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A Finite Deformation Variational Multiscale Framework for Modeling Strain Localization

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Variational Multiscale Method (VMM)

Previous work on VMM towards localization

- VMM was originally proposed by Hughes and coworkers [Hughes et al. 1998]
- Garikipati and Hughes applied VMM to analyze small-strain localization problem, in one and two dimensions [Garikipati and Hughes 1998, Garikipati and Hughes 2000]
  $\boldsymbol{u} = \bar{\boldsymbol{u}} + \boldsymbol{u}'$
- Hund and Ramm applied VMM to small-strain localized phenomena, where focus lies on the analysis of locality constrains. [Hund and Ramm 2007]

Key points of this work

- Finite deformation region: two-scale decomposition of deformation fields
- Potential energy functional and variational principles
- Completely general, independent of specific constitutive models
- Use FEM to discretize and solve both scales
- Issues to address: locality constraint, non-local regularization

Kinematics and Deformation Mapping

Two scale deformation mapping

$$\bar{\boldsymbol{X}} = \bar{\varphi}(\boldsymbol{X}), \quad \boldsymbol{x} = \varphi'(\bar{\boldsymbol{X}})$$

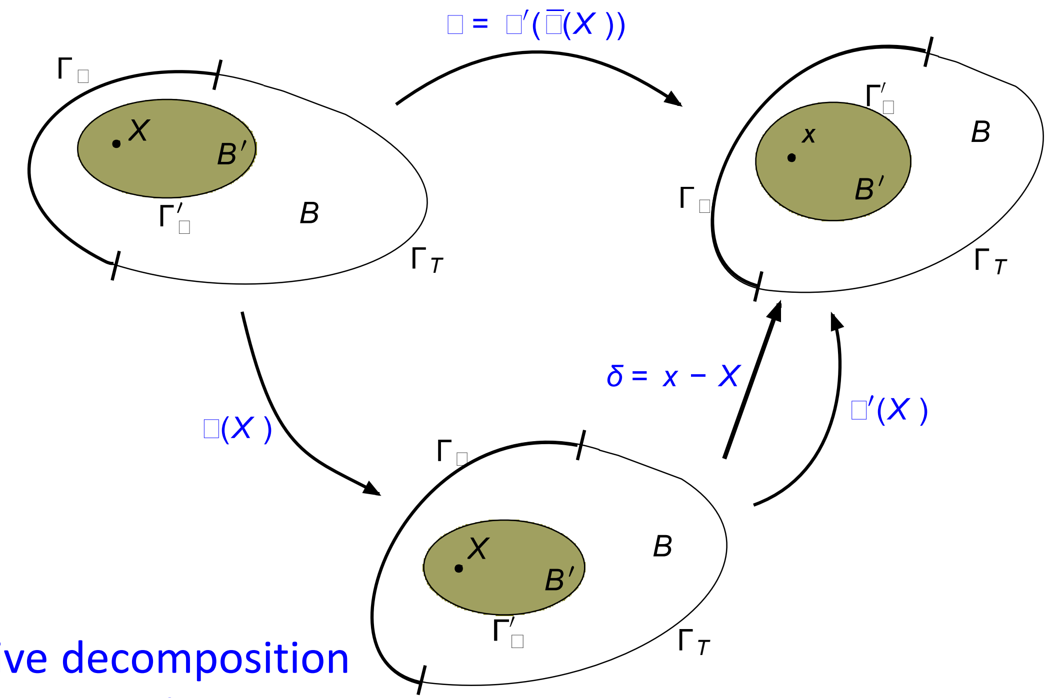
Total deformation mapping

$$\varphi(\boldsymbol{X}) = \varphi'(\bar{\varphi}(\boldsymbol{X}))$$

Introduce fine scale field

$$\boldsymbol{\delta} = \boldsymbol{x} - \bar{\boldsymbol{X}}$$
$$= \varphi'(\bar{\varphi}(\boldsymbol{X})) - \bar{\varphi}(\boldsymbol{X})$$

Decomposition of deformation mapping



Additive decomposition of deformation mapping

$$\varphi = \underbrace{\bar{\varphi}}_{\text{coarse}} + \underbrace{\boldsymbol{\delta}}_{\text{fine}}$$

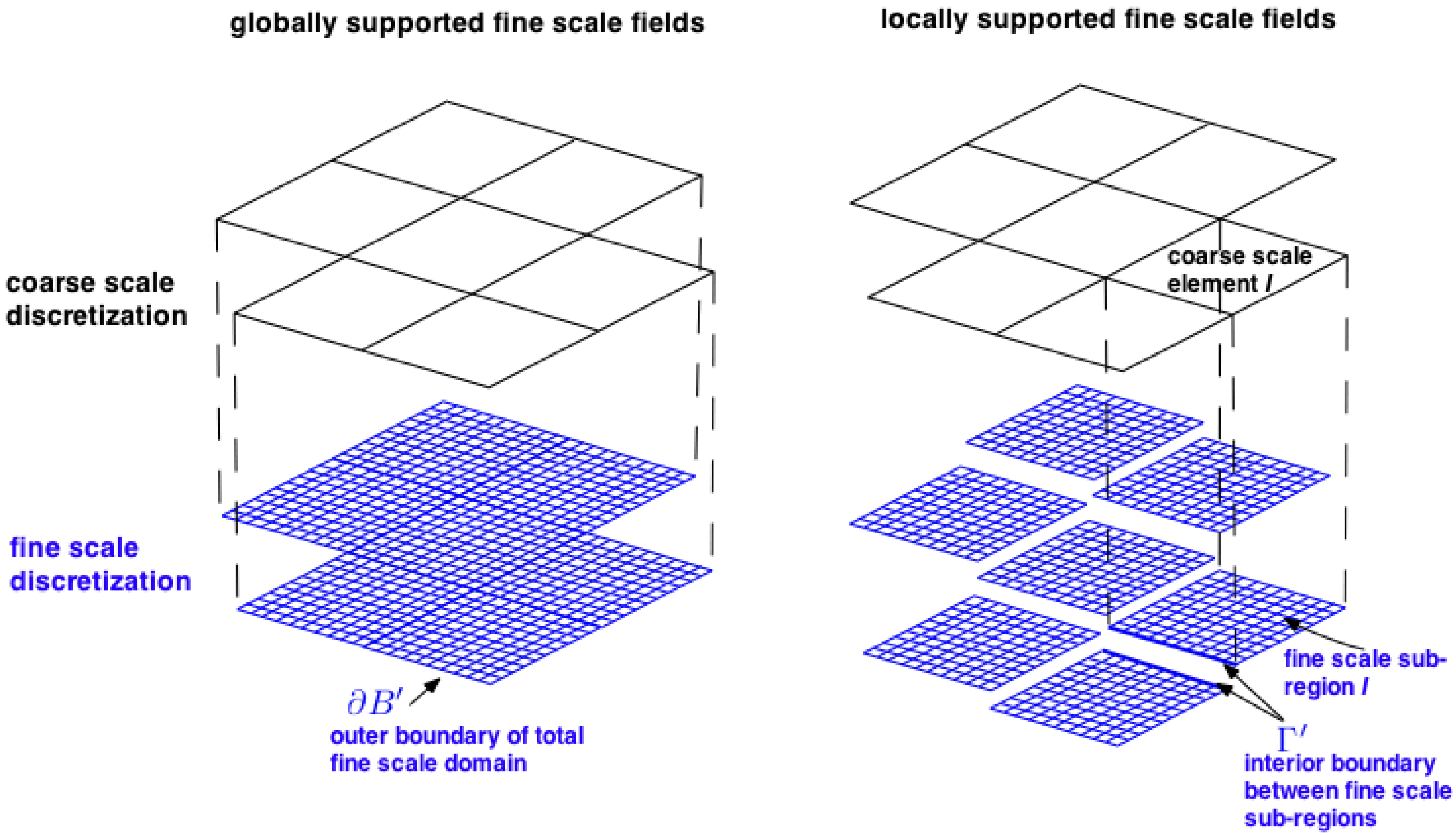
Multiplicative decomposition of deformation gradient

$$\boldsymbol{F} = \frac{\partial \boldsymbol{x}}{\partial \bar{\boldsymbol{X}}} \frac{\partial \bar{\boldsymbol{X}}}{\partial \boldsymbol{X}} = \boldsymbol{F}' \bar{\boldsymbol{F}}$$

Small strain contourpart [Garikipati and Hughes 1998, Garikipati and Hughes 2000]

$$\boldsymbol{u} = \bar{\boldsymbol{u}} + \boldsymbol{u}'$$

Global vs. locally supported fine scale domain



Boundary condition: $\delta = 0 \;\; \text{on } \partial B'$

$$\delta = 0 \;\; \text{on } \partial B'$$

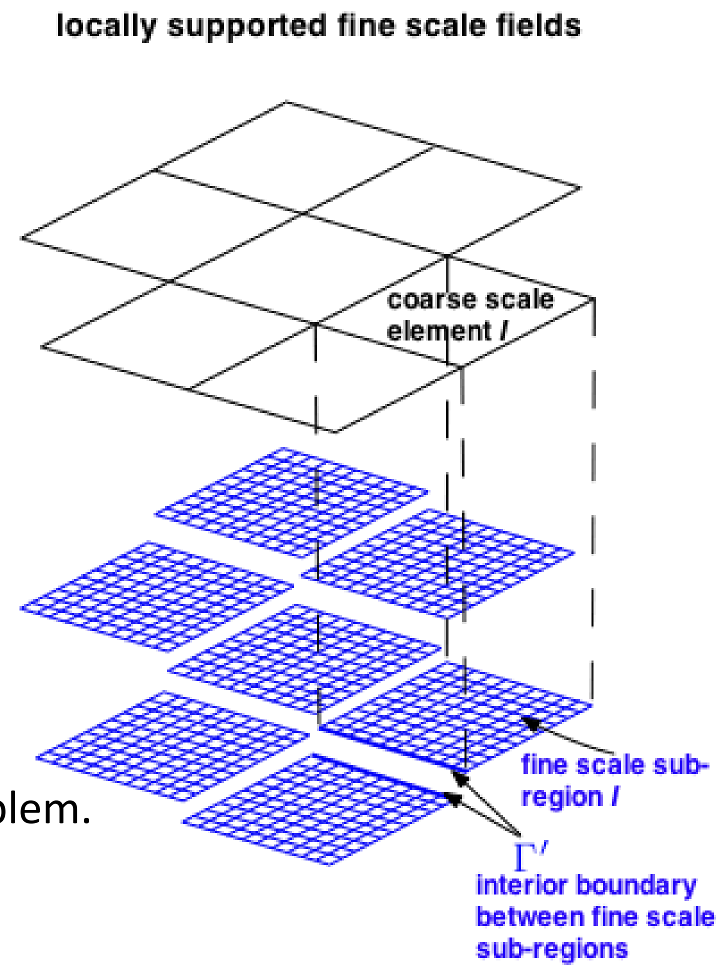
$$\delta = ? \;\; \text{on } \Gamma'$$

Constraints on fine scale problem

- Locality assumption generates additional interior boundaries Γ' between fine scale sub-regions. Different options are being explored in this work

1. Homogeneous boundary condition with $\boldsymbol{\delta} = 0$
   - Commonly used in VMM
   - Less numerical efforts
   - Rough approximation

1. Continuity boundary condition with $[\![\boldsymbol{\delta}]\!] = 0$
   1) Constraint by penalty method
   2) Constraint by point-wise Lagrange multiplier
   3) **Constraint by Lagrange multiplier in weak sense**



- Alternative option is globally constrained fine scale problem. However, the formulation is <u>not stable</u>, need stabilization technique.

The potential energy formulation

Two-Field Functional $\quad \boldsymbol{\varphi} = \bar{\boldsymbol{\varphi}} + \boldsymbol{\delta}$

$$I[\bar{\boldsymbol{\varphi}}, \boldsymbol{\delta}] = \int_B W(\boldsymbol{F}, \boldsymbol{Z})\ dV - \int_B R\boldsymbol{B} \cdot \boldsymbol{\varphi}\ dV - \int_{\partial_\Gamma B} \boldsymbol{T} \cdot \boldsymbol{\varphi}\ dS$$

where $\quad W(\boldsymbol{F}, \boldsymbol{Z}) \quad$ Stored strain energy function

For equilibrium, the first variations of the total potential energy mush vanish

Coarse scale:

$$DI[\bar{\boldsymbol{\varphi}}, \boldsymbol{\delta}] \cdot \delta\bar{\boldsymbol{\varphi}} = \int_B \boldsymbol{P}(\boldsymbol{F}, \boldsymbol{Z}) : D\boldsymbol{F} \cdot \delta\bar{\boldsymbol{\varphi}}\ dV - \int_B R\boldsymbol{B} \cdot \delta\bar{\boldsymbol{\varphi}}\ dV - \int_{\partial_\Gamma B} \boldsymbol{T} \cdot \delta\bar{\boldsymbol{\varphi}} \mathrm{d}S = 0$$

Fine scale:

$$DI[\bar{\boldsymbol{\varphi}}, \boldsymbol{\delta}] \cdot \delta\boldsymbol{\delta} = \int_{B'} \boldsymbol{P}(\boldsymbol{F}, \boldsymbol{Z}) : D\boldsymbol{F} \cdot \delta\boldsymbol{\delta}\ dV - \int_{B'} R\boldsymbol{B} \cdot \delta\boldsymbol{\delta}\ dV - \int_{\partial_\Gamma B'} \boldsymbol{T} \cdot \delta\boldsymbol{\delta} \mathrm{d}S = 0$$

- A single stored strain energy function is assumed, i.e., essentially the same systems of PDEs are assumed to describe the physics at all scales.
- ***F*** is the total deformation gradient, therefore, coarse and fine scales equations are coupled.
- FEM will be used to discretize both scales.
- Locality constraint will introduce additional energy term.

Enforcing locality constrains

In the Lagrange method, additional energy is introduced into the system.
The potential energy becomes three-field, **Λ** is the Lagrange multiplier

$$I[\bar{\boldsymbol{\varphi}}, \boldsymbol{\delta}, \boldsymbol{\Lambda}] = \int_B W(\boldsymbol{F}, \boldsymbol{Z})\, dV + \boxed{\int_{\Gamma'} \boldsymbol{\Lambda} \cdot [\![\boldsymbol{\delta}]\!]\, dS} - \int_B R\boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_\Gamma B} \boldsymbol{T} \cdot \boldsymbol{\varphi}\, dS$$

The same variation principle is applied, and the resulting residual equations are written as

$$\bar{\boldsymbol{R}} = \int_B \boldsymbol{P} \cdot \mathrm{Grad}\, \delta\bar{\boldsymbol{\varphi}}\, dV - \int_B R\boldsymbol{B} \cdot \delta\bar{\boldsymbol{\varphi}}\, dV - \int_{\partial_\Gamma B} \boldsymbol{T} \cdot \delta\bar{\boldsymbol{\varphi}}\, dS = 0$$

Within each coarse element I :

$$\boldsymbol{R}' = \int_{B'} \boldsymbol{P} \cdot \mathrm{Grad}\, \delta\boldsymbol{\delta}\, dV - \int_{B'} R\boldsymbol{B} \cdot \delta\boldsymbol{\delta}\, dV \pm \int_{\Gamma'} \boldsymbol{\Lambda} \cdot \delta\boldsymbol{\delta}\, dS = 0$$

$$\boldsymbol{R}^{\Lambda} = \int_{\Gamma'} \delta\boldsymbol{\Lambda} \cdot [\![\boldsymbol{\delta}]\!]\, dS = 0$$

- $\boldsymbol{R}^{\Lambda}$ is the residual for Lagrange multiplier d.o.f.
- Coarse scale residual is unchanged, while fine scale residual includes additional term.
- $[\![\boldsymbol{\delta}]\!] = \boldsymbol{\delta}^I - \boldsymbol{\delta}^J$, where *I* and *J* associate with two sides of the interior boundary

Finite Element Discretization

Introduce finite element discretization

Coarse scale: $$\bar{\boldsymbol{\varphi}} = \sum_{a=1}^{\mathrm{n_{node}}} N_a \bar{\boldsymbol{\varphi}}_a$$

Fine scale: $$\boldsymbol{\delta} = \sum_{\alpha=1}^{\mathrm{n_{node}}} \lambda_\alpha \boldsymbol{\delta}_\alpha$$

Lagrange multiplier: $$\boldsymbol{\Lambda} = \sum_{i=1}^{nl} \boldsymbol{\phi}_A \boldsymbol{\Lambda}_A$$

Remarks:

- Different interpolation functions may be chosen for three-fields
- Inf-sup condition governs the selection of possible interpolation functions (under investigation).

Discrete form of governing equations

$$\bar{\boldsymbol{R}}_a = \int_B \boldsymbol{P} \cdot \mathrm{Grad}\, N_a \; dV - \int_B R\boldsymbol{B} N_a \; dV - \int_{\partial_\Gamma B} \boldsymbol{T} N_a \; dS = \boldsymbol{0}$$

$$\text{Within each coarse element } I :$$

$$\boldsymbol{R}'_\alpha = \int_{B'} \boldsymbol{P} \cdot \mathrm{Grad}\, \lambda_\alpha \; dV - \int_{B'} R\boldsymbol{B} \lambda_\alpha \; dV \pm \int_{\Gamma'} N_a \boldsymbol{\phi}_a \cdot \lambda_\alpha \; dS = \boldsymbol{0}$$

$$\boldsymbol{R}^\phi_a = \int_{\Gamma'} N_a (\lambda^I_\alpha \boldsymbol{\delta}^I_\alpha - \lambda^J_\alpha \boldsymbol{\delta}^J_\alpha) \; dS = 0$$

Linearization of Governing Equations

the discrete linearized system of equations for the variational multsicale problem can be written as

$$\bar{\boldsymbol{K}}_{ab}\Delta\bar{\boldsymbol{\varphi}}_b + \sum_{I=1}^{\bar{n}} \boldsymbol{H}^T_{a\beta}\Delta\boldsymbol{\delta}_\beta = -\bar{\boldsymbol{R}}_a$$

$$\boldsymbol{H}_{\alpha b}\Delta\bar{\boldsymbol{\varphi}}^I_b + \boldsymbol{K}'_{\alpha\beta}\Delta\boldsymbol{\delta}_\beta + \sum_{l=1}^{n_{\Gamma'}}\left[\pm\boldsymbol{H}^\Lambda_{\alpha B}\Delta\boldsymbol{\Lambda}^l_B\right] = -\boldsymbol{R}'_\alpha$$

$$\text{for the } lth\ \Gamma' : \quad \boldsymbol{H}^{\Lambda I}_{A\alpha}\Delta\boldsymbol{\delta}^I_\alpha - \boldsymbol{H}^{\Lambda J}_{A\alpha}\Delta\boldsymbol{\delta}^J_\alpha = -\boldsymbol{R}^\Lambda_A$$

The linearized terms will be

$$\bar{\boldsymbol{K}}_{ab} = \int_B \operatorname{Grad} N_a : \mathbb{C}(\boldsymbol{F}) : \operatorname{Grad} N_b \; dV$$

$$\boldsymbol{K}'_{\alpha\beta} = \int_{B'} \operatorname{Grad} \lambda_\alpha : \mathbb{C}(\boldsymbol{F}) : \operatorname{Grad} \lambda_\beta \; dV$$

$$\int$$

$$\boldsymbol{H}^T_{a\beta} = \int_{B'} \operatorname{Grad} N_a : \mathbb{C}(\boldsymbol{F}) : \operatorname{Grad} \lambda_\beta \; dV$$

$$\boldsymbol{H}_{\alpha b} = \int_{B'} \operatorname{Grad} \lambda_\alpha : \mathbb{C}(\boldsymbol{F}) : \operatorname{Grad} N_b \; dV$$

$$\boldsymbol{H}^\Lambda_{A\alpha} = \int_{\Gamma'} \boldsymbol{\phi}_A \boldsymbol{\lambda}_\alpha \; dS$$

The system of equations are coupled in that:

- ***F*** is the total deformation gradient
- The projection matrix *H* contains interpolation functions from both scales

the fourth-order elasticity tensor

$$\mathbb{C} := \partial\boldsymbol{P}/\partial\boldsymbol{F} = \partial^2 W/\partial\boldsymbol{F}\partial\boldsymbol{F}$$

Iterative solution procedure

$$\bar{\boldsymbol{K}}_{ab}\Delta\bar{\boldsymbol{\varphi}}_b + \sum_{I=1}^{\bar{n}} \boldsymbol{H}^T_{a\beta}\Delta\boldsymbol{\delta}_\beta = -\bar{\boldsymbol{R}}_a$$

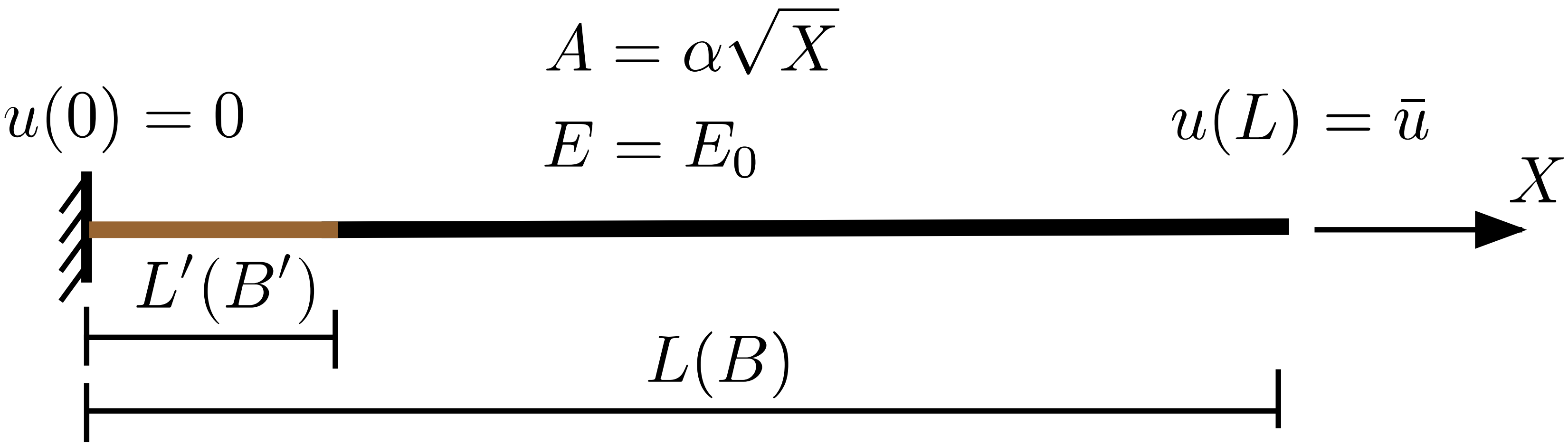
Update coarse incremental fields within each coarse element

Static condensation to eliminate fine scale fields

$$\boldsymbol{H}_{\alpha b}\Delta\bar{\boldsymbol{\varphi}}^I_b + \boldsymbol{K}'_{\alpha\beta}\Delta\boldsymbol{\delta}_\beta + \sum_{l=1}^{n_{\Gamma'}}\left[\pm\boldsymbol{H}^{\Lambda}_{\alpha B}\Delta\boldsymbol{\Lambda}^l_B\right] = -\boldsymbol{R}'_\alpha$$

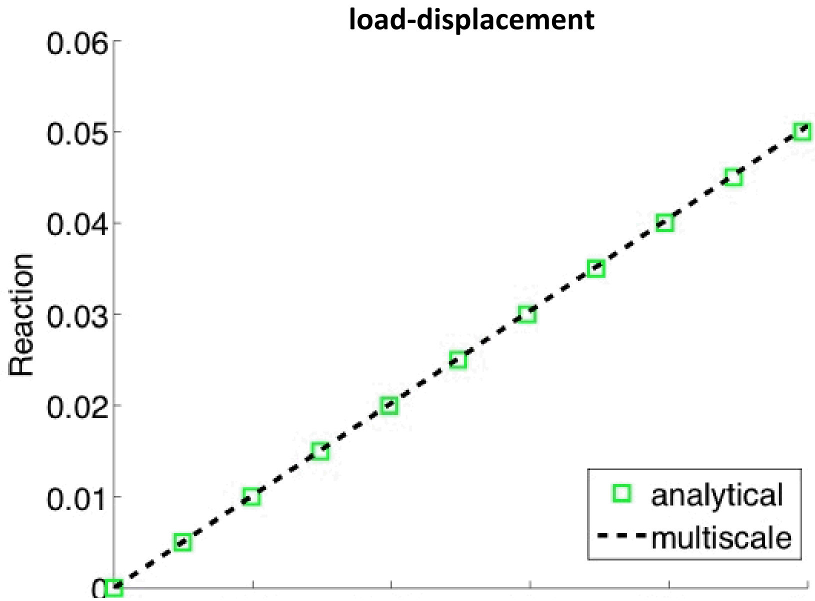
$$\text{for the } lth\ \Gamma' : \quad \boldsymbol{H}^{\Lambda I}_{A\alpha}\Delta\boldsymbol{\delta}^I_\alpha - \boldsymbol{H}^{\Lambda J}_{A\alpha}\Delta\boldsymbol{\delta}^J_\alpha = -\boldsymbol{R}^{\Lambda}_A$$

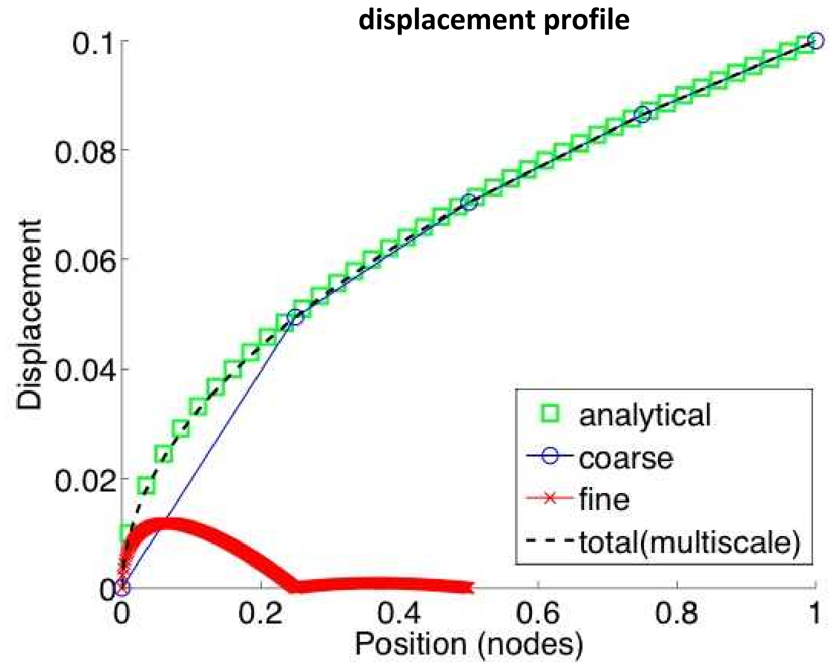
1D Example: Foulk's Singular Bar (2008)

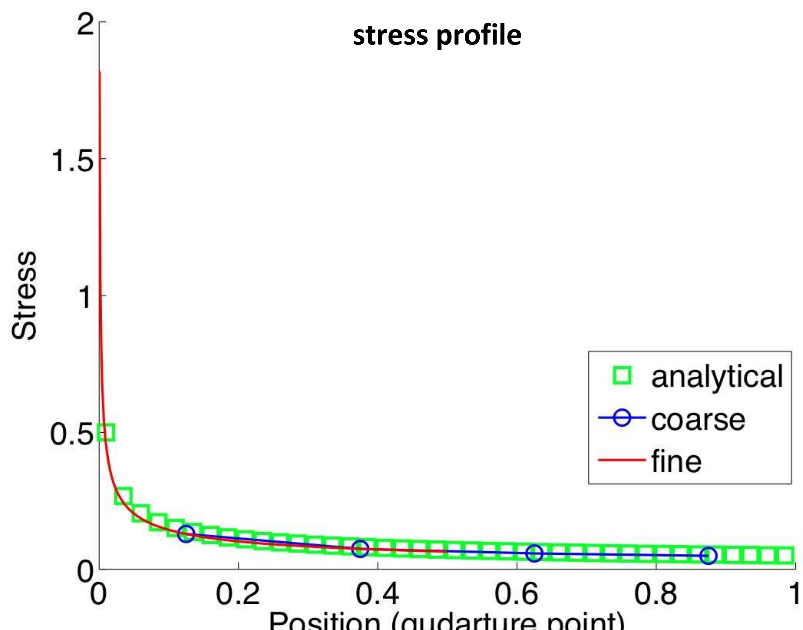


- Area proportional to square root of length
- Strong singularity at the left end of bar
- Fine scale resolutions are desirable around left end (region L')
- Constitutive model:
  elasticity without damage, hyper-elasticity with damage
- Conforming meshes

Elasticity without damage (analytical solution by Jay Foulk)

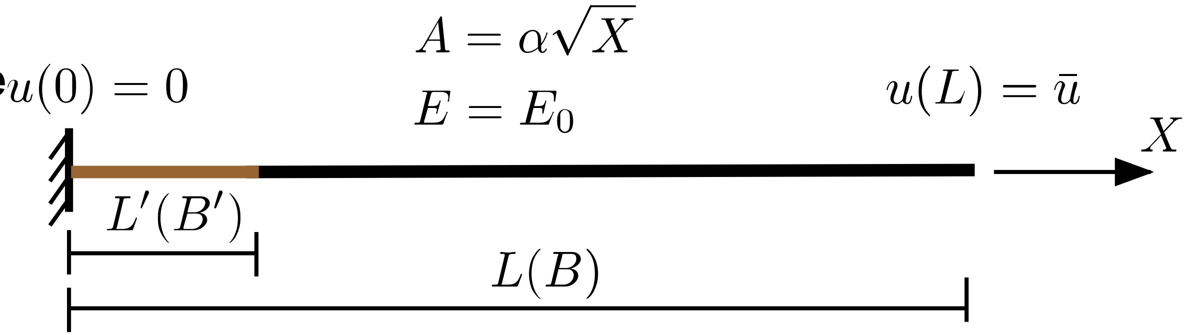






- 4 coarse elements are used to obtain the solution
- Multiscale computation matches well with analytical solution

Hyper-elasticity with damage



Material model:

Total strain-energy function $W(\boldsymbol{C}, \xi) = (1 - \xi) W_0(\boldsymbol{C})$ $\boldsymbol{C} = \boldsymbol{F}^T \boldsymbol{F}$

Effective strain energy $W_0(\boldsymbol{C}) = W_0^{\mathrm{vol}}(\theta) + W_0^{\mathrm{dev}}(\bar{\boldsymbol{\epsilon}})$

where the volumetric and deviatoric parts are given by

$$W_0^{\mathrm{vol}}(\theta) = \frac{\kappa}{4}[\exp(2\theta) - 1 - 2\theta] \quad W_0^{\mathrm{dev}}(\bar{\boldsymbol{\epsilon}}) = \frac{\mu}{2}[\mathrm{tr}(\exp(\bar{\boldsymbol{\epsilon}}) - 3]$$

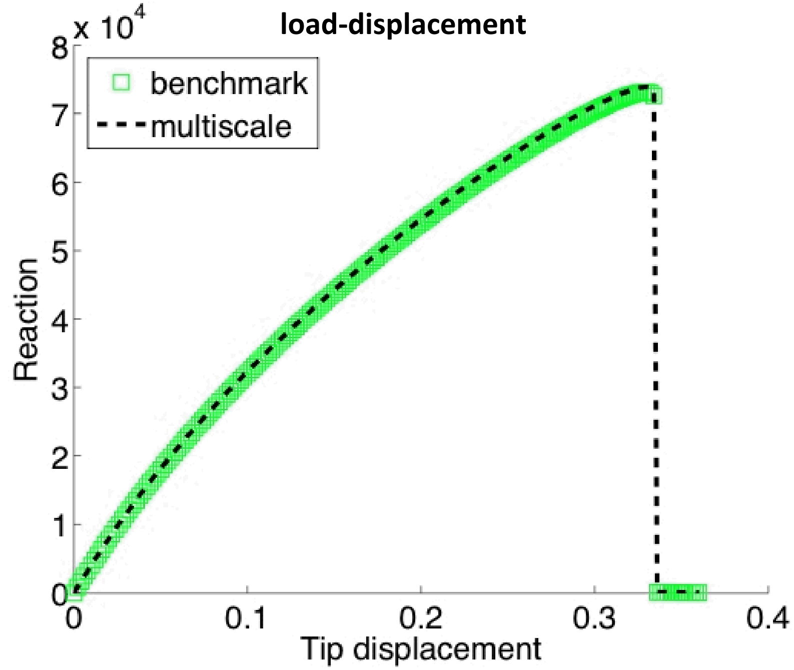
where

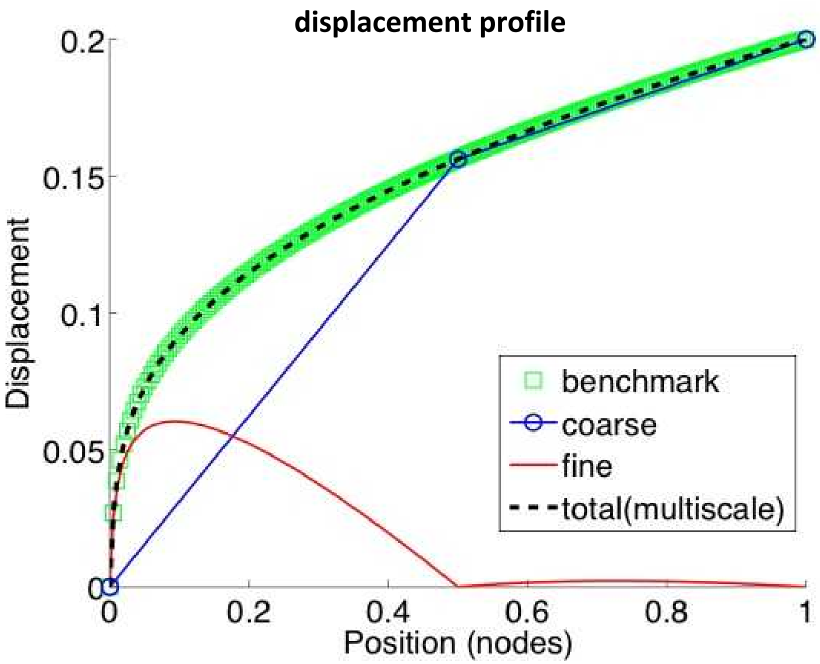
$$\boldsymbol{\epsilon} = \frac{1}{2}\log(\boldsymbol{C}), \;\; \bar{\boldsymbol{\epsilon}} = \mathrm{dev}(\boldsymbol{\epsilon}), \;\; \theta = \mathrm{tr}(\boldsymbol{\epsilon})$$

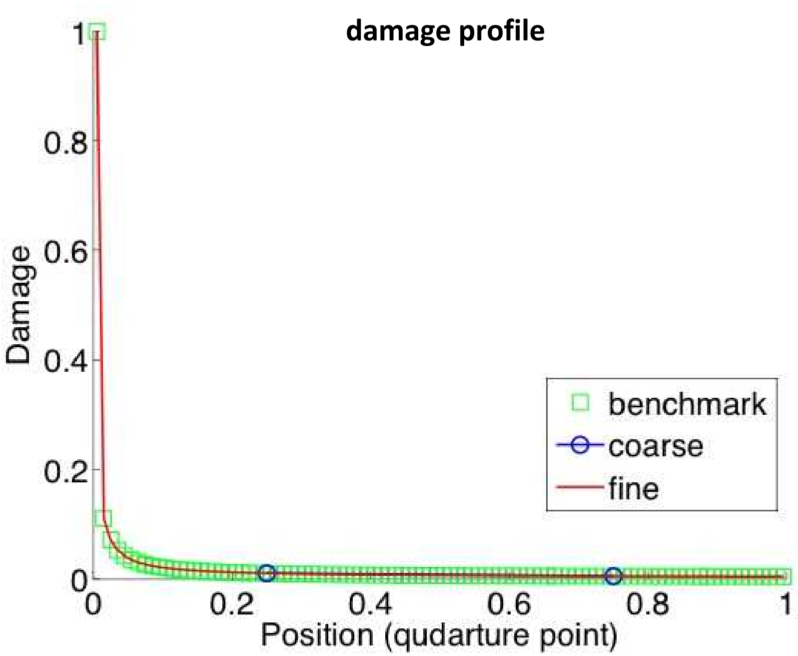
Damage evolution: simple exponential law

$$\xi(\alpha) = \xi_\infty[1 - \exp(\alpha/\tau)] \qquad \alpha(t) = \max[W_0(s)], \;\; s \in [0, t]$$

Hyper-elasticity with damage





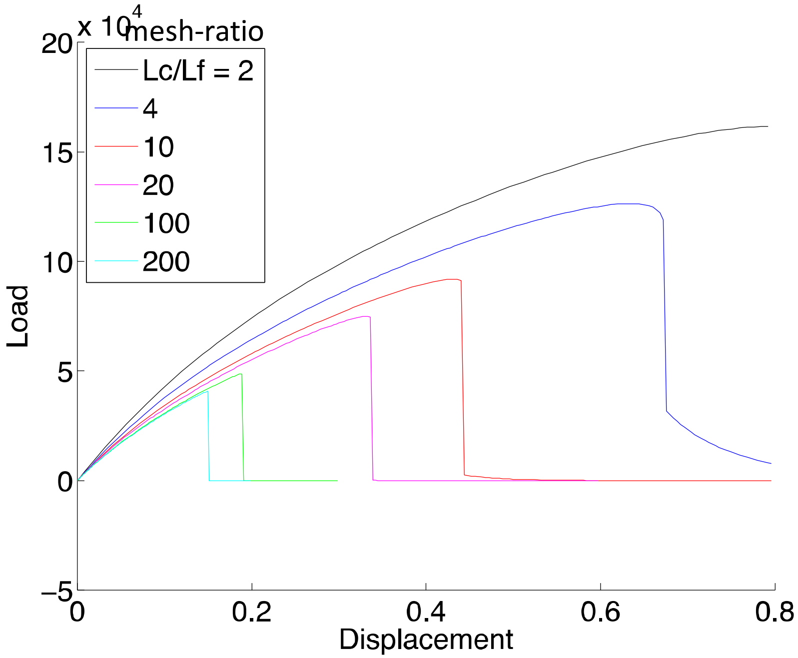


- Benchmark solution by full-single scale computation
- Material properties

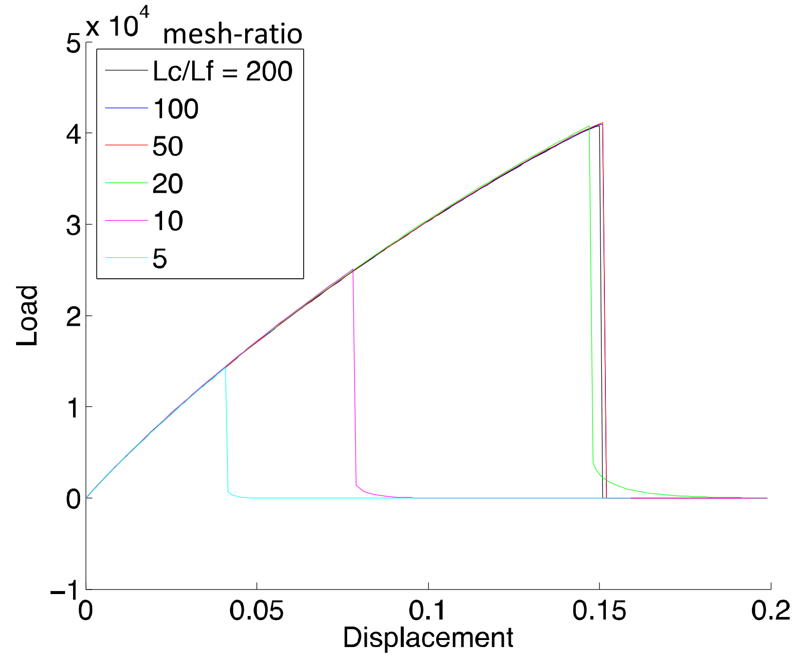
$$E = 200 \text{ GPa}$$
$$\nu = 0.25$$
$$\kappa = 133 \text{ GPa}$$
$$\mu = 67 \text{ GPa}$$
$$\xi_\infty = 1.0$$
$$\tau = 100 \text{ GJm}^{-3}$$

Hyper-elasticity with damage: mesh-dependent responses

Keep coarse scale fixed, refine fine scale



Keep fine scale element fixed, vary coarse scale



solution needs regularization!

Non-local variational regularization

Discrete Statement of Equilibrium,

Internal Variables and Conjugate Forces:

$$\int_B \boldsymbol{P} \cdot \operatorname{Grad} N_a \, dV - \int_B \rho_0 \boldsymbol{B} N_a \, dV - \int_{\partial_T B} \boldsymbol{T} N_a \, dS = \boldsymbol{0},$$

$$\bar{\boldsymbol{Y}} = \lambda_\alpha \left(\int_B \lambda_\alpha \lambda_\beta \, dV \right)^{-1} \int_B \lambda_\beta \boldsymbol{Y} \, dV,$$

$$\bar{\boldsymbol{Z}} = \lambda_\alpha \left(\int_B \lambda_\alpha \lambda_\beta \, dV \right)^{-1} \int_B \lambda_\beta \boldsymbol{Z} \, dV,$$

Unit Interpolation, Regularized Variables:

$$\lambda_\alpha = 1, \; \lambda_\beta = 1 \quad \Longrightarrow$$

$$\bar{\boldsymbol{Y}} = \frac{1}{\operatorname{vol}(D)} \int_D \boldsymbol{Y} \, dV,$$

$$\bar{\boldsymbol{Z}} = \frac{1}{\operatorname{vol}(D)} \int_D \boldsymbol{Z} \, dV,$$

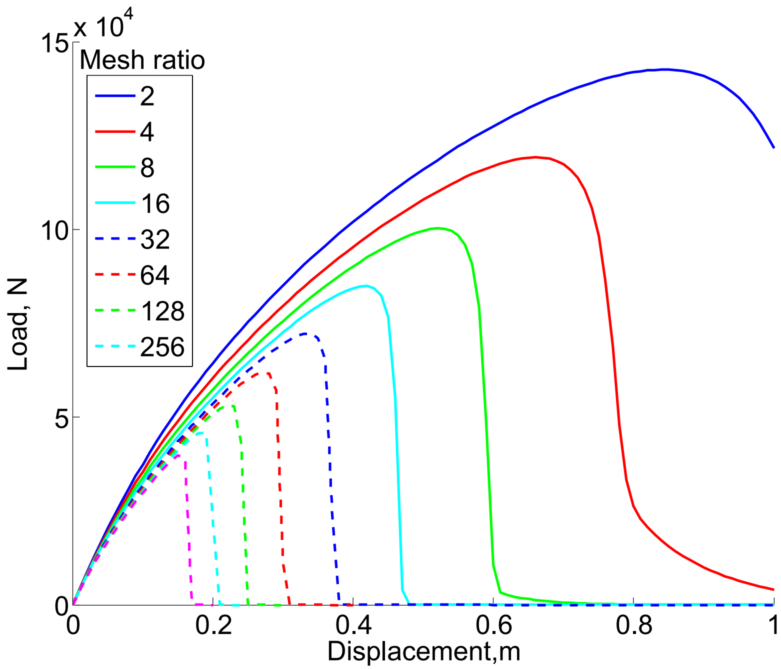
$$\operatorname{vol}(\bullet) := \int_{(\bullet)} dV,$$

Mota.et al. 2011

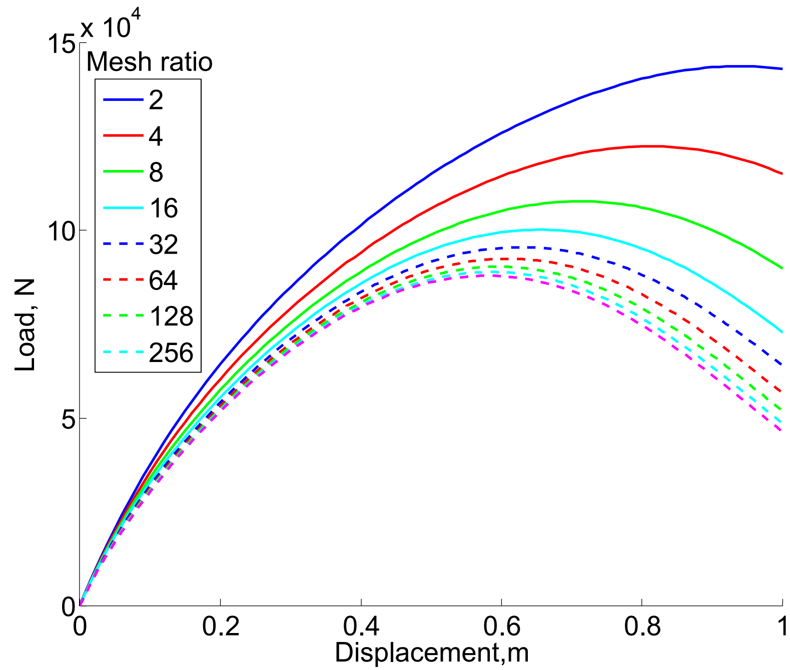
Regularization through non-local variational approach

Foulk's Singular Bar (2008) with hyper-elastic damage model

Classical mesh-dependent behavior without regularization



Solutions converge with regularization



Concluding remarks and future work

- Finite-deformation variational multiscale framework is proposed
- The formulation is potential-energy based and is independent of constitutive law
- FEM is used for discretizing both fine and coarse fields
- Additional field (Lagrange multiplier) is introduced to enforce constraint
- Solution is regularized by non-local variational approach

Future work for FY13

- Stabilization of the methods
- Expand to dynamic problems
- Expand to multi-dimensional problems (implementation in LCM)