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Variational Nonlocal Regularization in Finite-Deformation Inelasticity

Alejandro Mota, James W. Foulk III, Jakob T. Ostien

Sandia National Laboratories

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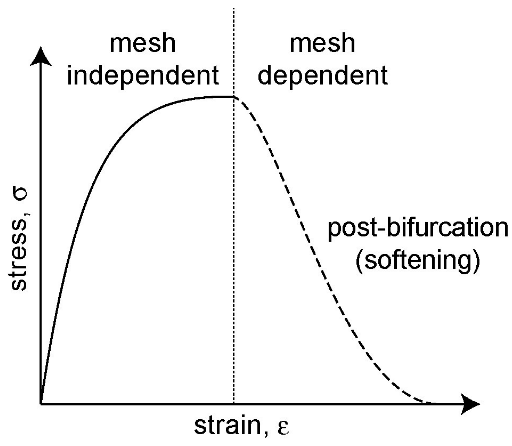
Loss of Ellipticity



Softening behavior

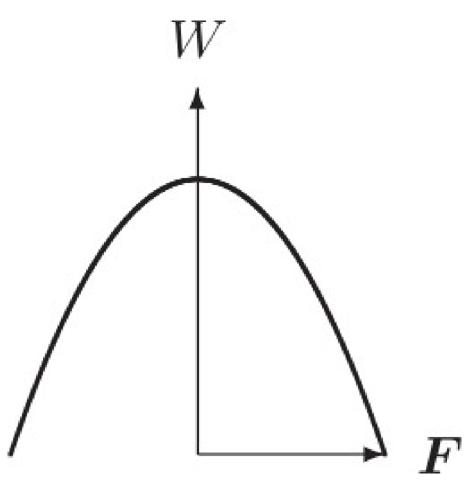
Stress-strain curve has one or more peaks.

Loss of ellipticity

Governing partial differential equation changes character.

$$\mathrm{Div}\,\boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$

Loss of convexity



Stored energy function becomes non-convex.

$$\Phi[\varphi] = \int_B W(\boldsymbol{F}, \boldsymbol{Z}, T)\, dV - \int_B \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_T B} \bar{\boldsymbol{T}} \cdot \boldsymbol{\varphi}\, dS$$

Non-positive-definite Hessian

Tangent modulus becomes non-positive definite (singular acoustic tensor).

$$\mathbb{C} = 4 \frac{\partial^2 W}{\partial \boldsymbol{C}^2}$$

Non-positive-definite stiffness

Stiffness has one or more null or negative eigenvalues.

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Regularization Methods

Gradient Formulations

$$\Phi[\boldsymbol{\varphi}] = \int_{\mathcal{B}} A(\boldsymbol{F}, \mathcal{K}, \boldsymbol{Z}, T)\, dV + \Phi^{\text{ext}}[\boldsymbol{\varphi}]$$

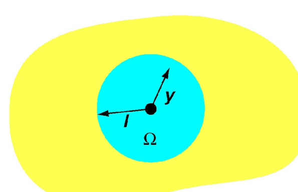
$$\bar{\boldsymbol{Z}} = \boldsymbol{Z}_0 + \nabla^2 \boldsymbol{Z}(\boldsymbol{X}_0) : \boldsymbol{H}(D) + \cdots$$

✓By-passes loss of ellipticity entirely.
✓Capable of modeling post-peak behavior.
✘Special boundary considerations.
✘Constitutive models require modifications.

Nonlocal FE Formulations

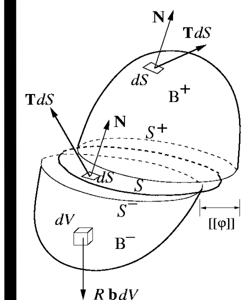
$$\bar{\boldsymbol{F}}(\boldsymbol{X}) := \frac{1}{\Psi(\boldsymbol{X})} \int_D \psi(\boldsymbol{X}, \boldsymbol{Y}) \boldsymbol{F}(\boldsymbol{Y})\, dV$$

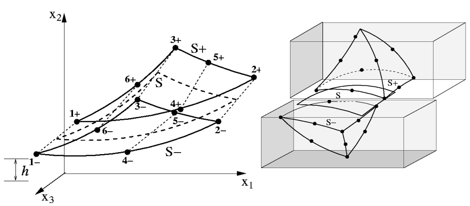
$$\Psi(\boldsymbol{X}) := \int_D \psi(\boldsymbol{X}, \boldsymbol{Y})\, dV$$

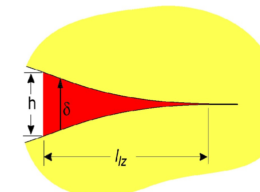


✓Confine localization to nonlocal domain.
✓Use constitutive behavior as-is.
✘Special boundary considerations.
✘Requires "cut off" approaches.

Localization Elements







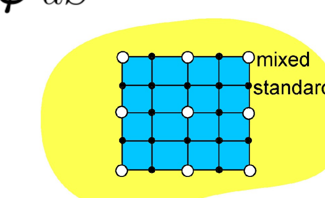
$$\boldsymbol{F}^{\parallel} \boldsymbol{F}^{\perp} \qquad \boldsymbol{F}^{\perp} = \boldsymbol{I} + \frac{\boldsymbol{\delta}}{h} \otimes \boldsymbol{N}$$

✓Use constitutive behavior as-is.
✓Accurate and efficient.
✘Failure follows mesh geometry.
✘Requires robust adaptive insertion.

(Yang, Mota, Ortiz; IJNME 2005)

Variational Nonlocal Method

$$\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}] := \int_B W(\boldsymbol{F}, \bar{\boldsymbol{Z}}, \boldsymbol{Q}, T)\, dV + \int_B \bar{\boldsymbol{Y}} \cdot (\bar{\boldsymbol{Z}} - \boldsymbol{Z})\, dV$$
$$- \int_B \rho_0 \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_T B} \boldsymbol{T} \cdot \boldsymbol{\varphi}\, dS$$



✓Nonlocality defined naturally.
✓Use constitutive behavior as-is.

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Motivation for Variational Methods

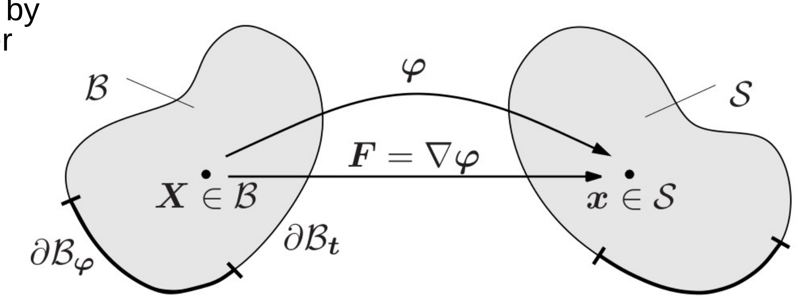
- Begin from fundamental physical principles.
- Governing equations from optimization.
- Allow better analysis for uniqueness of solutions.
- Lead to robust numerical methods.
- Help identify correct conjugate fields.
- Et cetera.

Variational Nonlocal Method

Three-Field Mixed Finite Element Formulation:

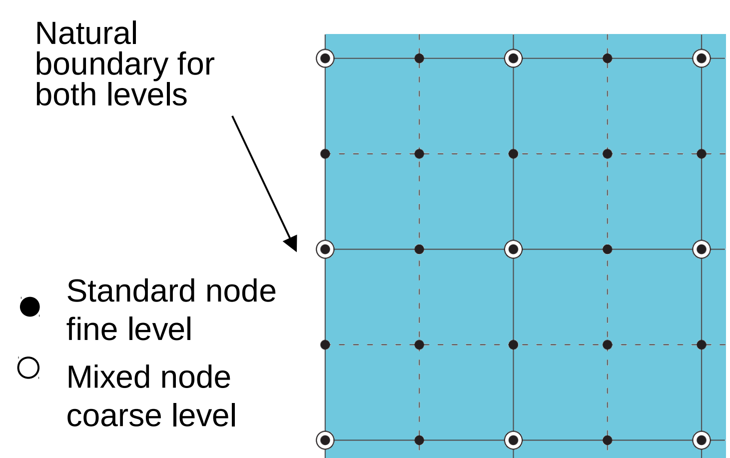
$$\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}] := \int_B W(\boldsymbol{F}, \bar{\boldsymbol{Z}}, \boldsymbol{Q}, T)\, dV + \int_B \bar{\boldsymbol{Y}} \cdot (\bar{\boldsymbol{Z}} - \boldsymbol{Z})\, dV - \int_B \rho_0 \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_T B} \boldsymbol{T} \cdot \boldsymbol{\varphi}\, dS$$

Deformation Mapping — Helmholtz Free Energy — Nonlocal Internal Variable — Constraint Enforced by Lagrange Multiplier



Deformation Mapping

- Motivated through studies of non-locality
- Fully variational approach.
- Entirely by-passes ad hoc approaches.
- Does not require any modifications to constitutive models.
- Nonlocal domain is defined naturally by support of mixed interpolation functions.
- Natural parallelization by domain decomposition of coarse discretization.
- Does not require cut-off approaches at boundary.
- Weight functions are unit interpolation functions.



Finite Element Formulation

Three-Field Mixed Finite Element Formulation:

$$\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}] := \int_B W(\boldsymbol{F}, \bar{\boldsymbol{Z}}, \boldsymbol{Q}, T)\, dV + \int_B \bar{\boldsymbol{Y}} \cdot (\bar{\boldsymbol{Z}} - \boldsymbol{Z})\, dV - \int_B \rho_0 \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_T B} \boldsymbol{T} \cdot \boldsymbol{\varphi}\, dS$$

Variations:

$$\boldsymbol{\varphi} \in V_\varphi := (W_2^1(B))^3,\ \bar{\boldsymbol{Z}} \in V_Z := (W_2^1(B))^q \text{ and } \bar{\boldsymbol{Y}} \in V_Y := (W_2^1(B))^q$$

$$\boldsymbol{\eta} \in V_\varphi,\ \boldsymbol{\zeta} \in V_Z \text{ and } \boldsymbol{\xi} \in V_Y$$

$$D\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}](\boldsymbol{\eta}) = \int_B \boldsymbol{P} : \mathrm{Grad}\, \boldsymbol{\eta}\, dV - \int_B \rho_0 \boldsymbol{B} \cdot \boldsymbol{\eta}\, dV - \int_{\partial_T B} \boldsymbol{T} \cdot \boldsymbol{\eta}\, dS = 0,$$

$$D\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}](\boldsymbol{\zeta}) = \int_B (\bar{\boldsymbol{Y}} - \boldsymbol{Y}) \cdot \boldsymbol{\zeta}\, dV = 0,$$

$$D\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}](\boldsymbol{\xi}) = \int_B (\bar{\boldsymbol{Z}} - \boldsymbol{Z}) \cdot \boldsymbol{\xi}\, dV = 0,$$

$$\boldsymbol{P} := \partial W / \partial \boldsymbol{F} \qquad \boldsymbol{Y} := -\partial W / \partial \bar{\boldsymbol{Z}}$$

Regularization

Discrete Statement of Equilibrium,

Internal Variables and Conjugate Forces:

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

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

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

Unit Interpolation, Regularized Variables:

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

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

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

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

Connection to Gradients

Expansion in Taylor Series:

$$\boldsymbol{Z} = \boldsymbol{Z}_0 + \frac{\partial \boldsymbol{Z}}{\partial \boldsymbol{X}}(\boldsymbol{X}_0) \cdot (\boldsymbol{X} - \boldsymbol{X}_0) + \frac{1}{2}(\boldsymbol{X} - \boldsymbol{X}_0) \cdot \frac{\partial^2 \boldsymbol{Z}}{\partial \boldsymbol{X}^2}(\boldsymbol{X}_0) \cdot (\boldsymbol{X} - \boldsymbol{X}_0) + \cdots$$

Apply to Regularized Variables:

$$\bar{\boldsymbol{Z}} = \boldsymbol{Z}_0 + \frac{1}{2\,\mathrm{vol}(D)} \frac{\partial^2 \boldsymbol{Z}}{\partial \boldsymbol{X}^2}(\boldsymbol{X}_0) : \int_D (\boldsymbol{X} - \boldsymbol{X}_0) \otimes (\boldsymbol{X} - \boldsymbol{X}_0)\, dV + \cdots$$

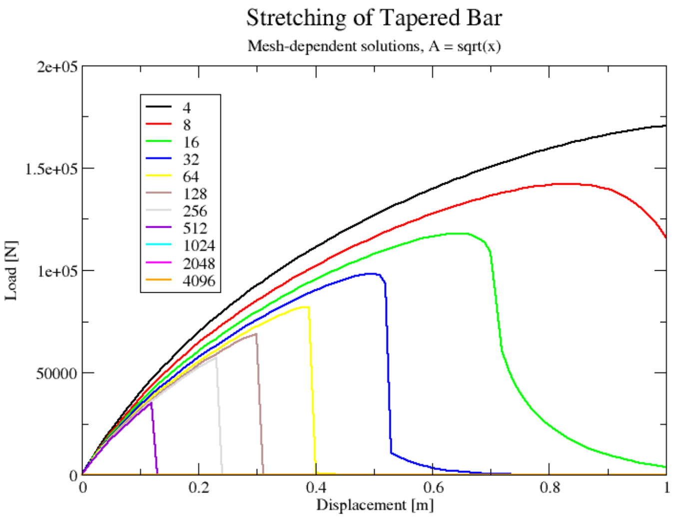
Obtain Gradient Regularization:

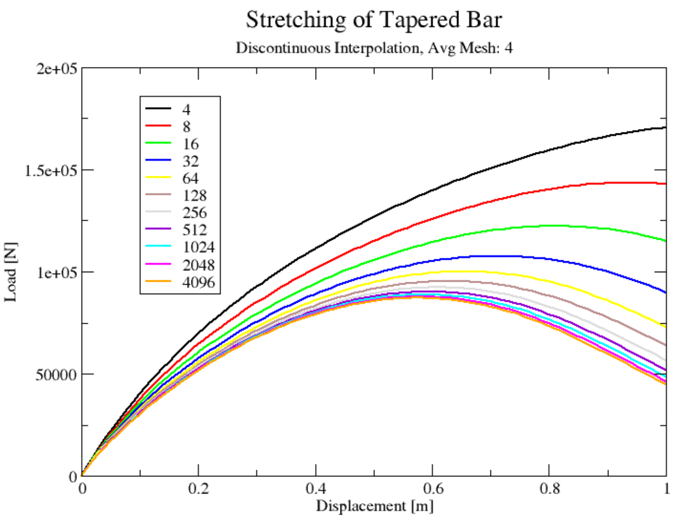
$$\bar{\boldsymbol{Z}} = \boldsymbol{Z}_0 + \nabla^2 \boldsymbol{Z}(\boldsymbol{X}_0) : \boldsymbol{H}(D) + \cdots$$

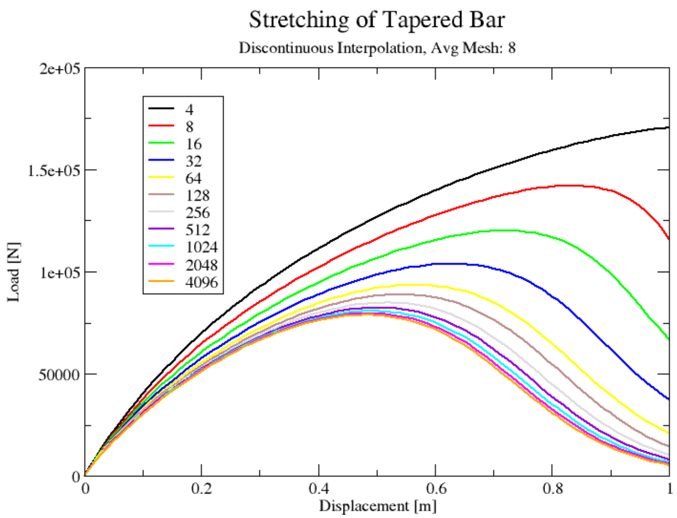
1D Problem – Stretching of Bar

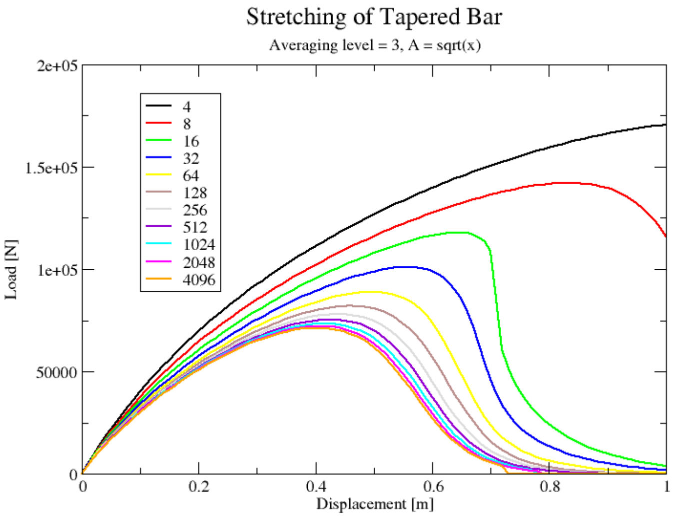
- Proof of concept problem.
- Area proportional to square root of length.
- Strong singularity on left end of bar.
- Simple hyperelestic model with damage.
- Code written in Matlab.
- Two interpolation schemes.

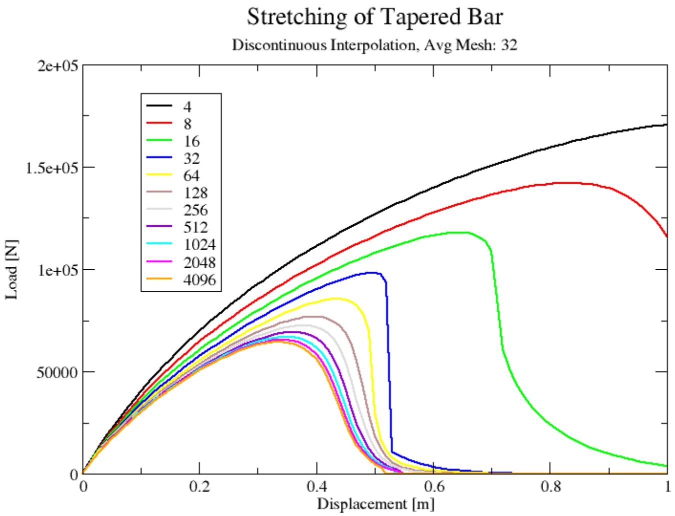
Constant Unit Interpolation

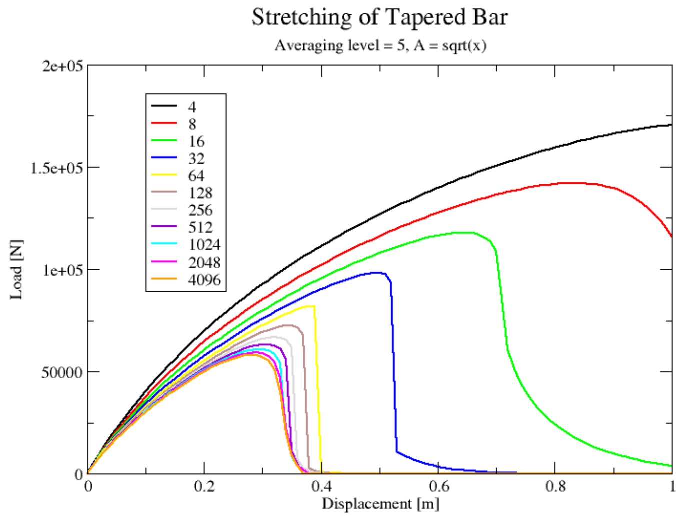












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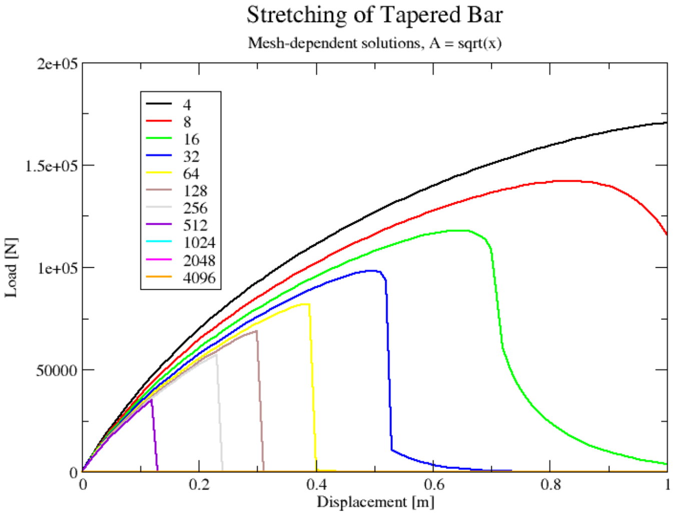
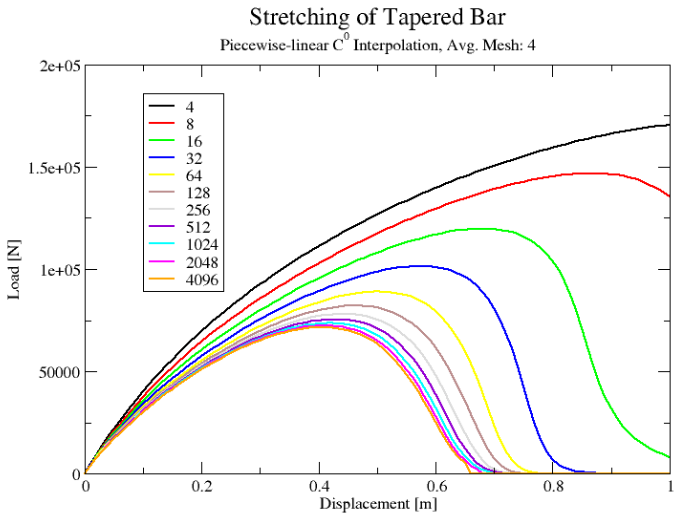
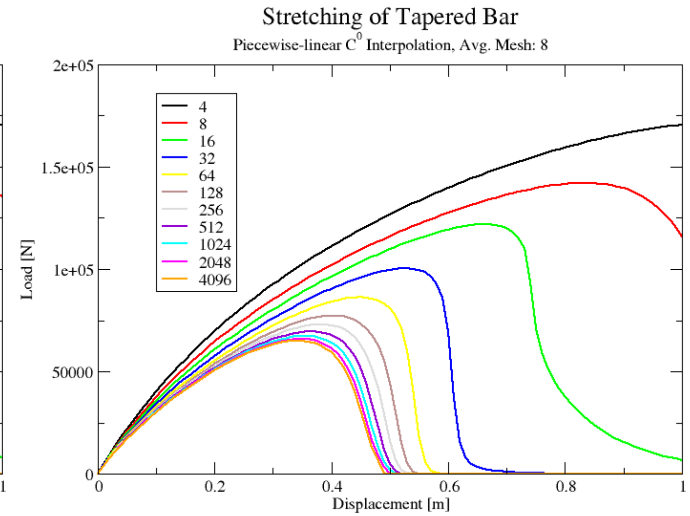
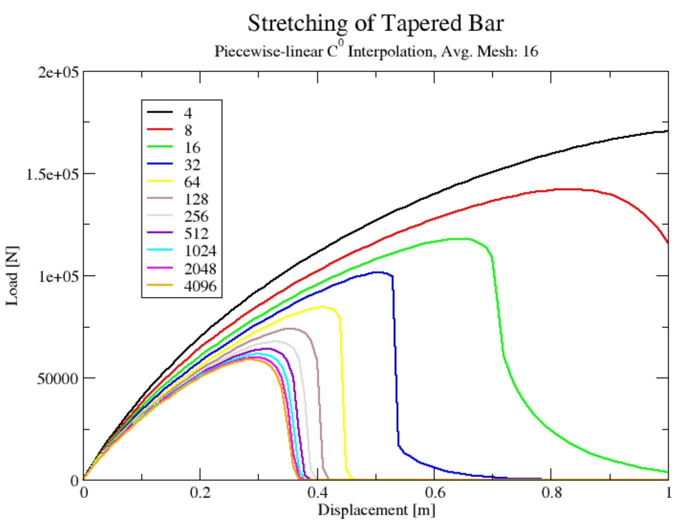
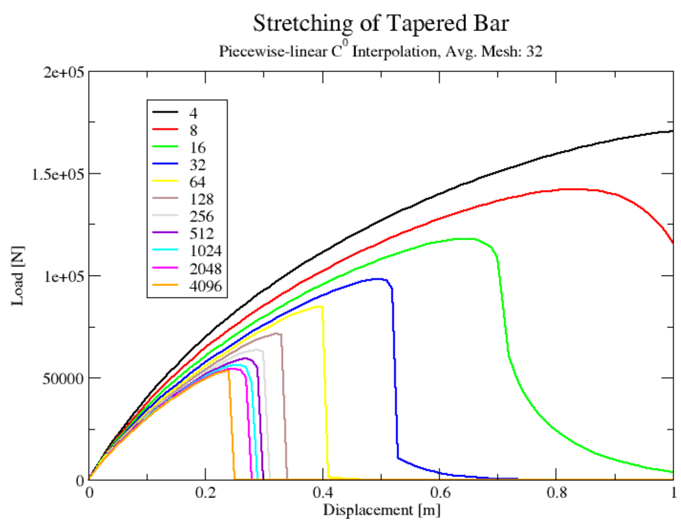
Linear Interpolation

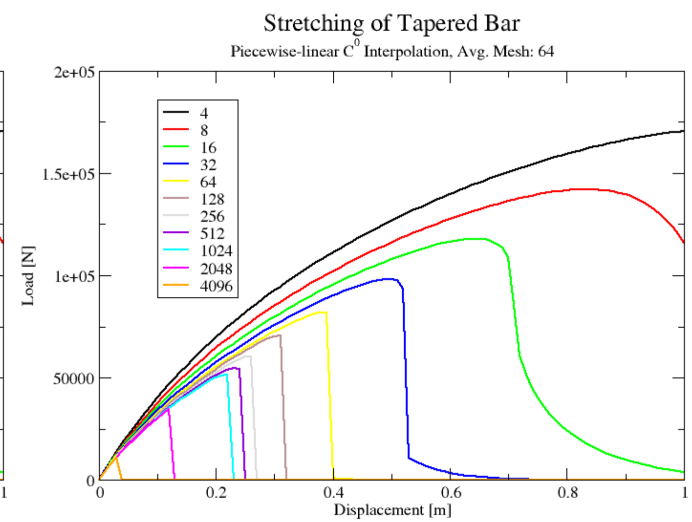




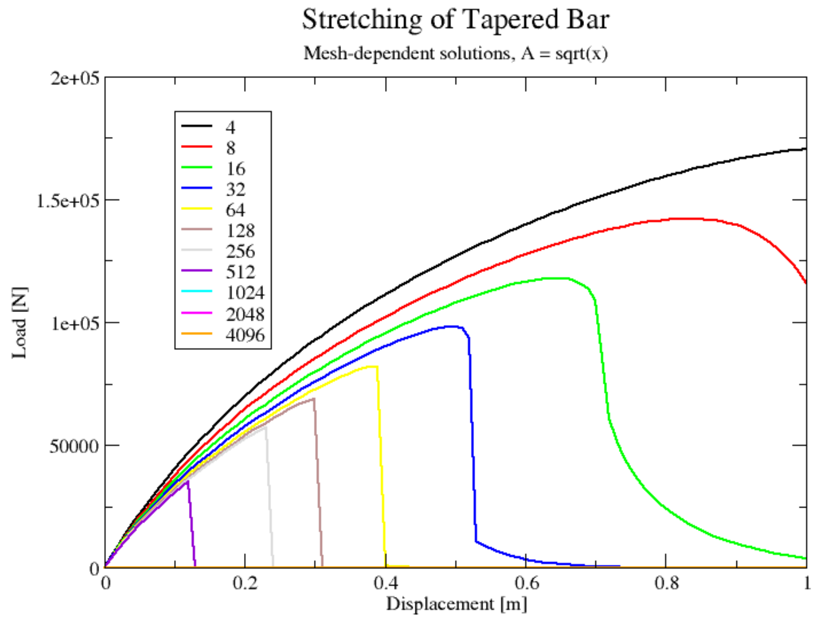


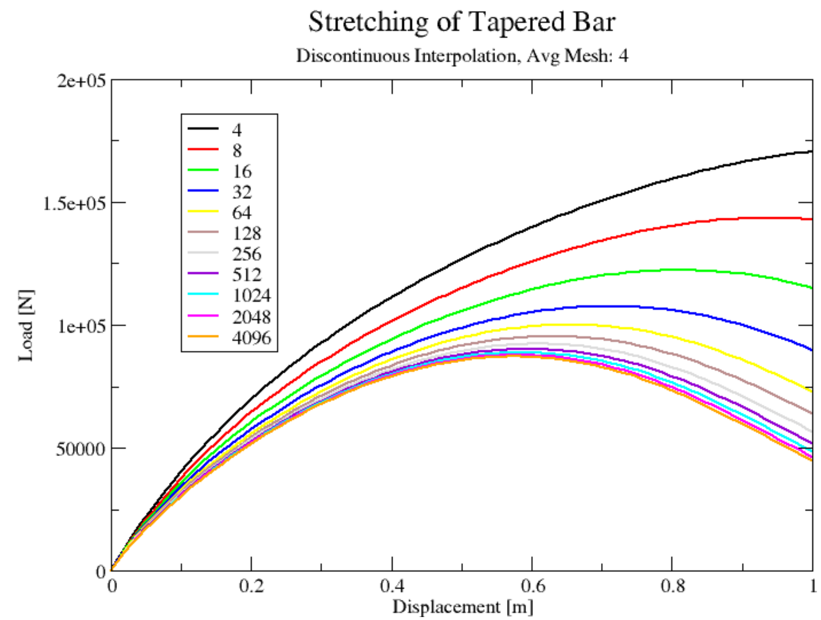


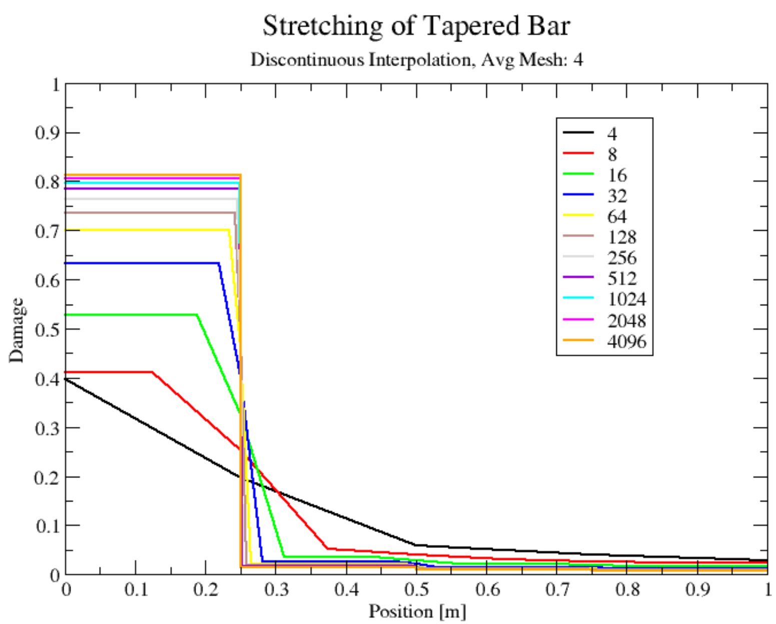


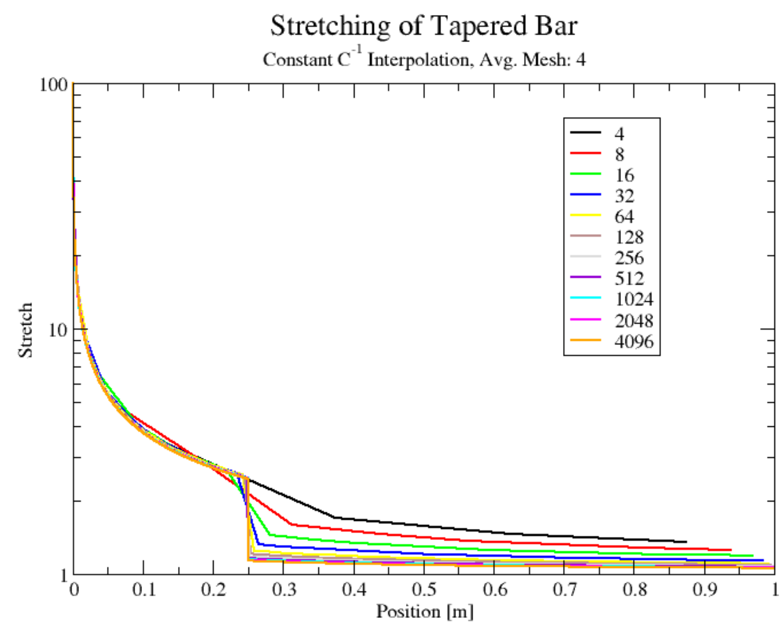


Avg Mesh 4, Unit Interpolation

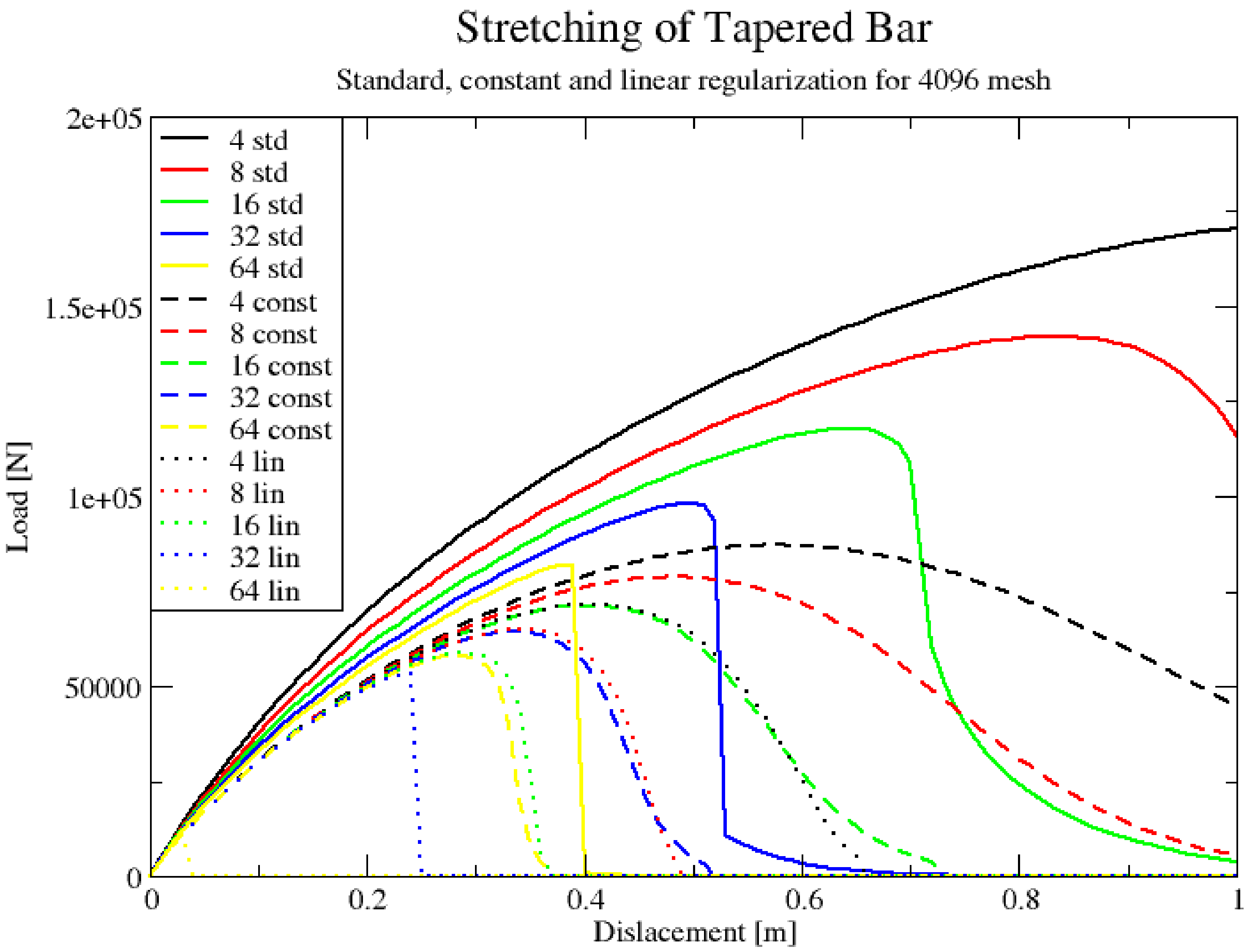








Effect of Order of Interpolation



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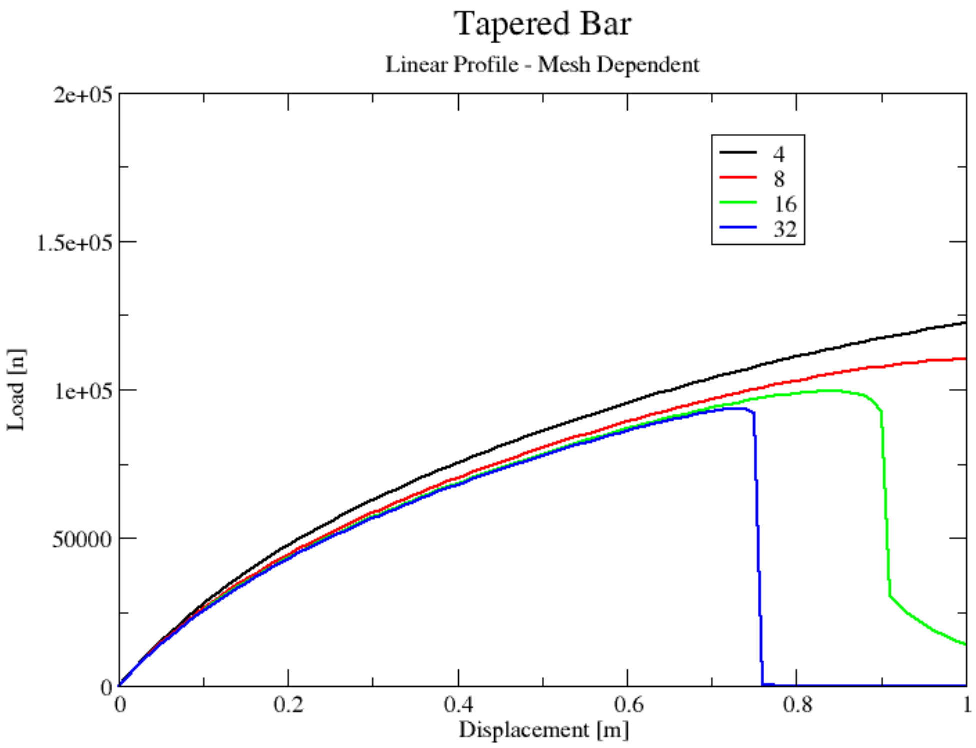
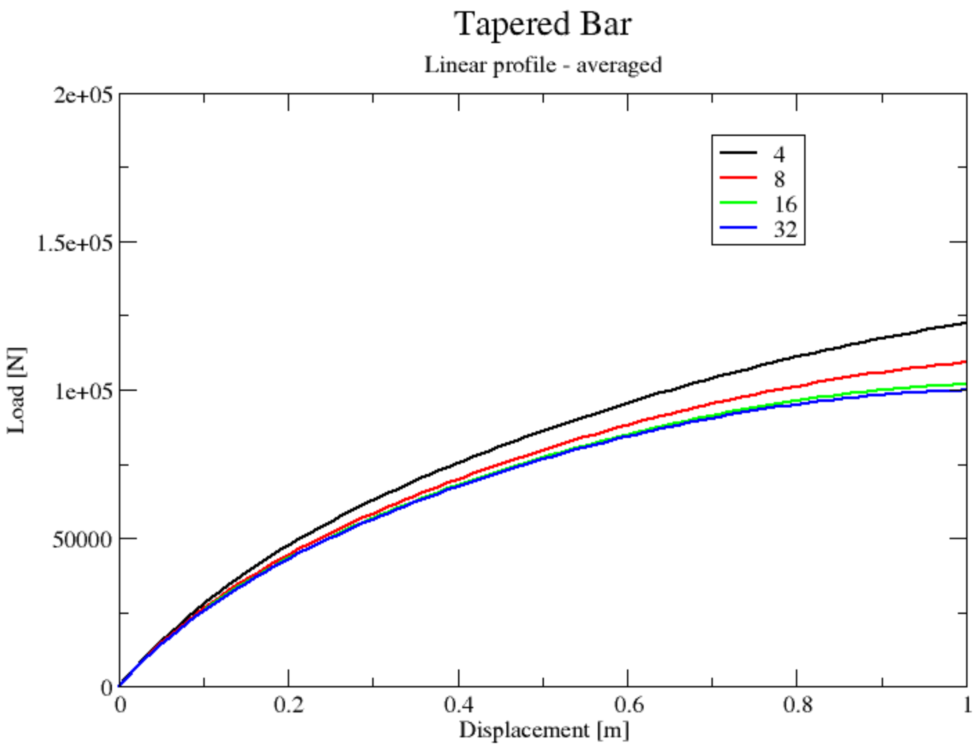
Weaker Defect – V Profile Bar



Mesh Dependent



Regularized

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Mesh Dependence

Simple finite-deformation elastic model with damage:

$$W(\boldsymbol{C}, \zeta) = (1 - \zeta) W_0(\boldsymbol{C})$$

$$\boldsymbol{\epsilon} = \frac{1}{2} \log(\boldsymbol{C})$$

$$\bar{\boldsymbol{\epsilon}} = \mathrm{dev}(\boldsymbol{\epsilon}), \quad \theta = \mathrm{tr}(\boldsymbol{\epsilon}),$$

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

$$W_0^{\mathrm{vol}}(\theta) = \frac{\kappa}{4}\left[\exp(2\theta) - 1 - 2\theta\right],$$

$$W_0^{\mathrm{dev}}(\bar{\boldsymbol{\epsilon}}) = \frac{\mu}{2}\left[\mathrm{tr}(\exp \bar{\boldsymbol{\epsilon}}) - 3\right].$$

$$\zeta(\alpha) := \zeta_\infty [1 - \exp(-\alpha/\iota)]$$

$$\alpha(t) := \max_{s \in [0,t]} W_0(s)$$

ζ_∞: maximum possible damage

ι: damage saturation parameter

$E = 200\mathrm{GPa}$

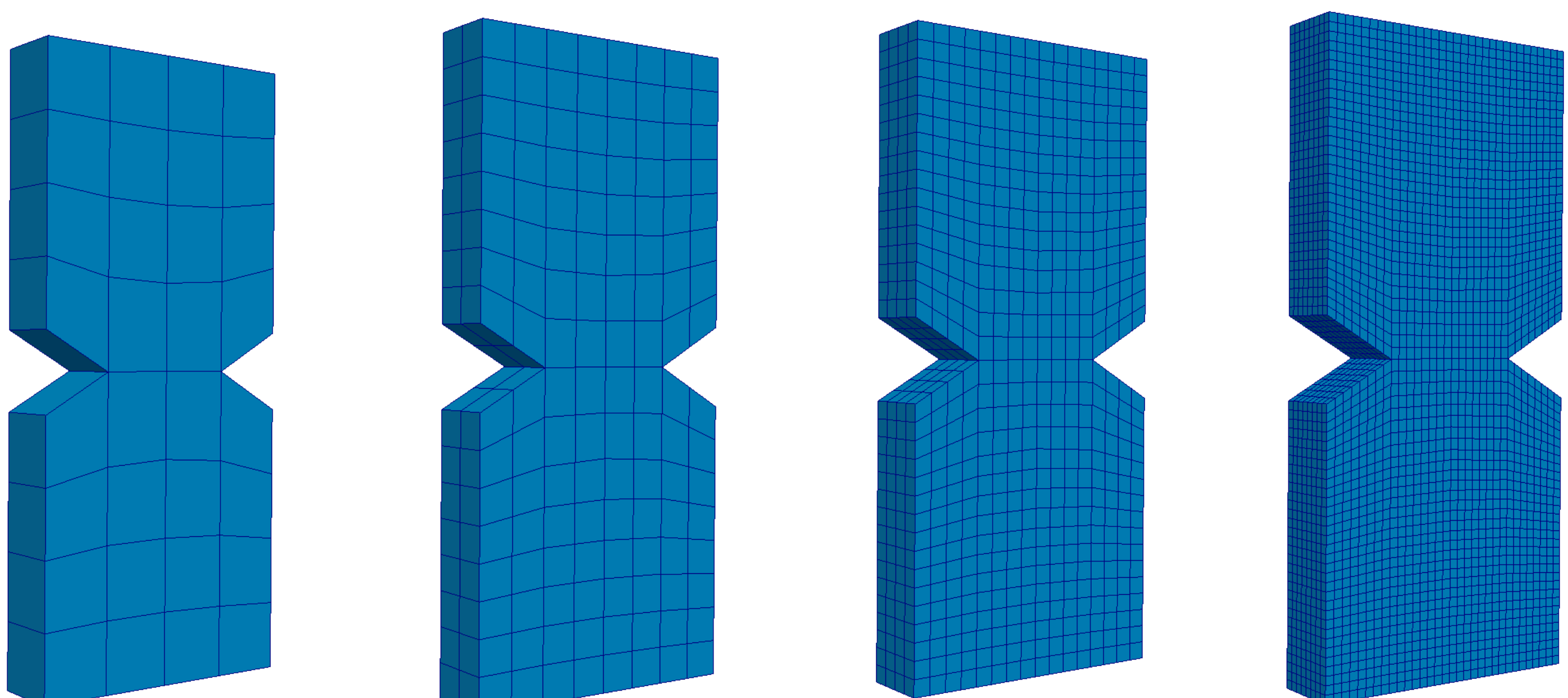
$\nu = 0.25$

$\kappa = 133\mathrm{GPa}$

$\mu = 67\mathrm{GPa}$

$\zeta_\infty = 1.0$

$\iota = 100\mathrm{GJm}^{-3}$



N=32 h~1mm | N=256 h~0.5mm | N=2048 h~0.25mm | N=16384 h~0.125mm

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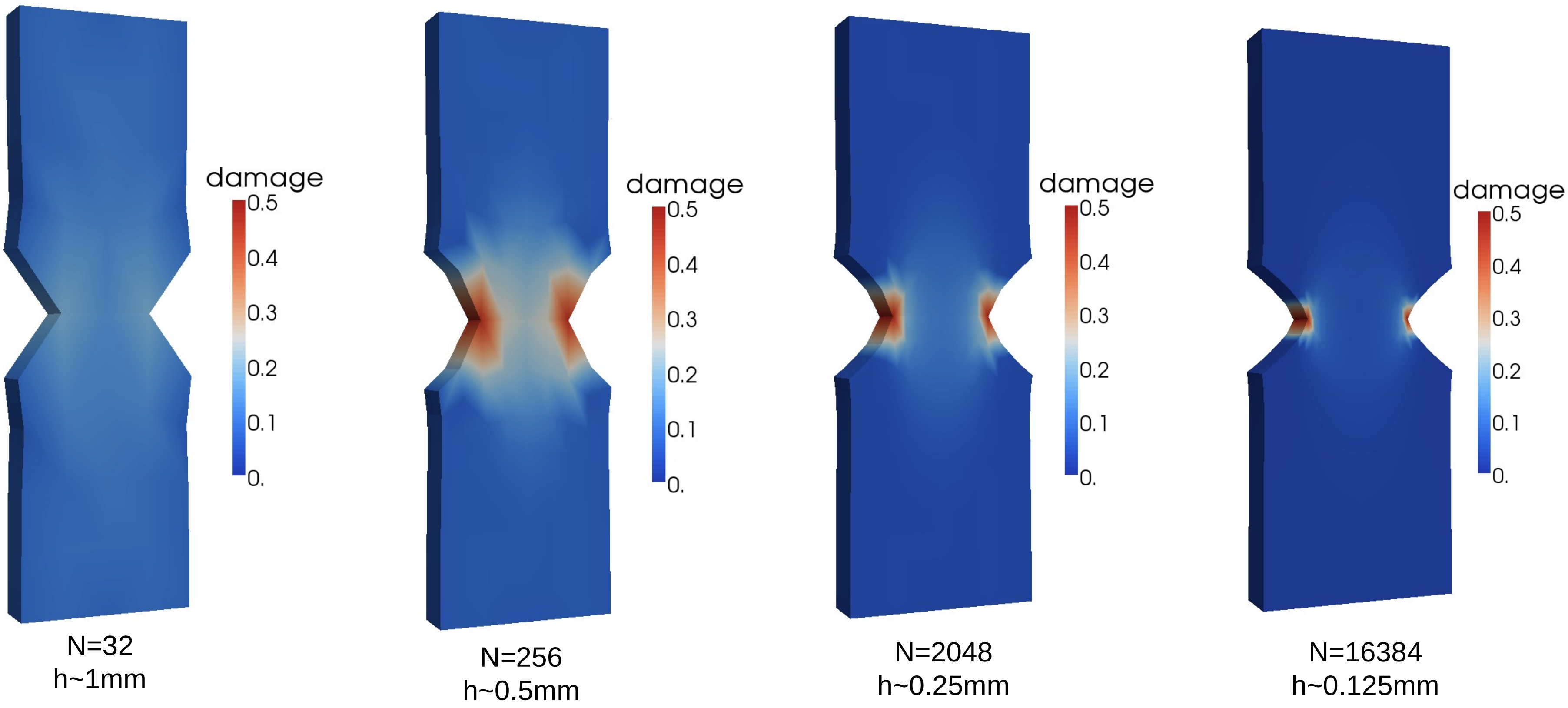
Mesh Dependence



Damage

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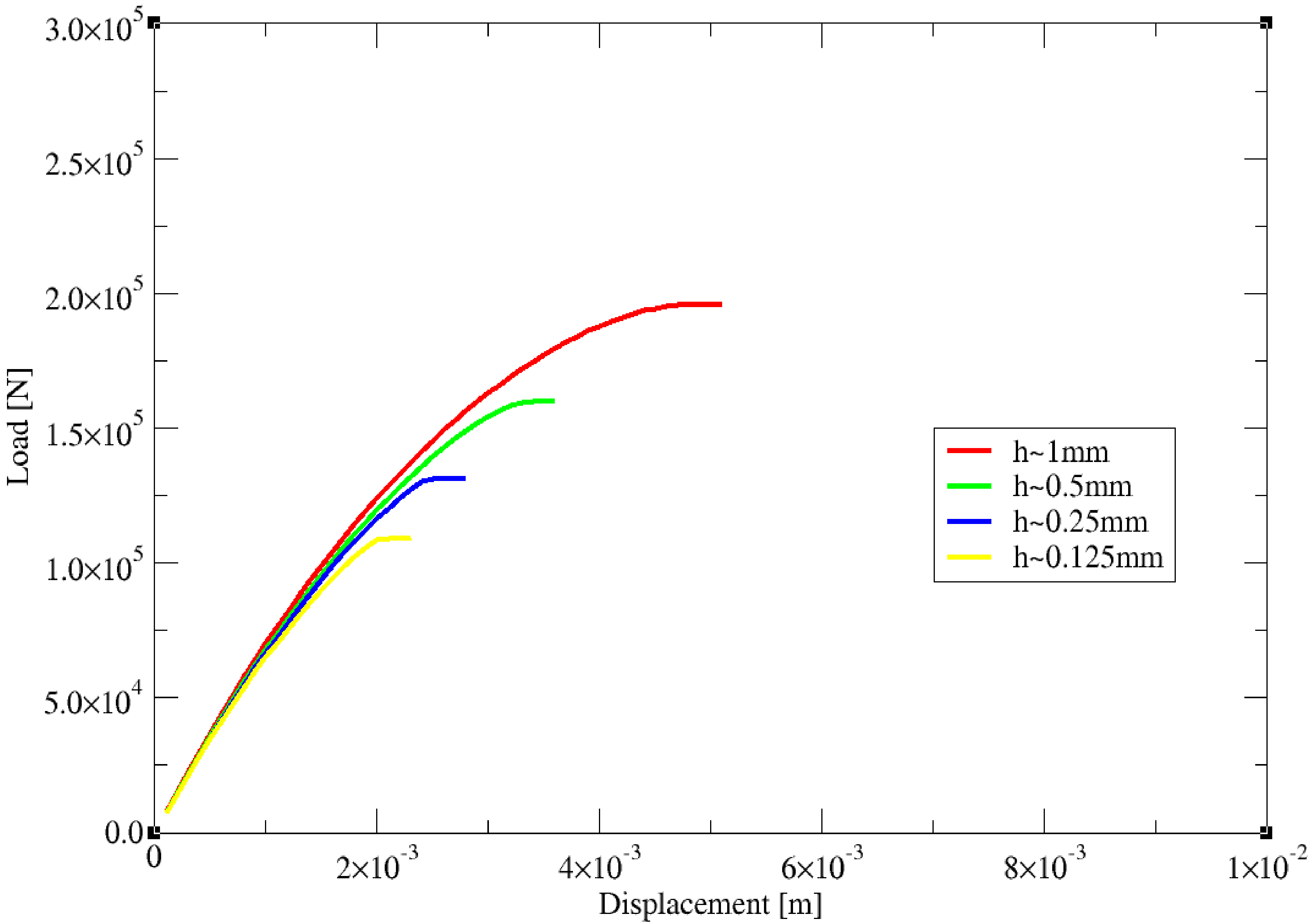
Mesh Dependence



Load - Displacement

Implementation

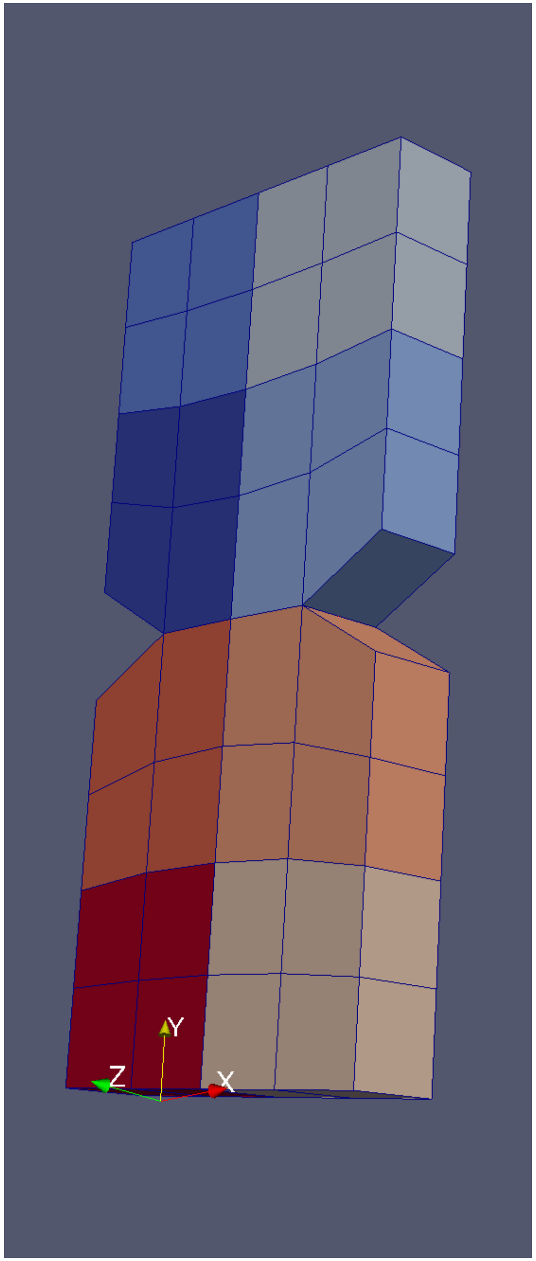
$$\bar{\boldsymbol{Y}} = \frac{1}{\text{vol}(D)} \int_D \boldsymbol{Y}\ dV,$$
$$\bar{\boldsymbol{Z}} = \frac{1}{\text{vol}(D)} \int_D \boldsymbol{Z}\ dV,$$
$$\text{vol}(\bullet) := \int_{(\bullet)} dV,$$

Constant interpolation leads to simple averaging:

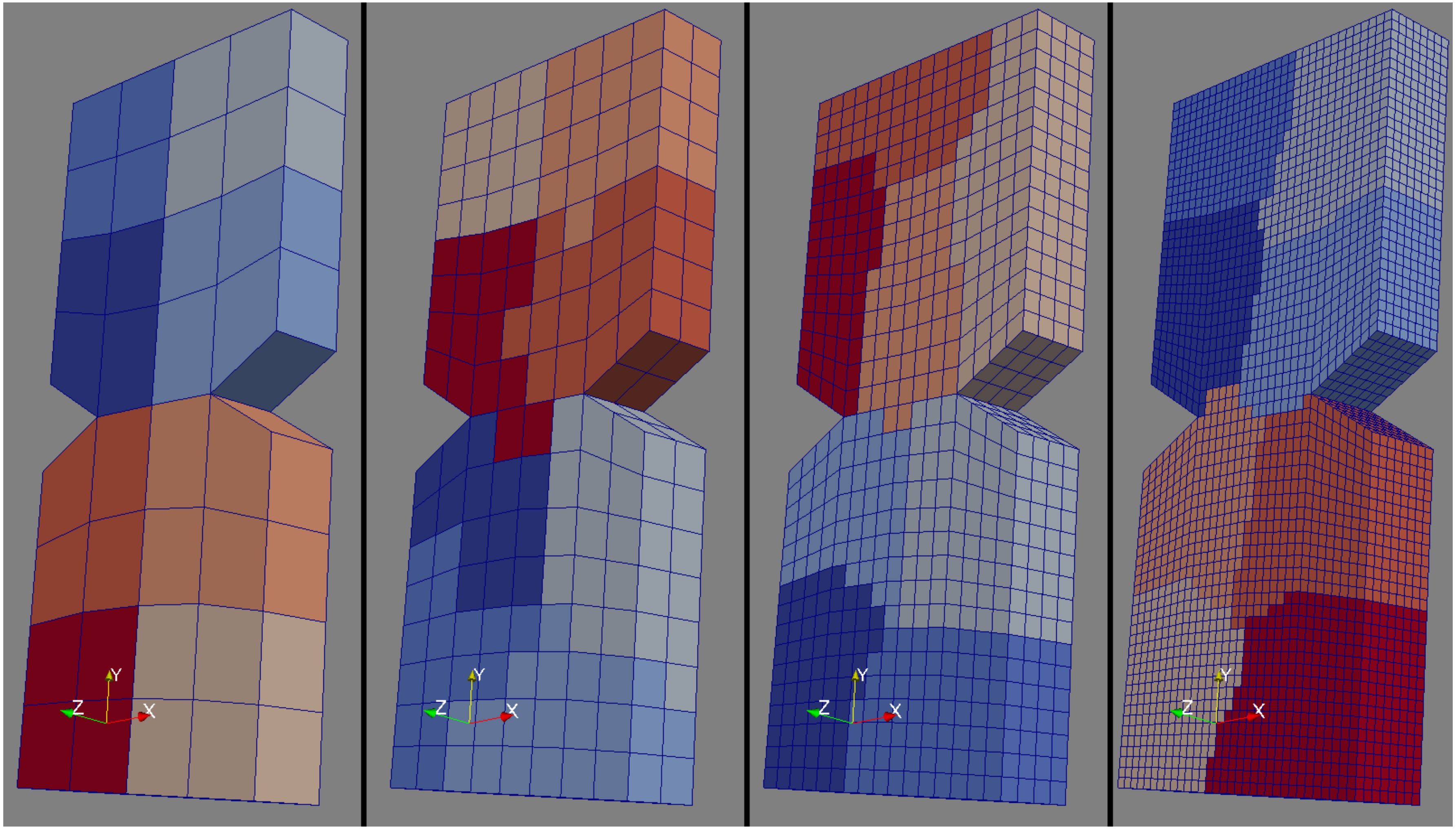
$$\text{vol}(D) = \sum_{i=0}^{n} \text{vol}(E_i),$$
$$\int_D \boldsymbol{Y}\ dV = \sum_{i=0}^{n} \int_{E_i} \boldsymbol{Y}\ dV,$$
$$\int_D \boldsymbol{Z}\ dV = \sum_{i=0}^{n} \int_{E_i} \boldsymbol{Z}\ dV.$$

Use METIS to create domains *D*

vol(*D*)=(lengh scale)^3=(1.6mm)^3



Partitions



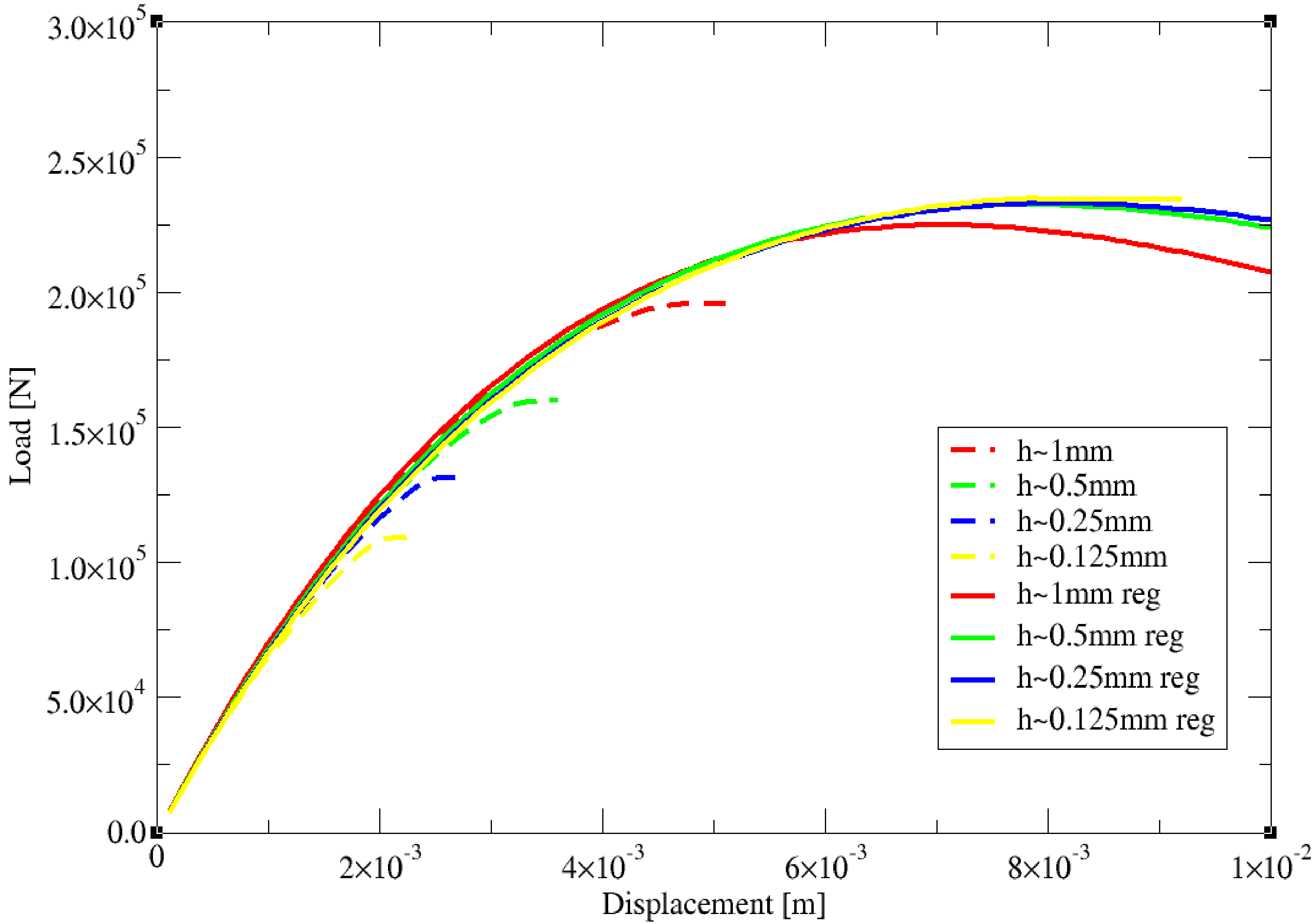
N=32
h~1mm

N=256
h~0.5mm

N=2048
h~0.25mm

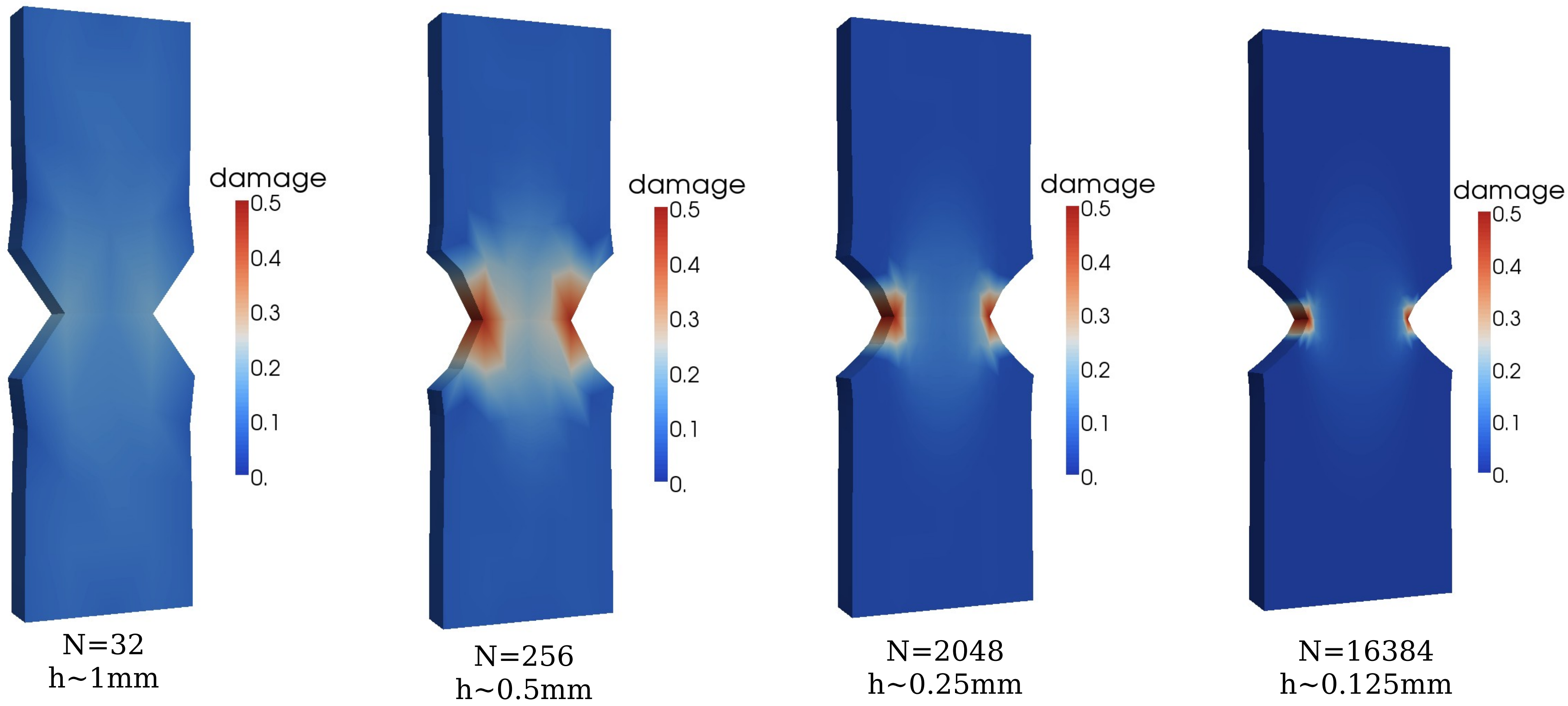
N=16384
h~0.125mm

Regularized Solution



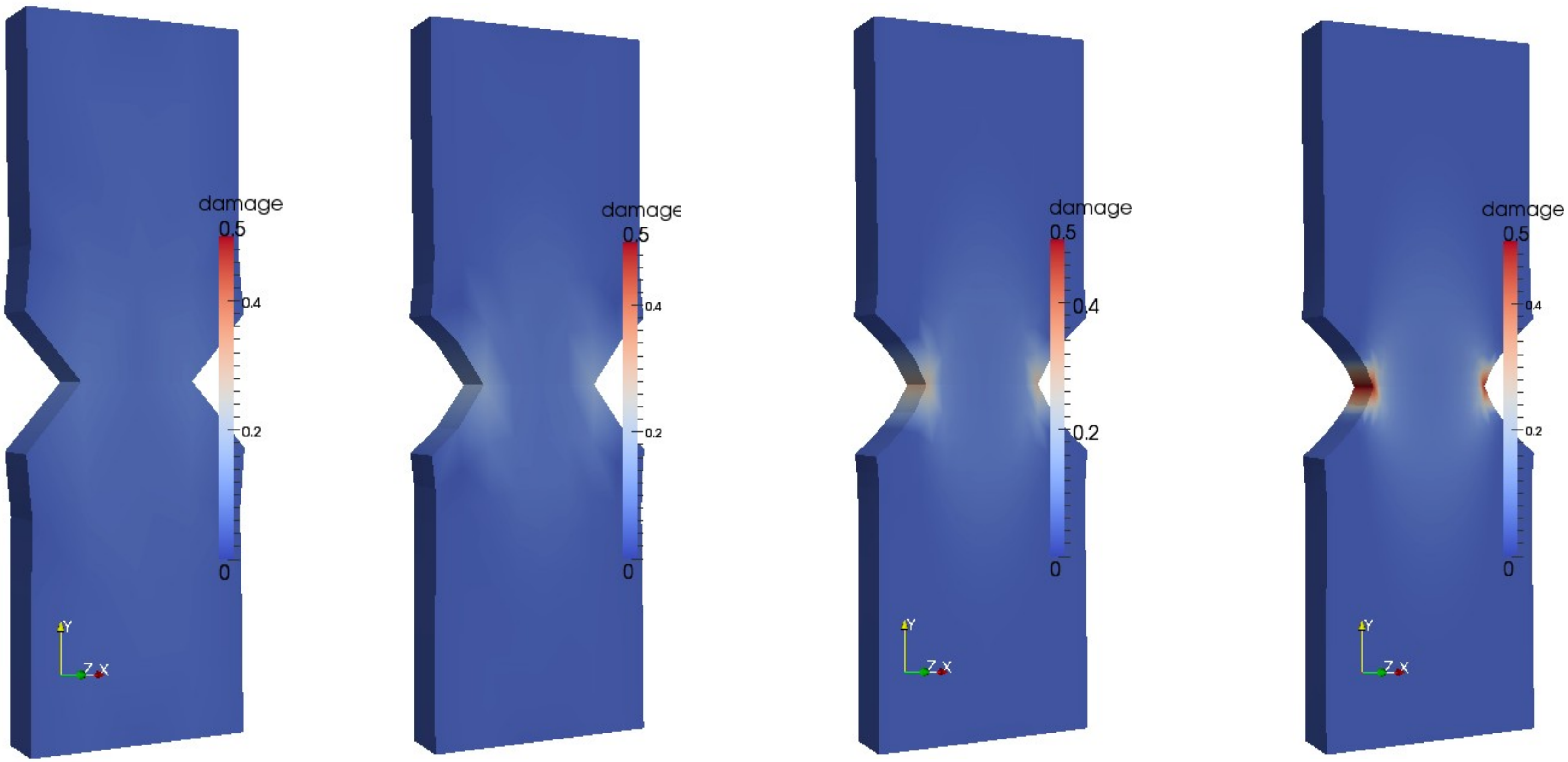
Load - Displacement

Mesh Dependence



Damage

Regularized Solution



N=32 h~1mm

N=256 h~0.5mm

N=2048 h~0.25mm

N=16384 h~0.125mm

Damage

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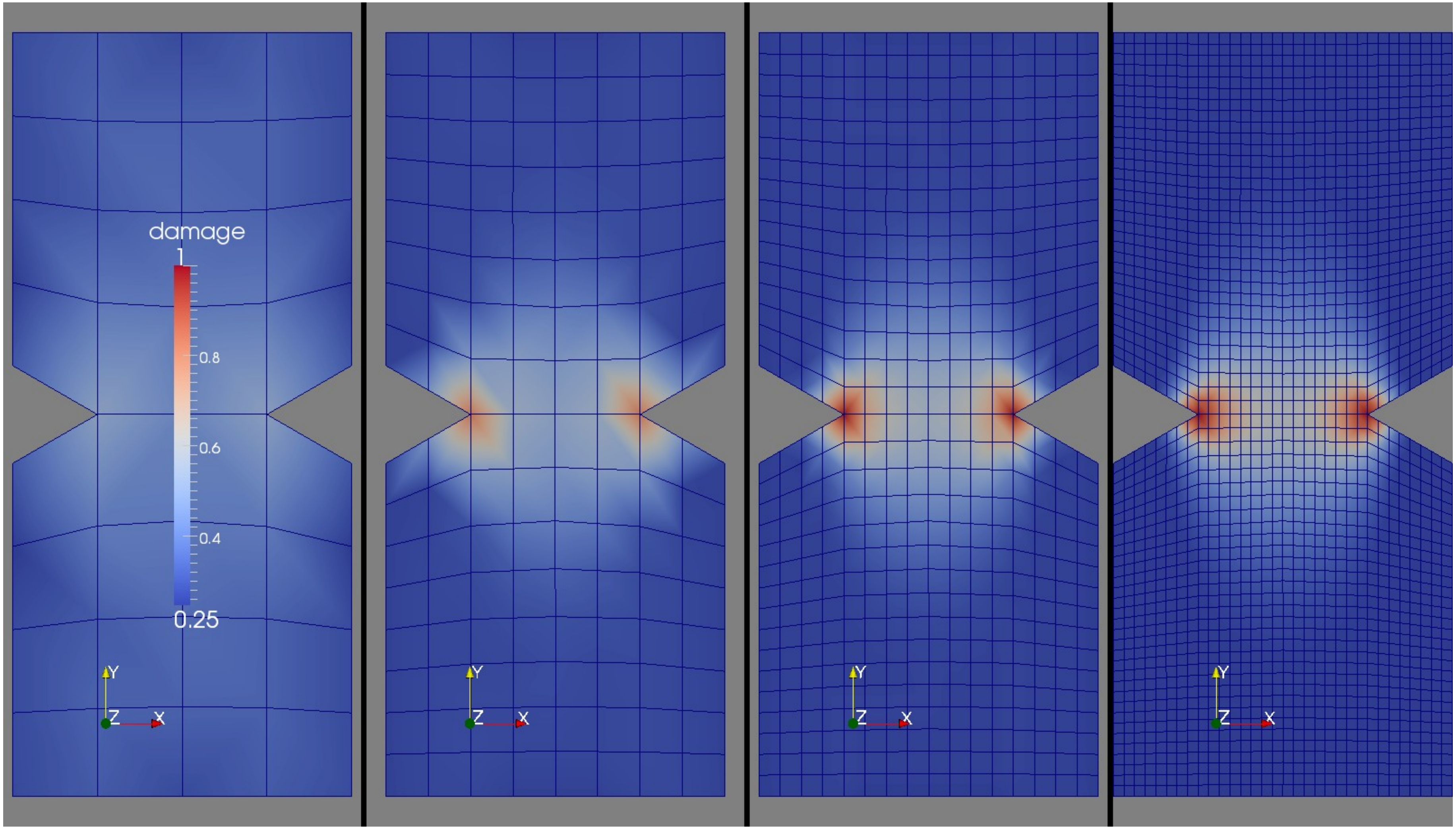
Regularized Solution (reference)



N=32
h~1mm

N=256
h~0.5mm

N=2048
h~0.25mm

N=16384
h~0.125mm

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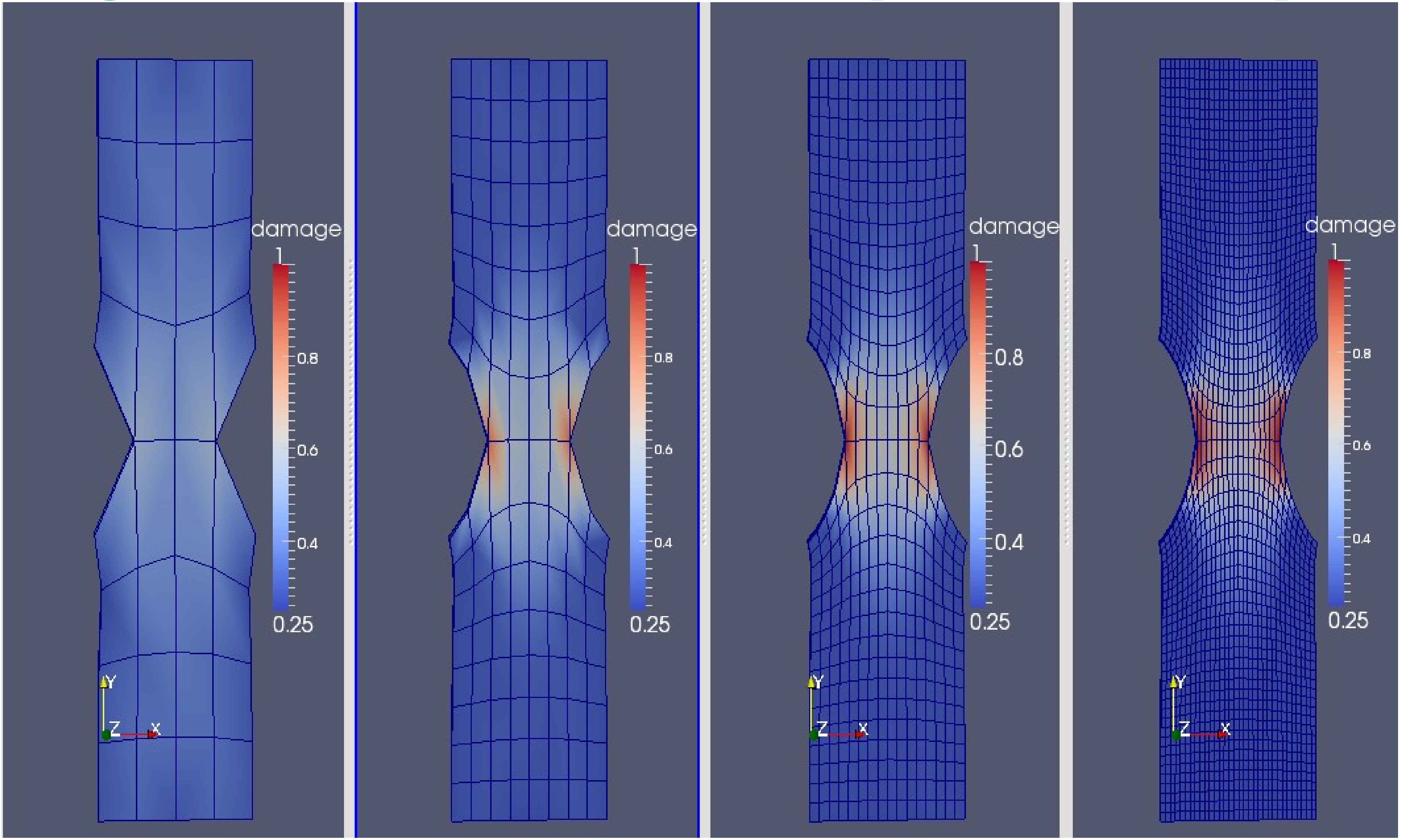
Regularized Solution (deformed)



N=32
h~1mm

N=256
h~0.5mm

N=2048
h~0.25mm

N=16384
h~0.125mm

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Conclusions

- Regularization effective.
- Derived naturally from variational principle.
- Strong connection to gradient methods.
- No special boundary considerations.
- Simple form with unit interpolation functions.

Work in Progress

- Test in large 3D problems.
- Use same variational principle for mapping of internal variables.

Acknowledgments

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