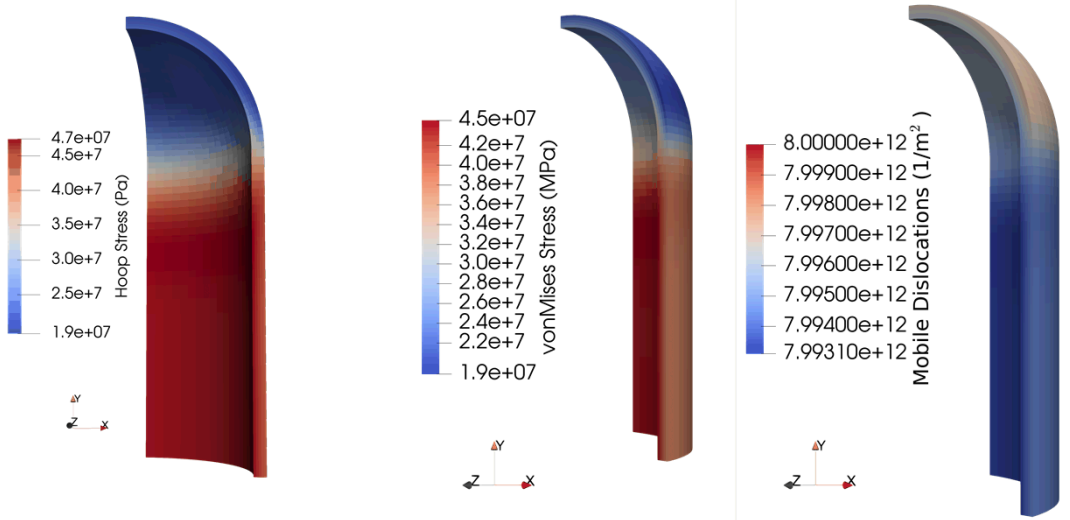
Use 1/8 symmetry geometry

- 5cm height, 2cm radius, 0.2cm thickness
- Apply internal pressure, uniaxial tension to outer cap

Allowable ranges limited:

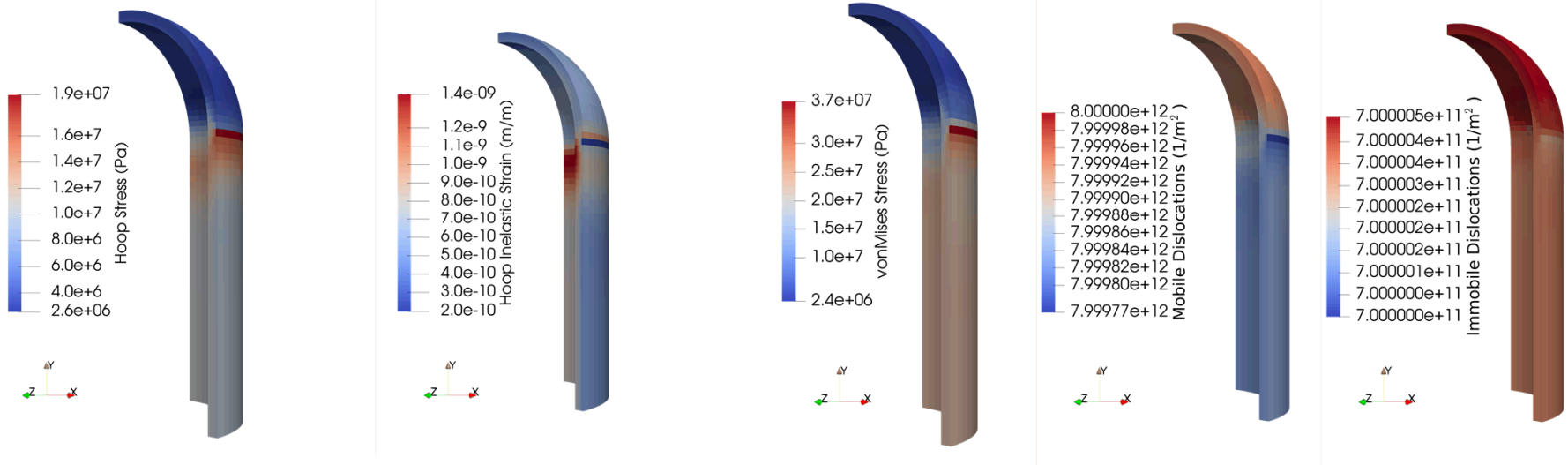
- Effective stress: 2MPa – 50MPa
- Temperature: use 801°C

Similar hoop and von Mises stress values with internal pressure only



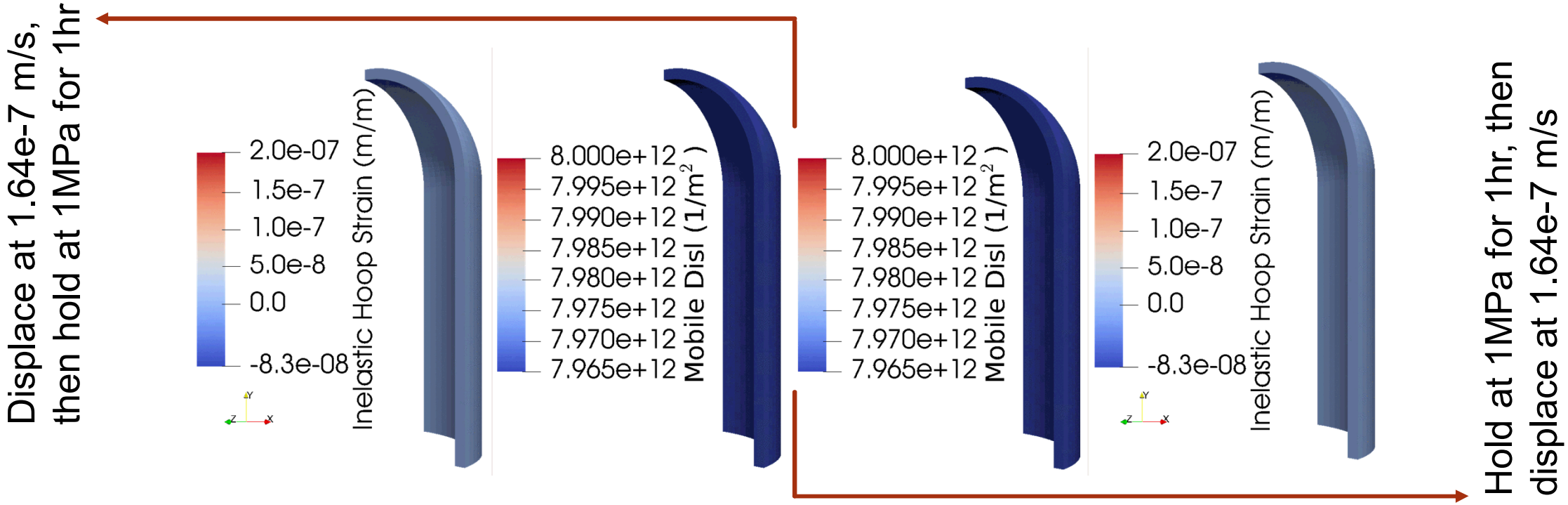
Simplified Uniaxial Tension Cases

- Different strain rates (1.64e-8 to 1.64e-5 m/s) to an approximate 0.01% strain with an internal pressure of 1.0 MPa (results shown for 1.64e-7 m/s)
- Achievable hoop stress is limited by the higher effective von Mises stress



- The evolution of the inelastic hoop strain and dislocation densities is strongly dependent on the displacement rate used; these increase with lower strain rates

Investigate Impact of Static Hold



The variation in the inelastic strain and mobile dislocation responses, with equivalent final stress states, shows the importance of using a constitutive model capable of capturing strain history influence

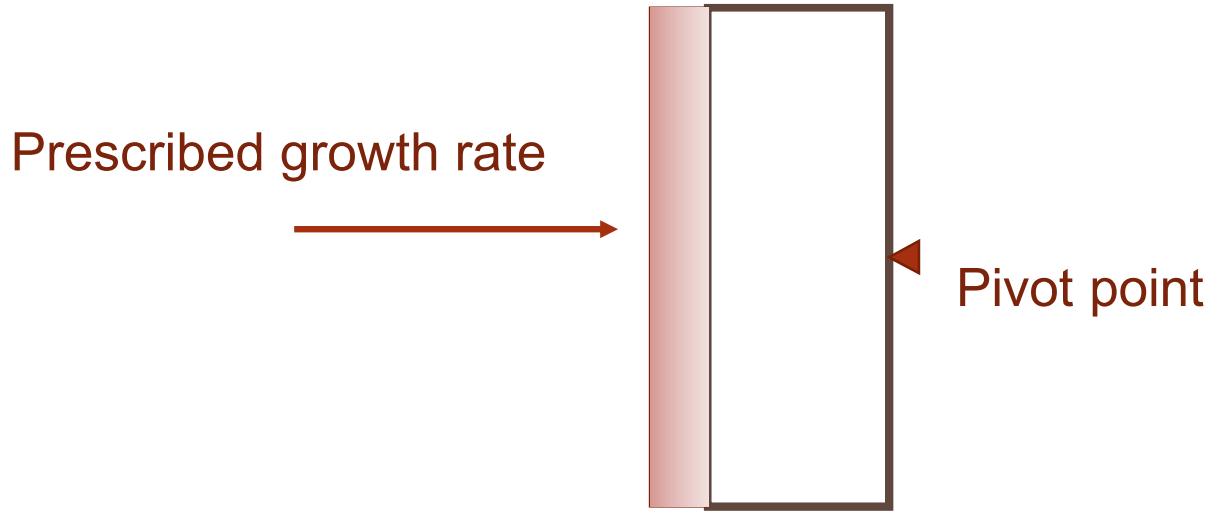
Oxide Growth Induced Eigenstrain

Demonstrate the mechanical response to an oxide growth induced eigenstrain with an engineering scale simulation as the oxide grows into the metal

- Focus on simulating the impact of the moving oxide interface on the mechanics
- Goal was to simulate both the oxide eigenstrain and the creep behavior
- Selected stainless steel 316H in order to use the LAROMANCE code

Assumptions for proof-of-concept:

- Stainless steel 316H
- Thick beam of 0.1mm x 0.4mm, with pivot and fixed points along the horizontal centerline



Prescribe Oxide Growth

Focusing only on the mechanics simulation at this stage, prescribed an approximate oxide thickness growth rate for SS316H at 801°C

- Assume only external oxidation, no internal oxidation
- Chromia as sole, prefect, and dense oxide
- Fit equation for k_p from mid-band for chromia formers (Gleeson 2010)

$$x = \frac{6.93\ cm^3/mol}{1.5 \cdot 15.99\ g/mol} \cdot (k_p \cdot t)^{1/2} \qquad k_p = 3.26 \times 10^{-20} \times e^{0.0176 \times T}$$

Apply a constant approximate volumetric eigenstrain to the oxide (Bernstein 1987)

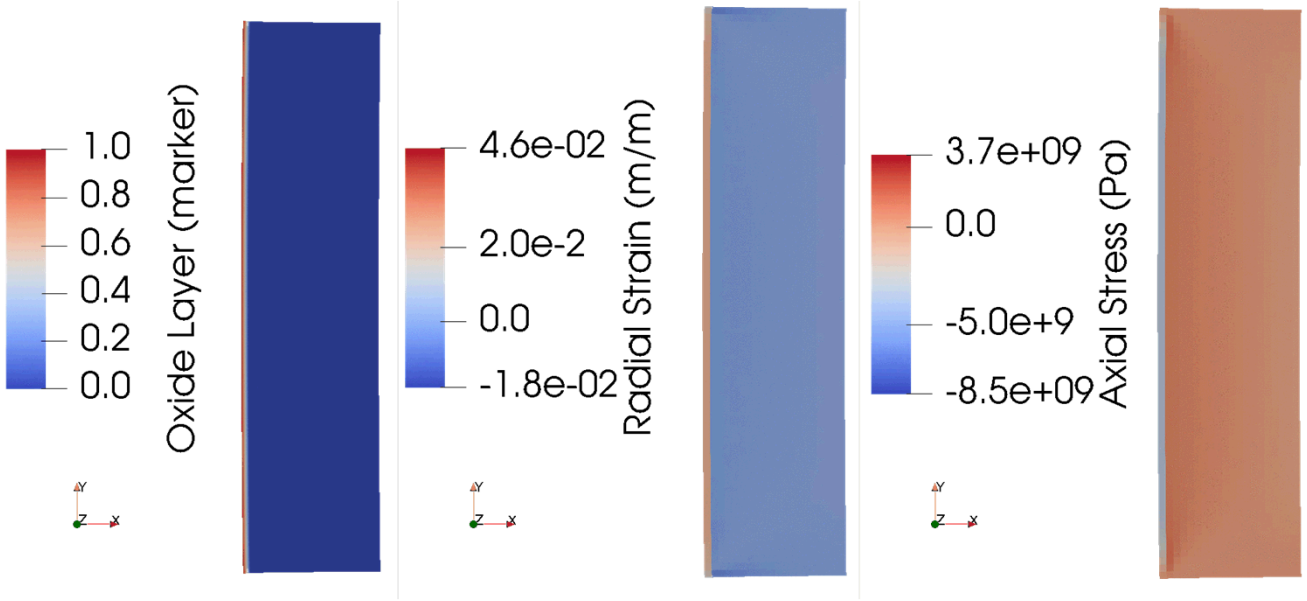
$$\epsilon_{ii} = \omega \cdot \left(\Phi^{1/3} - 1 \right)$$

Oxidized Plate Simulation

Preliminary moving oxide interface model demonstrates expected stress patterns

Challenges in modeling required additional simplifications:

- Small, total strain formulation
- Isotropic elastic materials
- Diffuse interface approach requires mesh adaptivity

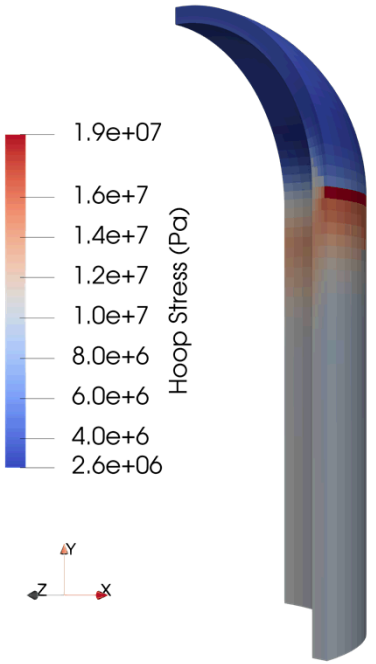


Continued development work required to address these challenges for mechanics simulation aspects of the oxidation modeling

Status Summary

These preliminary simulations demonstrate MOOSE capabilities:

- Pressurized capsule simulation using the LAROMANCE code demonstrate the ability to capture the dependence of the material response on different loading histories
- Initial oxidized plate simulations highlight the need for continued mechanics capability development

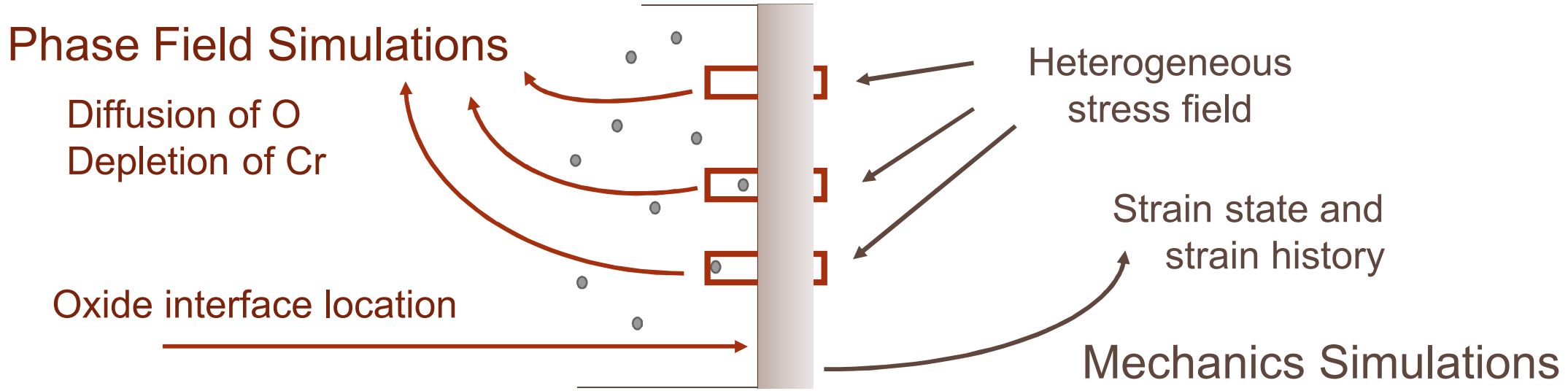


These proof-of-concept modeling efforts provide a basis for future development within the XMAT framework:

- Collaboration on additional LAROMANCE code for SS347H
- Assistance with phase field modeling for oxide interface modeling

Explore Coupling with Phase Field

Propose a multiscale simulation, using a set of phase field simulations to model the oxide layer growth and coupled to the mechanics



Hope to collaborate with Youhai Wen on phase field efforts to learn from and leverage the existing oxide kinetics modeling expertise in XMAT

Concurrent Modeling for Spallation

Tight coupling with mechanics adds the capability to model damage, including cracking in the alloy and spallation of the oxide

- Given oxidation kinetics we can work towards predicting spallation
- Challenge: Passing the high tensile stresses in metal due to oxide growth induced strain to the oxidation kinetic model to account of additional pathways

Goal: Capture the influence of oxide growth and internal stress within the metal on the conditions that lead to spallation

- Challenges to address include:
  - Predicting conditions that lead to cracking/buckling of the oxide (thermal expansion, microstructure)
  - Accounting for the metal-oxide interface characteristics

Summary

Task 2.5 Objective: Engineering scale simulations on the component scale using models informed by the lower-length scale physics involved in oxidation

- Preliminary proof-of-concept simulations to jump-start the engineering/component scale efforts using LAROMANCE codes
- Next steps involve coupling phase field simulations with mechanics to model the stress response to given oxide kinetics
- Focus on model predictions for spallation of the oxide