

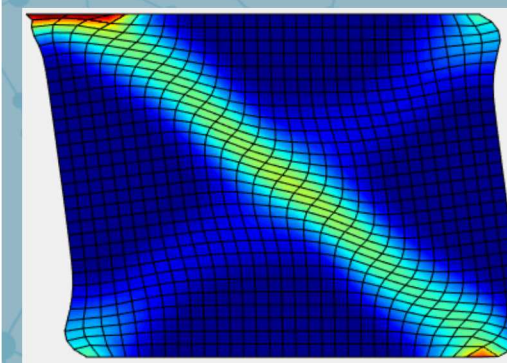
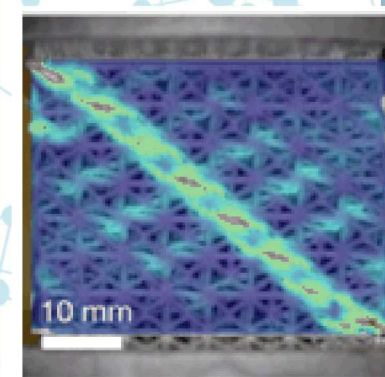
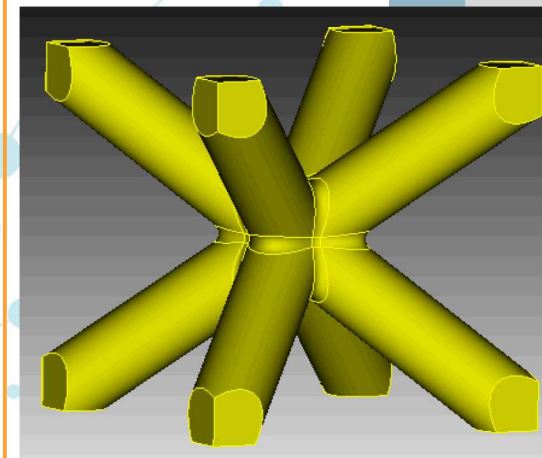
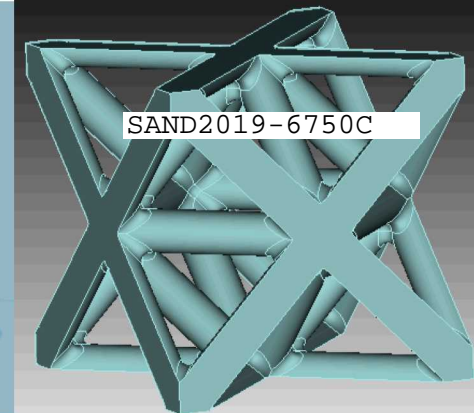
Nonlinear Topology Optimization with Microstructural Effects: A Micromorphic Approach

PRESENTED BY

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Nanostructure Physics Department

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Talking Points for Today



- Lattice Metamaterials for Novel Structural Designs
- Capturing Localization Effects through a Generalized Continuum Approach
- Topology Optimization for Structural Design
- Shear Band Localization and Dual-Lattice Metamaterials



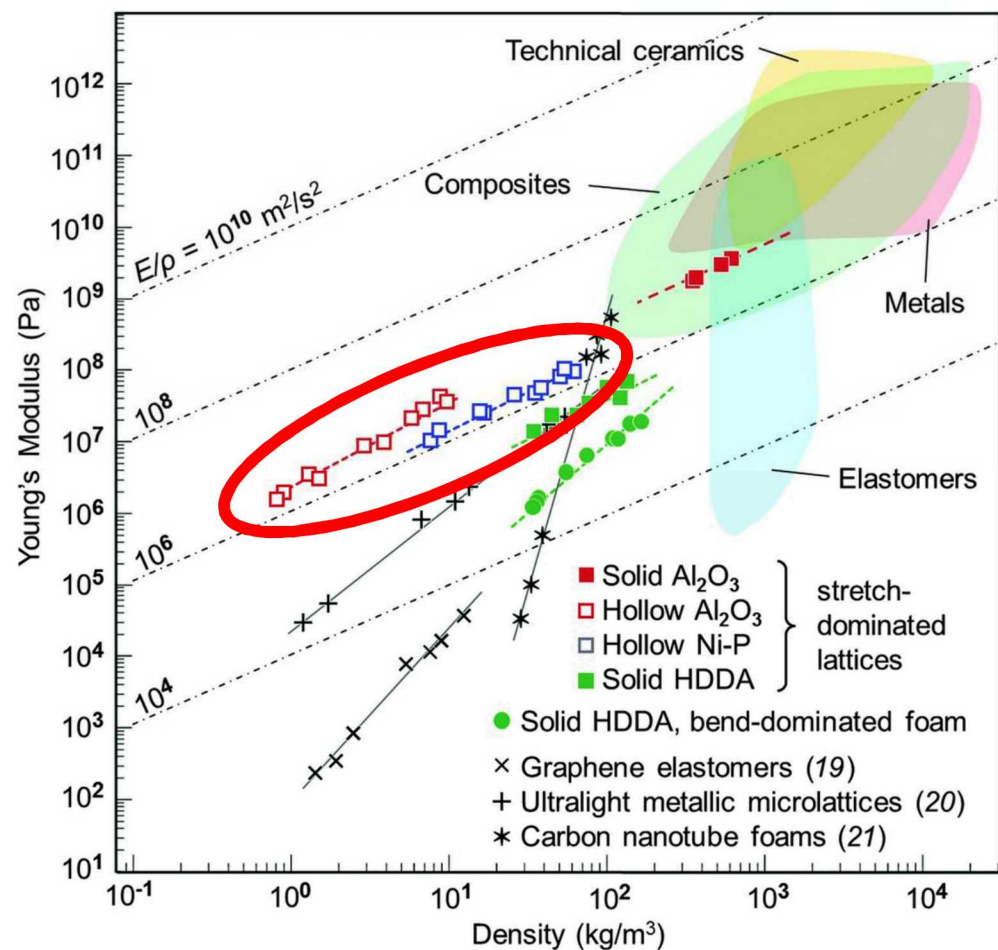
Lattice Metamaterials for Novel Structural Designs

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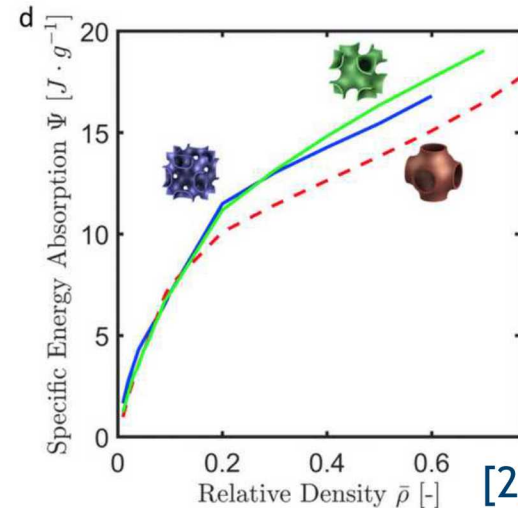
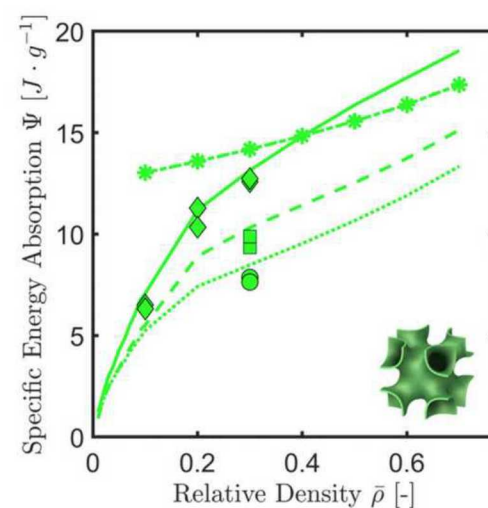
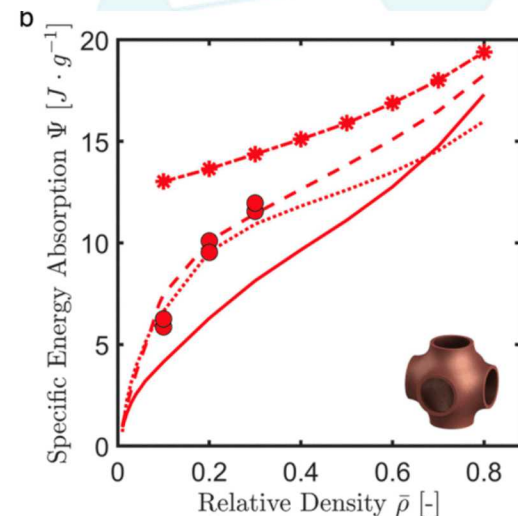
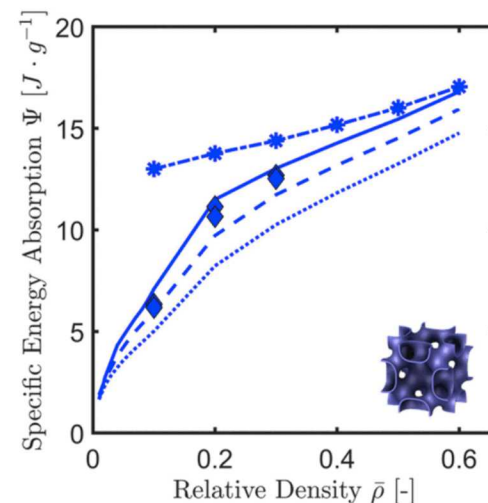
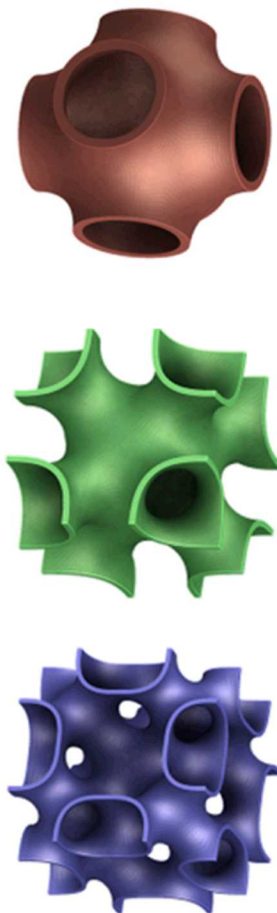


What Are Lattice Metamaterials?

- Exceptional weight-specific stiffness/strength^[1]



[1]



[2]

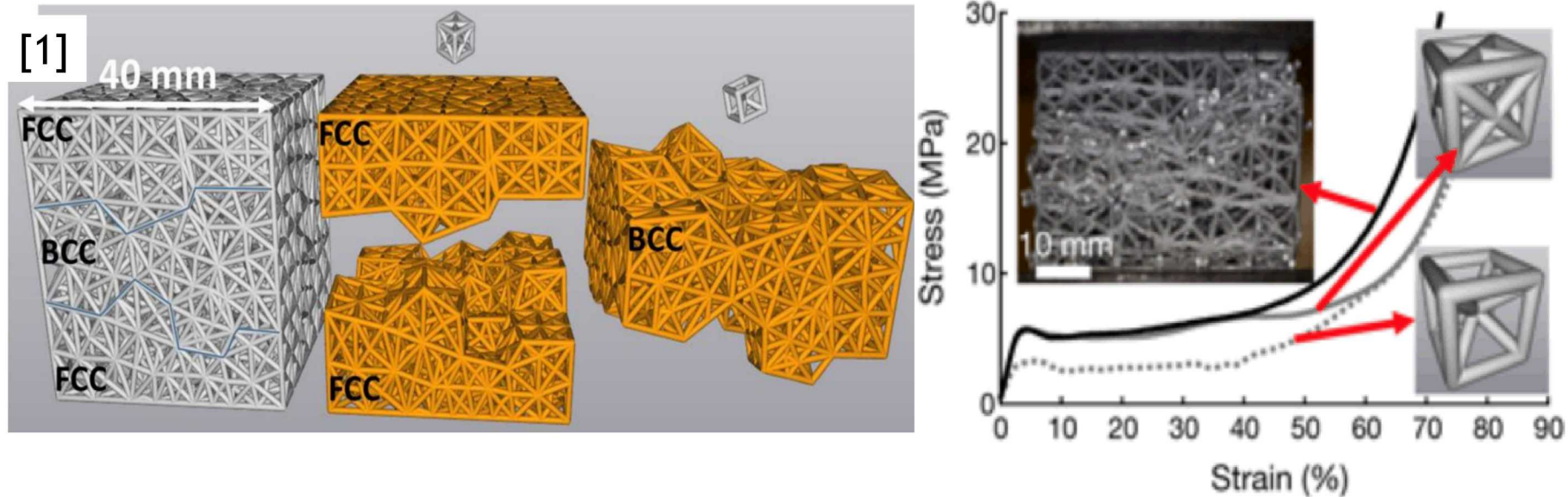
- High specific energy absorption – Ultralight energy absorbers^[2]

[1] Zhang, et al. *Ultralight, ultrastiff mechanical metamaterials*. Science, 2014. **344**: p. 1373-1377.

[2] Colin Bonatti and Mohr, D. *Smooth-shell metamaterials of cubic symmetry: Anisotropic elasticity, yield strength and specific energy absorption*. Acta Materialia, 2019. **164**: p. 301-321.

Design Considerations with Lattice Metamaterials is non-intuitive

- Design approaches with traditional materials don't apply to lattice metamaterials – non-intuitive
- Combining different lattice topologies can allow for tailoring of properties and control of localization^[1]



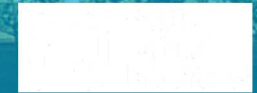
- Topology optimization provides rigorous way to explore design space
- Multiscale topology optimization approaches can account for microstructure but are based on homogenization
 - Becomes computationally **very expensive for nonlinear problems**
 - Homogeneous deformation of RVE **cannot capture localization**

[1] Pham, et al. *Damage-tolerant architected materials inspired by crystal microstructure*. Nature, 2019. **565**: p. 305-311.

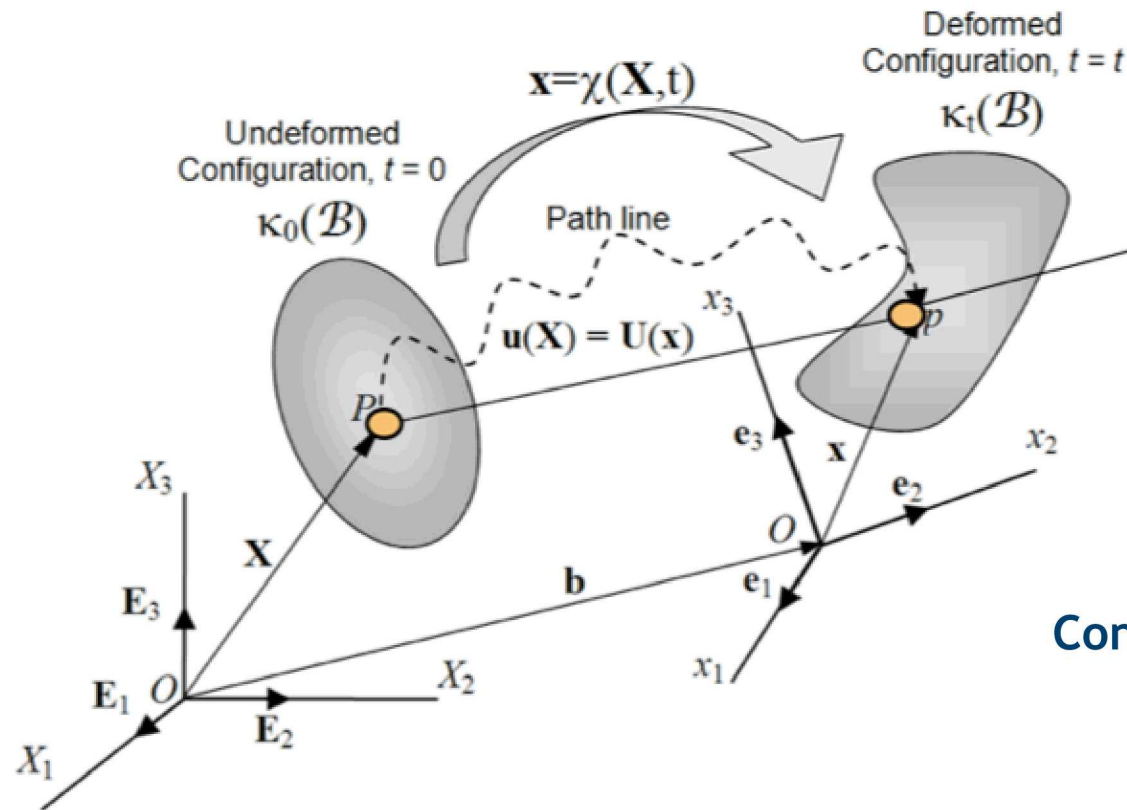


Capturing Localization Effects Through a Generalized Continuum Approach

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Accounting for Underlying “Microstructure” With Additional DOFs: Micromorphic Approach



Accounts for rotation and stretching
Geometry agnostic
Constitutive parameters contain microstructure info

- Can capture significant gradients in macroscopic loading over microstructural features which cause
 - Size dependent mechanical properties
 - Dispersion effects in wave propagation
 - Accumulation of plastic deformation in microstructure during localization

Calibrating Micromorphic Models to Specific Microstructures



**Direct Numerical Simulation
(DNS)**



Physical system	First order operator	Second order operator	Higher order terms
$L[\dots] \cong$	$c_1 L_1[\dots]$	$+ c_2 L_2[\dots]$	$+ h.o.t$

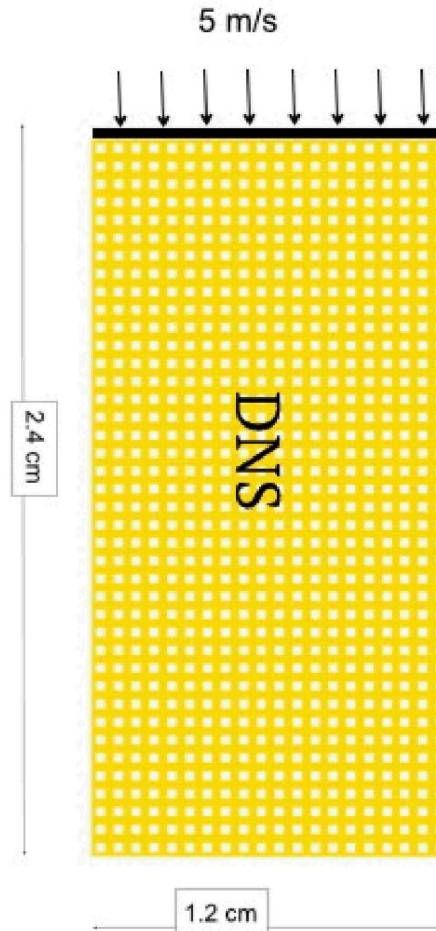


Component scale simulation

Example: Low Velocity Impact in Foam



Classical (200 x 100 elements):



Direct (800 x 400 elements):

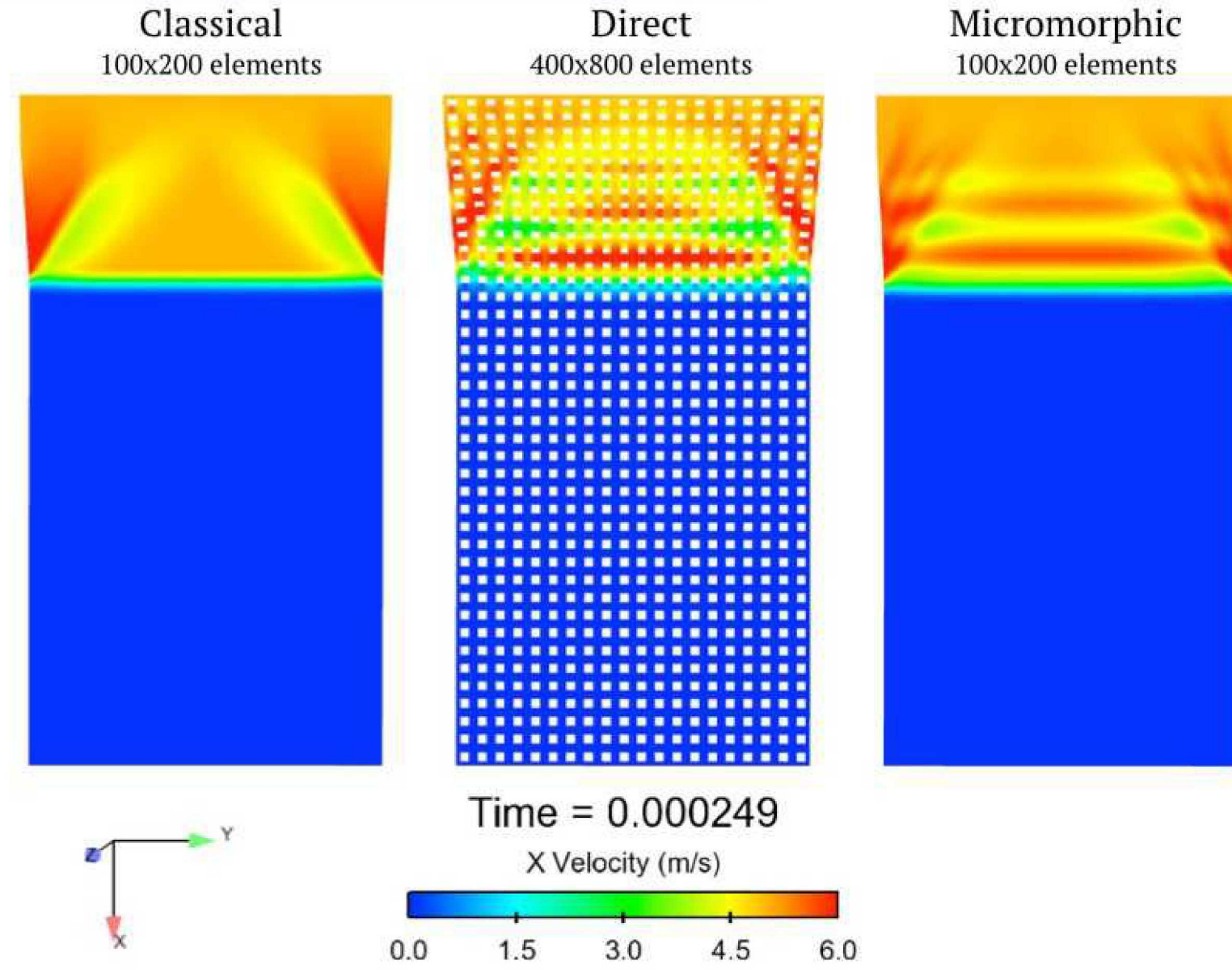
- 0.3 mm "pore" size (0.6 mm RVE)
- 25% porosity
- Solid density: 1100 kg/m³ (Matweb.com)
- Young's modulus: 0.851 MPa (Fan, 2011)
- Poisson's ratio: 0.4



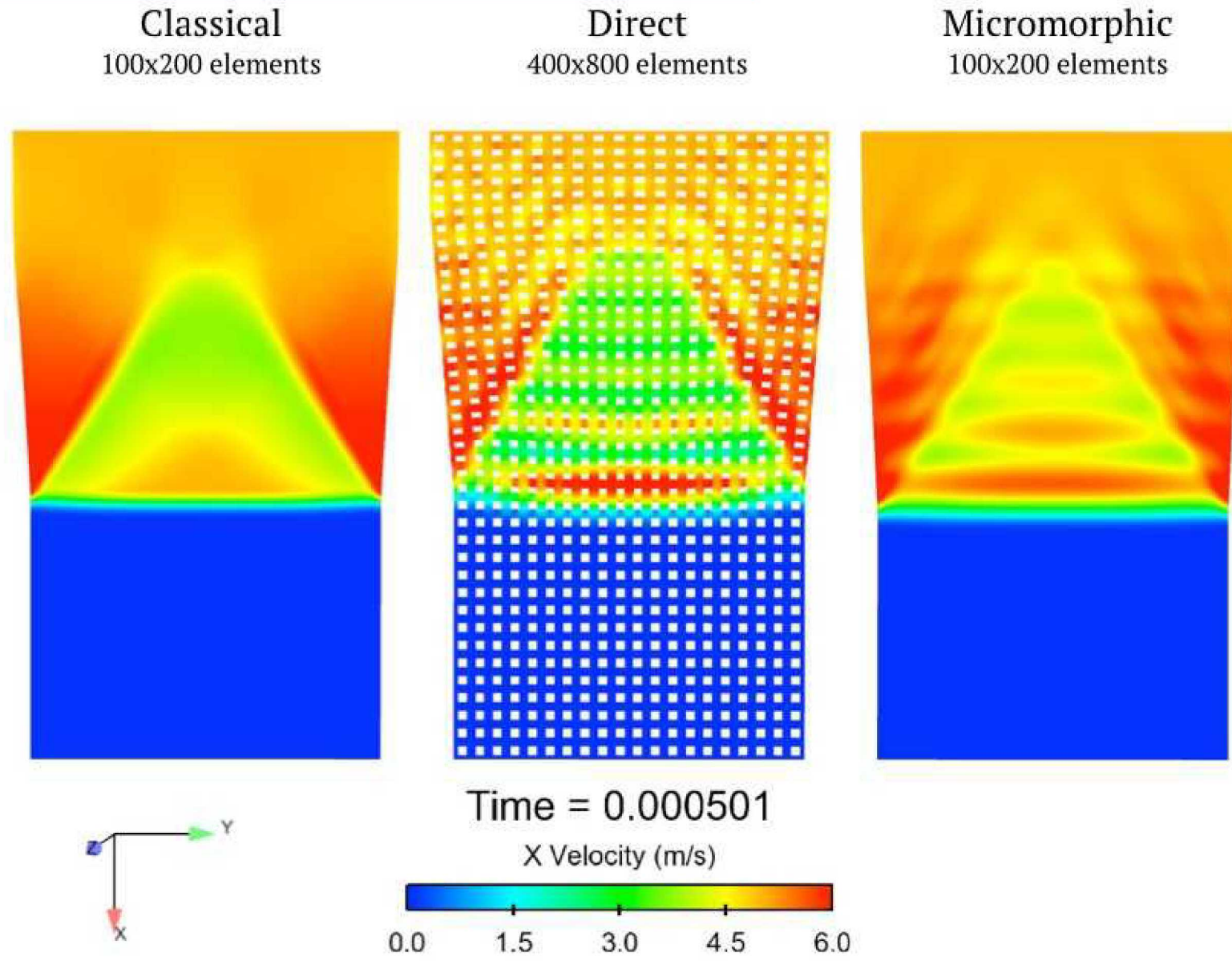
Micromorphic (200 x 100):

- microscale length: 0.6 mm
- Mindlin parameter (a.k.a. coupling constant): 0.3

Example: Low Velocity Impact in Foam



Example: Low Velocity Impact in Foam

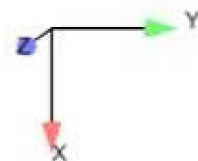
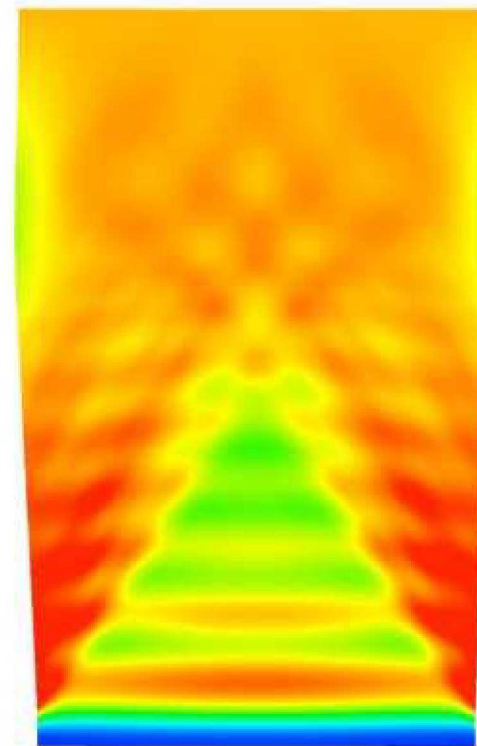
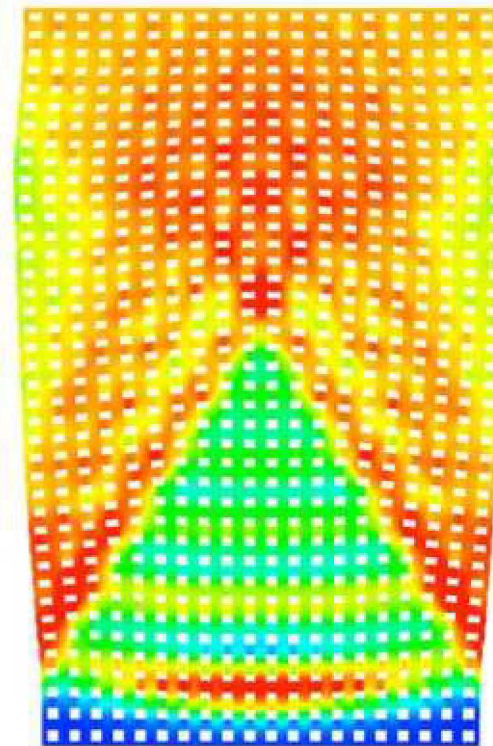
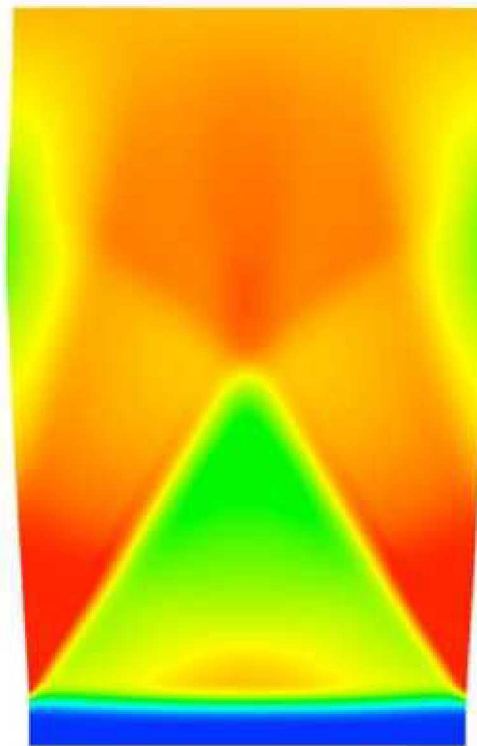


Example: Low Velocity Impact in Foam

Classical
100x200 elements

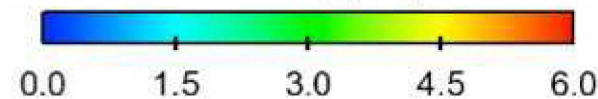
Direct
400x800 elements

Micromorphic
100x200 elements



Time = 0.000752

X Velocity (m/s)



Capturing Strain Softening and Localization: Regularization Through a Micromorphic Model



- Localization phenomena can lead to a loss of ellipticity in governing PDEs for classical continua
- Micromorphic continua involve length scale which regularizes this effect – suitable for **simulating localization phenomena in lattice metamaterials**
- Regularizing effect can be gained by replacing the microstrain tensor with a scalar plastic microstrain variable – only 1 additional DOF per continuum point
- Finite deformation theory considering elastoplastic softening and scalar plastic microstrain variable^[1]:

Free Energy

$$\psi(\mathbf{C}^e, \chi, \nabla \chi) = \psi_{ref}(\mathbf{C}^e, \alpha) + \frac{1}{2}H(\alpha - \chi)^2 + \frac{1}{2}\mathbf{K} \cdot \mathbf{A} \cdot \mathbf{K}$$

$$\mathbf{K} = \nabla \chi \quad \mathbf{A} = A\mathbf{I} \quad \psi_{ref}(\mathbf{C}^e, \alpha) \longrightarrow \text{Macroscale free energy}$$

Micro Momentum Balance

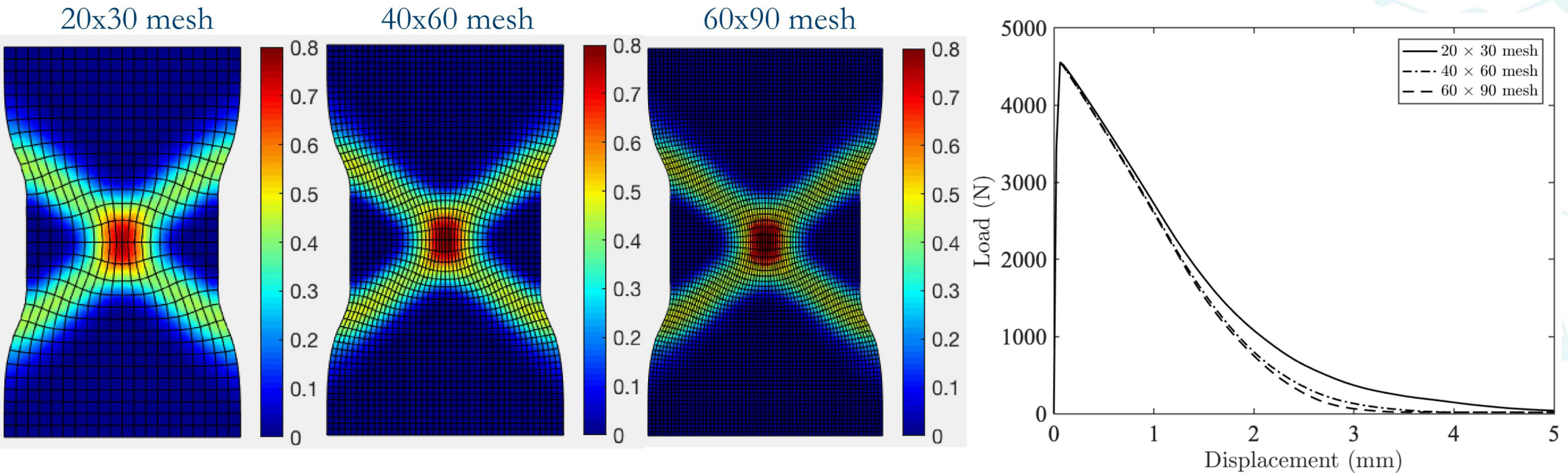
$$\nabla \cdot \mathbf{b}_0 - a_0 = A\Delta \chi - H\chi + H\alpha = \alpha - \chi + l^2 \Delta \chi = 0$$

$$l = \sqrt{A/H}$$

[1] Anand, et al. *A large-deformation gradient theory for elastic-plastic materials: Strain softening and regularization of shear bands*. International Journal of Plasticity, 2012. **30-31**: p. 116-145.

Shear Band Localization

- Localization bands have finite width dictated by micromorphic parameters A, H, Z and hardening/softening modulus
- Inhomogeneous deformation induced by finite deformation kinematics (necking/bulging)





Topology Optimization for Structural Designs

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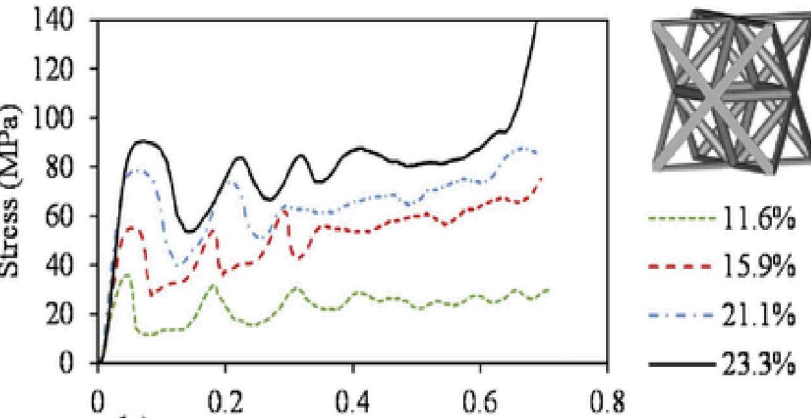
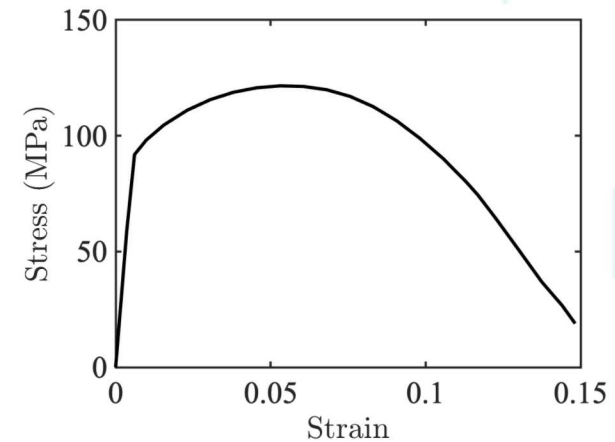
Combining Functionalities of FCC (Energy Dissipation) & BCC (No Softening) Lattices

FCC Lattice

- Higher stiffness and yield stress
- Peak stress reached $\sim 5\%$ strain
- Severe softening after peak stress

$$E \rightarrow 16.55 \text{ GPa} \quad \sigma_{max} \rightarrow 37.07 \text{ MPa}$$

$$\sigma_y \rightarrow 23.17 \text{ MPa} \quad K^h \rightarrow -220 \text{ MPa}$$



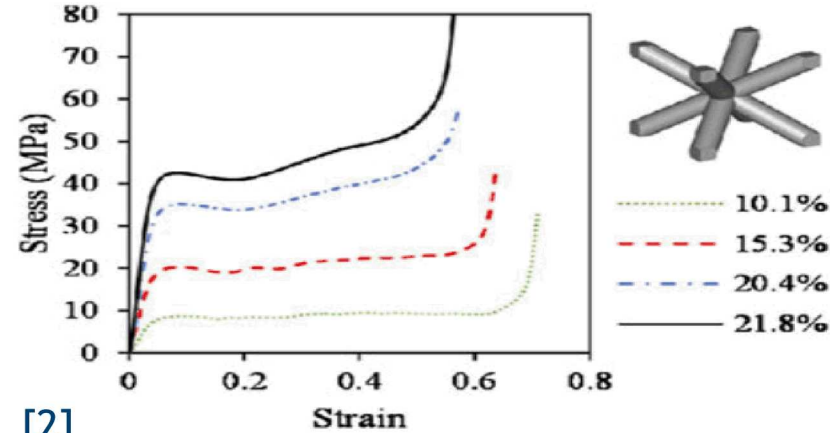
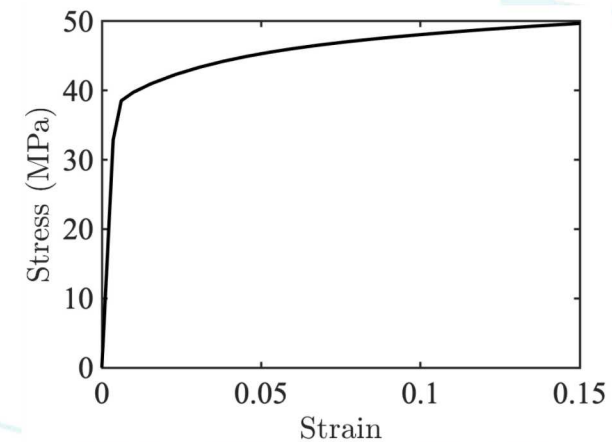
[1]

BCC Lattice

- Lower stiffness and yield stress
- Little to no softening
- Relatively level hardening until densification

$$E \rightarrow 9.31 \text{ GPa} \quad \sigma_{max} \rightarrow 11.47 \text{ MPa}$$

$$\sigma_y \rightarrow 9.57 \text{ MPa} \quad K^h \rightarrow -20 \text{ MPa}$$



[2]

The Math Slide: Formulating the Optimization Problem



Density-Based Parameterization

$$0 \leq \rho_e \leq 1$$

$$\text{BCC Phase } \rho_e = 0$$

$$\text{FCC Phase } \rho_e = 1$$

SIMP Interpolation

$$A_e = \rho_e^p A_{FCC} + (1 - \rho_e)^p A_{BCC}$$

$$A \in \{E, \sigma_y, \sigma_{max}, K^h\}$$

Design Problem

$$\min_{\mathbf{x}} f_0(\mathbf{x}) = - \int_t \int_{\Omega_0} \dot{w}^p dv dt$$

$$\text{s. t. } f_1(\mathbf{x}) = 1 - \frac{1}{V} \sum_e^{n_{ele}} \rho_e(\mathbf{x}) v_e - V_f \leq 0$$

$$f_2(\mathbf{x}) = \left[\sum_e^{n_{ele}} \sum_{r=1}^{n_{ipt}} (\alpha_{er}^N)^q \right]^{\frac{1}{q}} - \hat{\alpha} \leq 0$$

$$\mathbf{R}^k(\hat{\mathbf{u}}^k, \hat{\mathbf{u}}^{k-1}, \mathbf{c}^k, \mathbf{c}^{k-1}, \boldsymbol{\rho}(\mathbf{x})) = \mathbf{0},$$

$$k = 1, 2, \dots, N$$

$$\mathbf{H}^k(\hat{\mathbf{u}}^k, \hat{\mathbf{u}}^{k-1}, \mathbf{c}^k, \mathbf{c}^{k-1}, \boldsymbol{\rho}(\mathbf{x})) = \mathbf{0},$$

$$k = 1, 2, \dots, N$$

$$\mathbf{0} \leq \mathbf{x} \leq \mathbf{1}$$

Maximize Plastic Work

Volume Fraction Constraint (BCC Phase)

Maximum Accumulated Plastic Strain Constraint

Implicit Global Constraint

Explicit Global Constraint

Box Constraint

Adjoint Sensitivity Analysis: Defining Local and Global Variables and Associated Constraints



Global Variables and Constraints

Scalar plastic microstrain, F-bar elements for incompressibility

$$\hat{\mathbf{u}}^k = \begin{bmatrix} \mathbf{u}^k \\ \chi^k \end{bmatrix} \quad \mathbf{R}^k = \begin{bmatrix} \mathbf{R}_1^k \\ \mathbf{R}_2^k \end{bmatrix} = \begin{bmatrix} n_{ele} \mathcal{A} \mathbf{F}_{int}^{e,u^k} \\ n_{ele} \mathcal{A} \mathbf{F}_{int}^{e,\chi^k} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

$$\mathbf{F}_{int}^{e,u^k} = \sum_{r=1}^{n_{ipt}} w_r \mathbf{B}_{e_r}^{u^k T} r_{e_r}^{k-a} \bar{\mathbf{P}}_{e_r}^k \quad \mathbf{F}_{int}^{e,\chi^k} = \sum_{r=1}^{n_{ipt}} w_r \left(\mathbf{N}_{e_r}^{\chi^k T} \mathbf{N}_{e_r}^{\chi^k} \chi_e^k - \mathbf{N}_{e_r}^{\chi^k T} \alpha_{e_r}^k + \frac{A}{H} \mathbf{B}_{e_r}^{\chi^k T} \mathbf{B}_{e_r}^{\chi^k} \chi_e^k \right)$$

Local Variables and Constraints

Finite deformation isotropic elasto-viscoplasticity with micromorphic regularization

$$\mathbf{c}^k = \begin{bmatrix} \mathbf{c}_1^k & \dots & \mathbf{c}_{n_{ele}}^k \end{bmatrix}^T$$

$$\mathbf{c}_e^k = \begin{bmatrix} \mathbf{c}_{e_1}^k & \dots & \mathbf{c}_{e_{n_{ipt}}}^k \end{bmatrix}^T$$

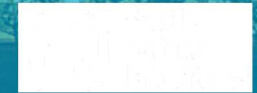
$$\mathbf{c}_{e_r}^k = \begin{bmatrix} \mathbf{b}_{e_r}^{e^k} & \alpha_{e_r}^k & \Delta \gamma_{e_r}^k \end{bmatrix}^T$$

$$\mathbf{H}_{e_r}^k = \begin{cases} \mathbf{h}_{e_{r1}}^k = \mathbf{b}_{e_r}^{e^k} - \mathbf{b}_{e_r}^{e,tr} \cdot \exp[-2\Delta t \mathbf{A}_{e_r}^k] = \mathbf{0} \\ \mathbf{h}_{e_{r2}}^k = \alpha_{e_r}^k - \alpha_{e_r}^{k-1} - \Delta \gamma_{e_r}^k \\ \mathbf{h}_{e_{r3}}^k = \sqrt{\frac{3}{2}} \|\mathbf{s}_{e_r}^k\| \left(\frac{\Delta t}{\mu \Delta \gamma_{e_r}^k + \Delta t} \right)^\vartheta - \zeta(\alpha_{e_r}^k, \chi_e^k) \end{cases}$$

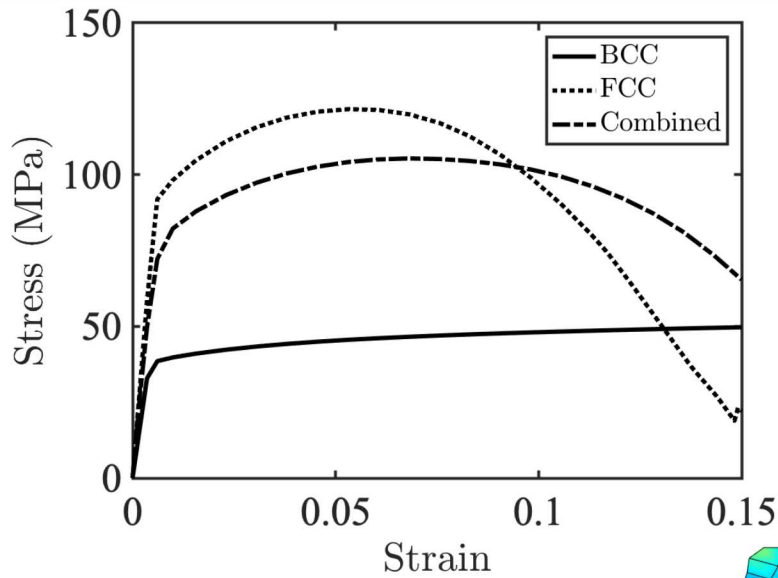


Examples for Shear Band Localization and Dual Lattice Optimization

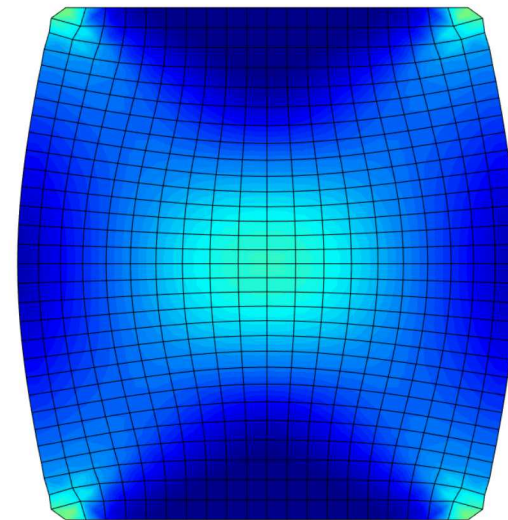
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Naïve Combination of Lattices Leads to Improvement in Energy Dissipation



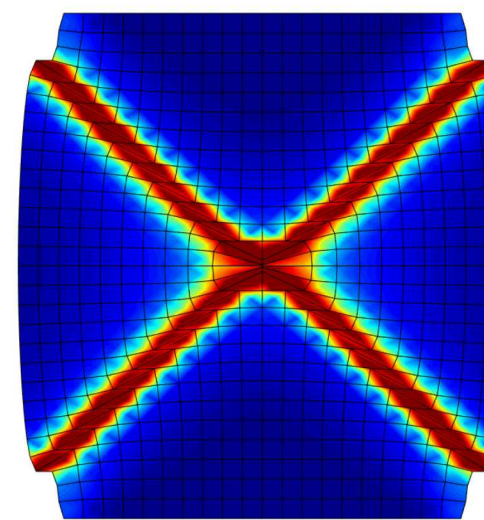
BCC



Dissipated energy:

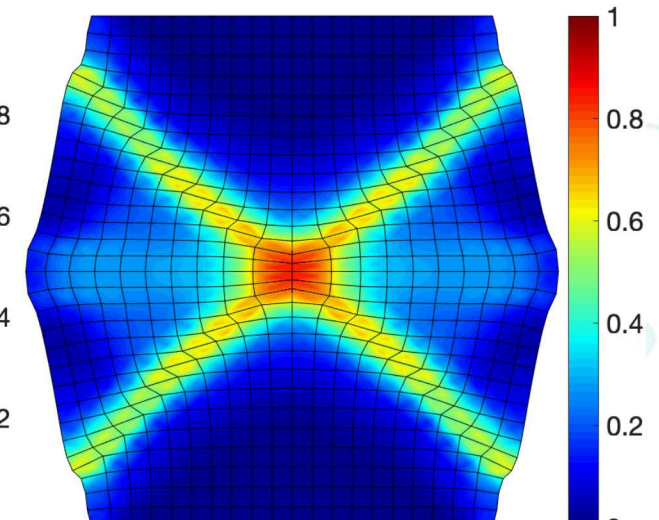
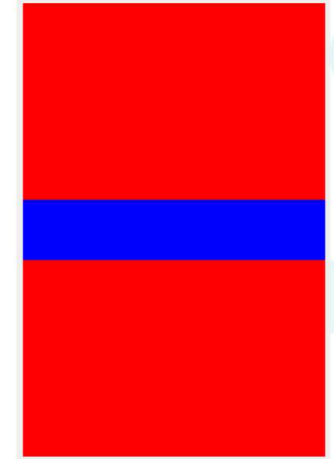
1.043 J

FCC



8.109 J

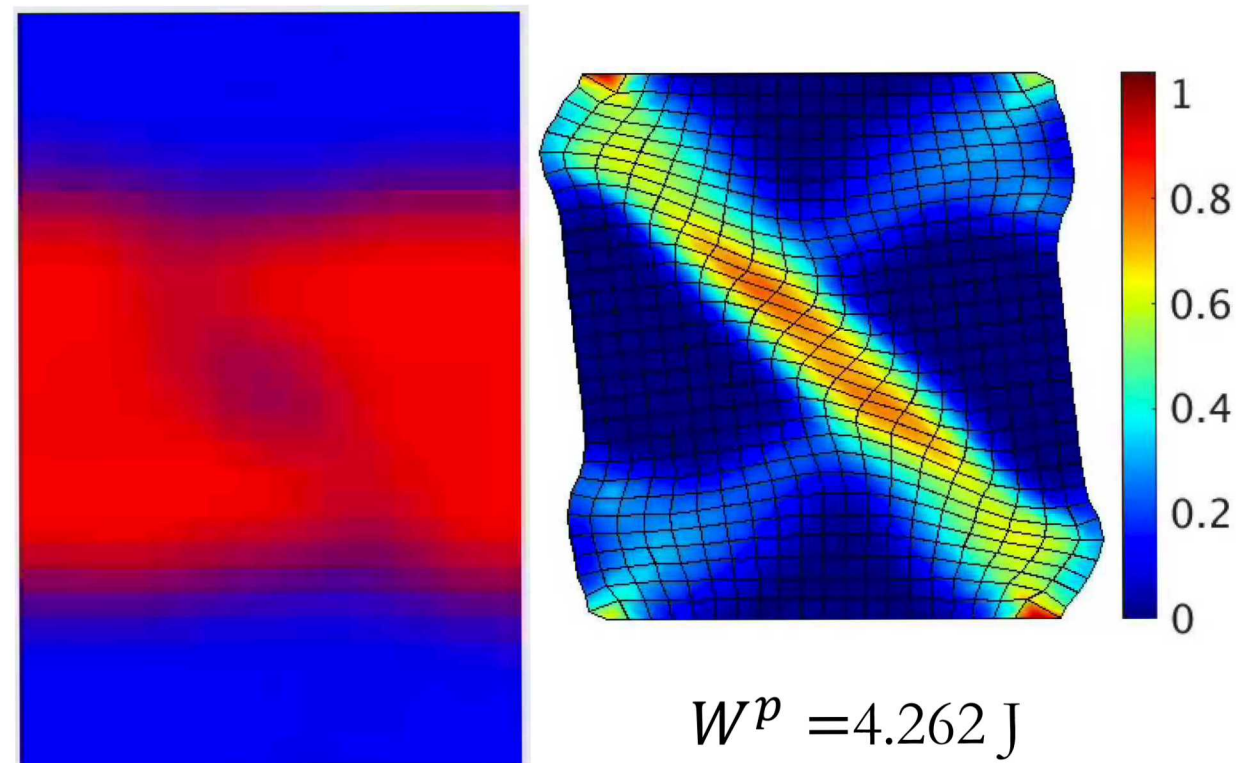
Combined (13% BCC)



8.218 J

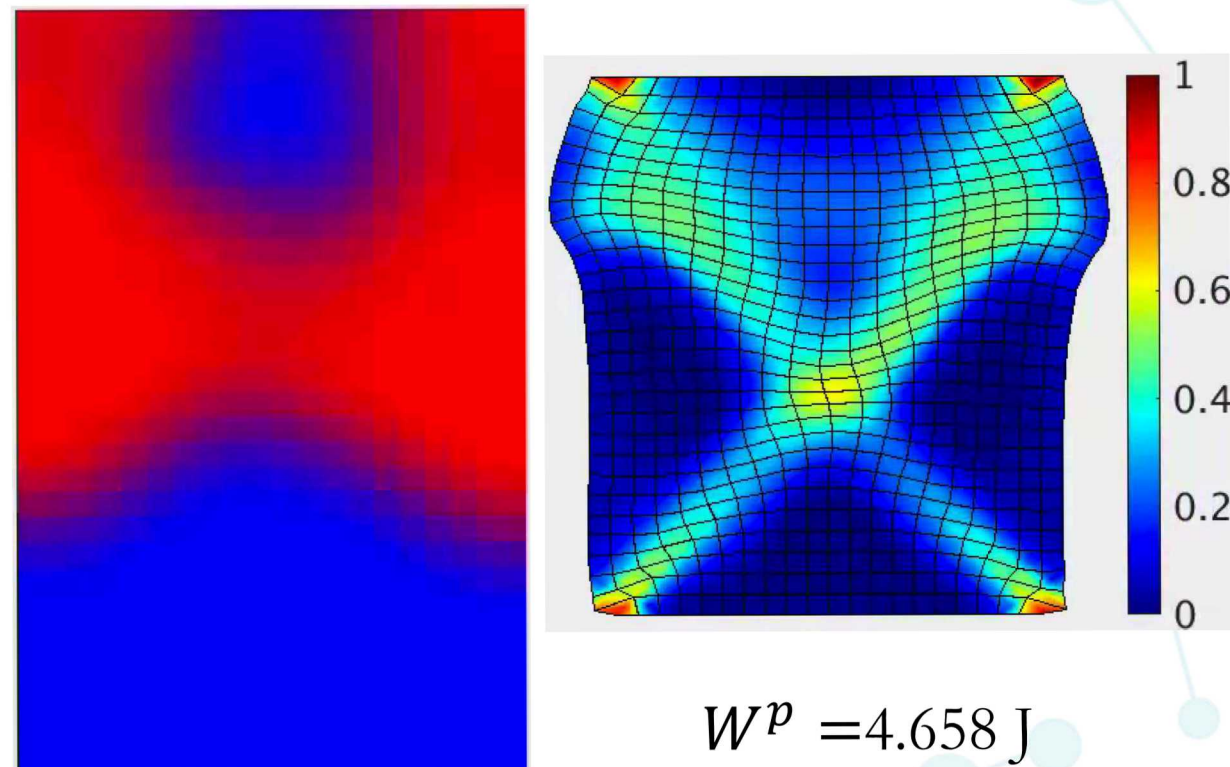
Preliminary Optimization Results

$$\underline{V_f = 0.5}$$



$$W^p = 4.262 \text{ J}$$

$$\underline{V_f = 0.9}$$



$$W^p = 4.658 \text{ J}$$

- Both designs experience less severe localization than FCC alone
- Problem is highly sensitive to changes in topology



Conclusions and Future Perspectives

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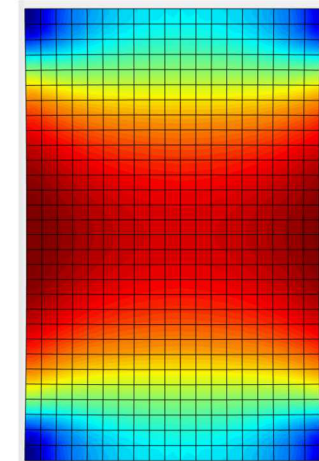
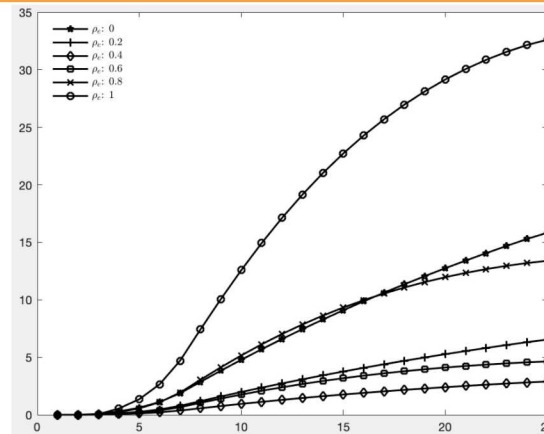
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Future Work

Optimization

- Better parameterization for intermediate density values
- More appropriate objective functions/constraints

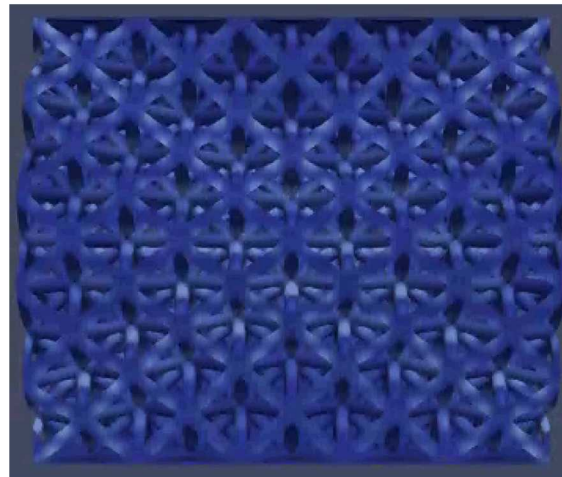
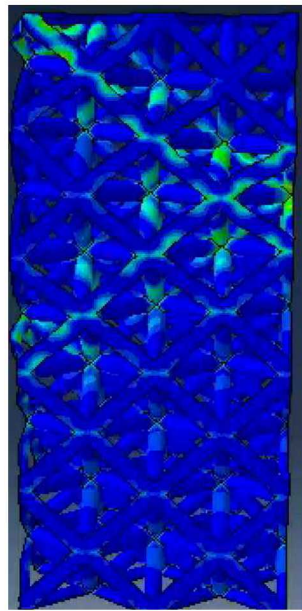


Model Extensions

- Pressure dependent plasticity models
- Full microstrain tensor

Calibration through DNS

$$f(\phi) = F(\hat{u}^1(\phi), \dots, \hat{u}^n(\phi)) = \sum_{k=1}^n \sum_{i=1}^{n_n} \|\bar{d}_i^k - d_i^k\|^2$$



Transient Analysis

- Account for dispersive effects
- Coupling with plasticity

