Peridynamic Modeling of Localization in Ductile Metals

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Peridynamics

WHAT IS PERIDYNAMICS?

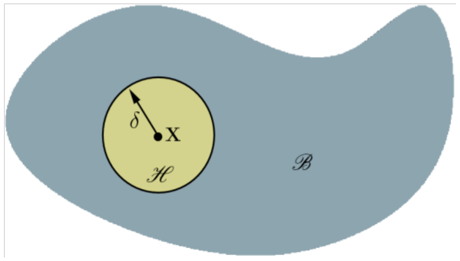
Peridynamics is a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles

HOW DOES IT WORK?

- Peridynamics is a *nonlocal* extension of continuum mechanics
- Remains valid in presence of discontinuities, including cracks
- Balance of linear momentum is based on an *integral equation*:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \underbrace{\int_{\mathscr{B}} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x}\rangle - \underline{\mathbf{T}}'[\mathbf{x}',t]\langle \mathbf{x} - \mathbf{x}'\rangle \right\} \mathrm{d}V_{\mathbf{x}'}}_{\text{Divergence of stress replaced with integral of nonlocal forces.}} + \mathbf{b}(\mathbf{x},t)$$

The point X interacts directly with all points within its horizon



S.A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48:175-209, 2000.

Silling, S.A. and Lehoucq, R. B. Peridynamic Theory of Solid Mechanics. *Advances in Applied Mechanics* 44:73-168, 2010.

Peridynamics

CONSTITUTIVE LAWS IN PERIDYNAMICS

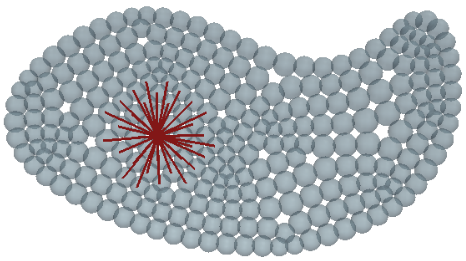
- Peridynamic *bonds* connect any two material points that interact directly
- Peridynamic forces are determined by *force states* acting on bonds

$$\underbrace{\underline{\mathbf{T}}[\mathbf{x}, t]}_{\text{Force State}} \; \underbrace{\langle \mathbf{x}_i' - \mathbf{x} \rangle}_{\text{Bond}}$$

- Force states are determined by constitutive laws and are functions of the deformations of all points within a neighborhood
- *Material failure* is modeled through the breaking of peridynamic bonds
  - Example: critical stretch bond breaking law

DISCRETIZATION OF A PERIDYNAMIC BODY

A body may be represented by a finite number of sphere elements



$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x}, t) = \sum_{i=0}^{N} \left\{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}_i' - \mathbf{x} \rangle - \underline{\mathbf{T}}'[\mathbf{x}_i', t] \langle \mathbf{x} - \mathbf{x}_i' \rangle \right\} \Delta V_{\mathbf{x}_i'} + \mathbf{b}(\mathbf{x}, t)$$

State-based Peridynamic Material Models

LINEAR PERIDYNAMIC SOLID (ELASTIC MODEL)

$$\theta\left(\underline{e}\right) = \frac{3}{m}\left(\underline{\omega}\,\underline{x}\right) \bullet \underline{e}$$

$$\underline{t} = \frac{3k\theta}{m}\,\underline{\omega}\,\underline{\mathrm{x}} + \frac{15\mu}{m}\,\underline{\omega}\,\underline{e}^{\mathrm{d}}$$

ELASTIC-PLASTIC MODEL

$$\underline{t} = \frac{3k\theta}{m}\,\underline{\omega}\,\underline{\mathrm{x}} + \frac{15\mu}{m}\,\underline{\omega}\,\left(\underline{e}^{\mathrm{d}} - \underline{e}^{\mathrm{dp}}\right)$$

S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.

J.A. Mitchell. A nonlocal, ordinary, state-based plasticity model for peridynamics. Sandia Report SAND2011-3166, 2011.

Adaptation of Classical Material Models for Peridynamics

APPROACH: NON-ORDINARY STATE-BASED PERIDYNAMICS

- Apply existing (local) constitutive models within nonlocal peridynamic framework
- Utilize approximate deformation gradient based on positions and deformations of all elements in the neighborhood

① Compute regularized deformation gradient

$$\bar{\mathbf{F}} = \left(\sum_{i=0}^{N} \underline{\omega}_i \, \underline{\mathbf{Y}}_i \otimes \underline{\mathbf{X}}_i \, \Delta V_{\mathbf{x}_i} \right) \mathbf{K}^{-1} \qquad \mathbf{K} = \sum_{i=0}^{N} \underline{\omega}_i \, \underline{\mathbf{X}}_i \otimes \underline{\mathbf{X}}_i \, \Delta V_{\mathbf{x}_i}$$

② Classical material model computes stress based on regularized deformation gradient

③ Convert stress to peridynamic force densities

$$\underline{\mathbf{T}} \langle \mathbf{x}' - \mathbf{x} \rangle = \underline{\omega} \, \sigma \mathbf{K}^{-1} \langle \mathbf{x}' - \mathbf{x} \rangle$$

④ Apply peridynamic hourglass forces as required to stabilize simulation (optional)

S. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari. Peridynamic states and constitutive modeling. *Journal of Elasticity*, 88(2):151-184, 2007.

Suppression of Zero-Energy Modes

APPROACH: PENALIZE DEFORMATION THAT DEVIATES FROM REGULARIZED DEFORMATION GRADIENT

Predicted location of neighbor

$$\mathbf{x}_n'^{\star} = \mathbf{x}_n + \bar{\mathbf{F}}_n \; (\mathbf{x}_o' - \mathbf{x}_o)$$

Hourglass vector

$$\mathbf{\Gamma}_{\text{hg}} = \mathbf{x}_n'^{\star} - \mathbf{x}_n'$$

Hourglass vector projected onto bond

$$\gamma_{\text{hg}} = \mathbf{\Gamma}_{\text{hg}} . \, (\mathbf{x}_n' - \mathbf{x}_n)$$

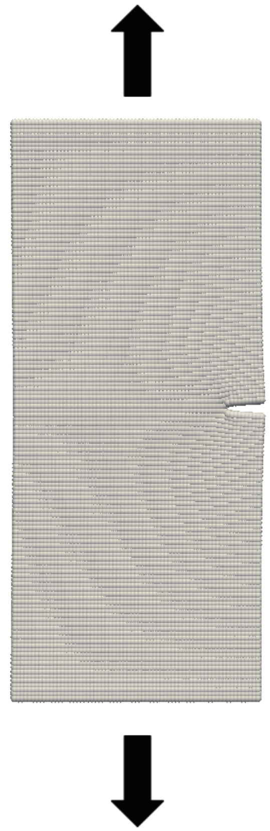
Hourglass force

$$\mathbf{f}_{\text{hg}} = -\text{C}_{\text{hg}} \underbrace{\left(\frac{18k}{\pi\delta^4}\right)}_{\text{micro-modulus}} \underbrace{\frac{\gamma_{\text{hg}}}{\|\mathbf{x}_o' - \mathbf{x}_o\|}}_{\text{hourglass stretch}} \underbrace{\frac{\mathbf{x}_n' - \mathbf{x}_n}{\|\mathbf{x}_n' - \mathbf{x}_n\|}}_{\text{bond unit vector}} \Delta V_{\text{x}} \, \Delta V_{\text{x}'}$$

Peridynamic Horizon Provides a Length Scale

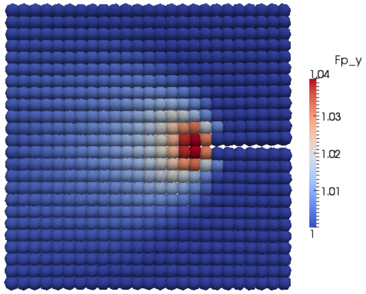
NONLOCALITY YIELDS MESH INDEPENDENCE AT CRACK TIP

- The peridynamic horizon introduces a length scale that is independent of the mesh size.
- Decoupling from the mesh size enables consistent modeling of material response in the vicinity of discontinuities.
- Example: Mesh independent plastic zone in the vicinity of a crack.

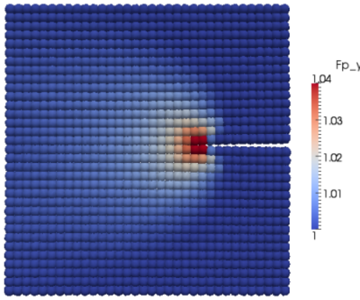


Pre-cracked specimen loaded in tension

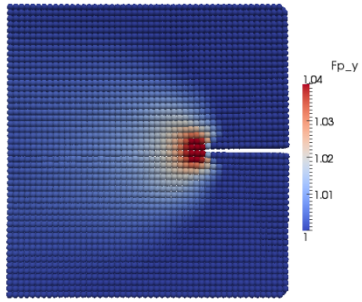
Coarse mesh



Medium mesh



Fine mesh

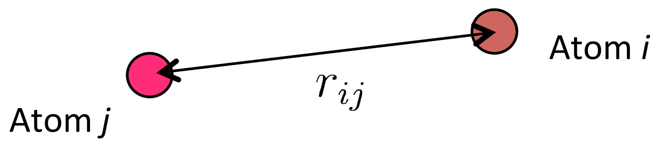


Component of plastic deformation gradient in loading direction

Can the Peridynamic Horizon Have Physical Meaning?

MANY PHYSICAL PROBLEMS HAVE NATURAL LENGTH SCALE(S)

- Interatomic forces

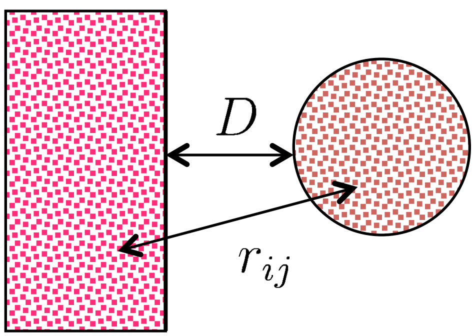


$$F_{ij} \sim \left(\frac{a}{r_{ij}}\right)^{12} - \left(\frac{a}{r_{ij}}\right)^{6}$$

- Van der Waals forces
  - Force between a pair of atoms as they are separated:

$$F_{ij} \sim 1/r_{ij}^6$$

  - Net force between half-space and sphere occurs over a much larger length scale*



$$F_{\text{sphere}} \sim 1/D$$

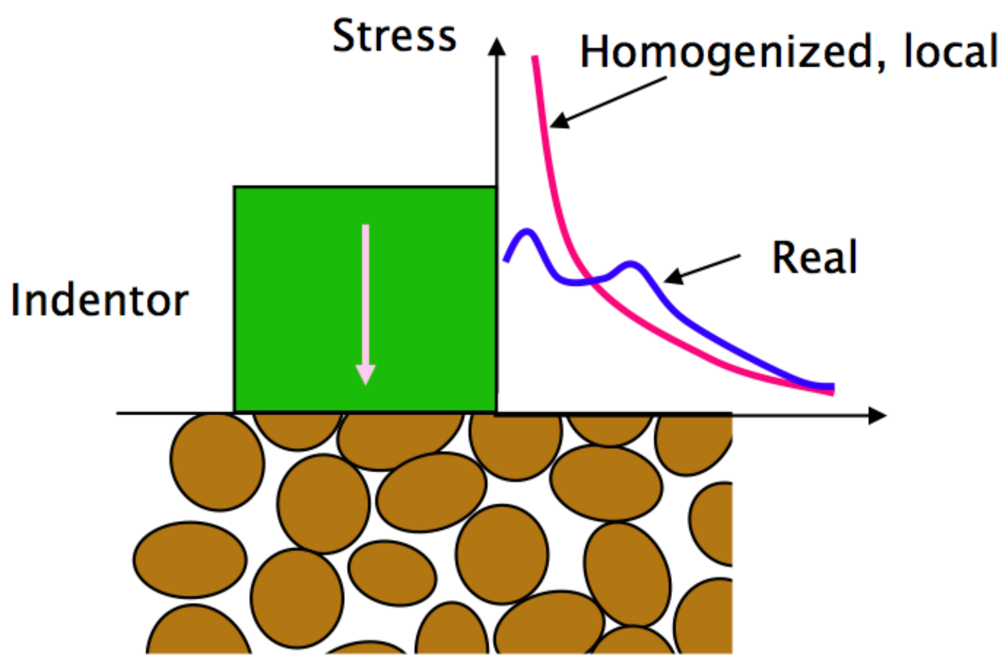
*See J. Israelachvili, *Intermolecular and Surfaces Forces*, pp. **177**.

[Courtesy S. Silling]

Physical Interpretation of Peridynamic Horizon

NONLOCALITY AS A RESULT OF HOMOGENIZATION

- Homogenization (neglecting natural length scales) often leads to poor results
- Nonlocality (length scale) can be an essential feature of a realistic homogenized model of a heterogeneous material
- Example: Concrete indentor

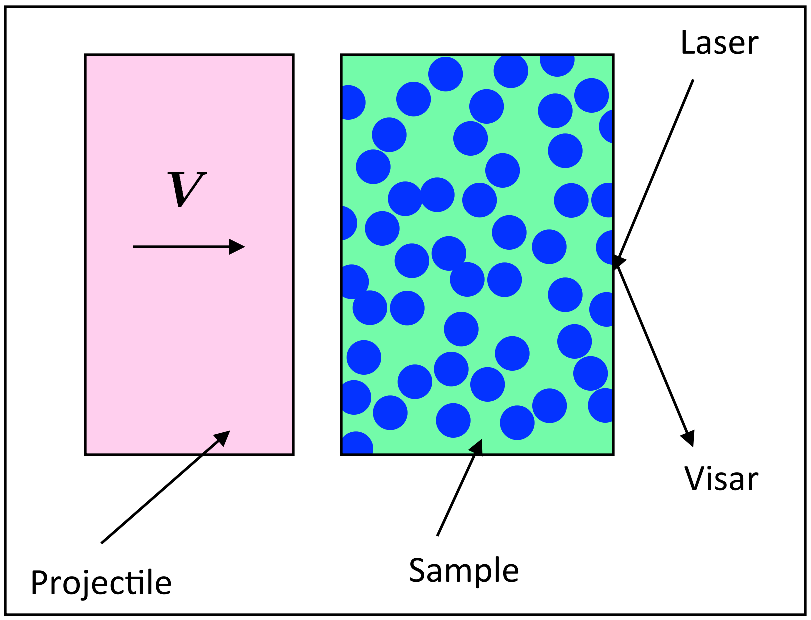


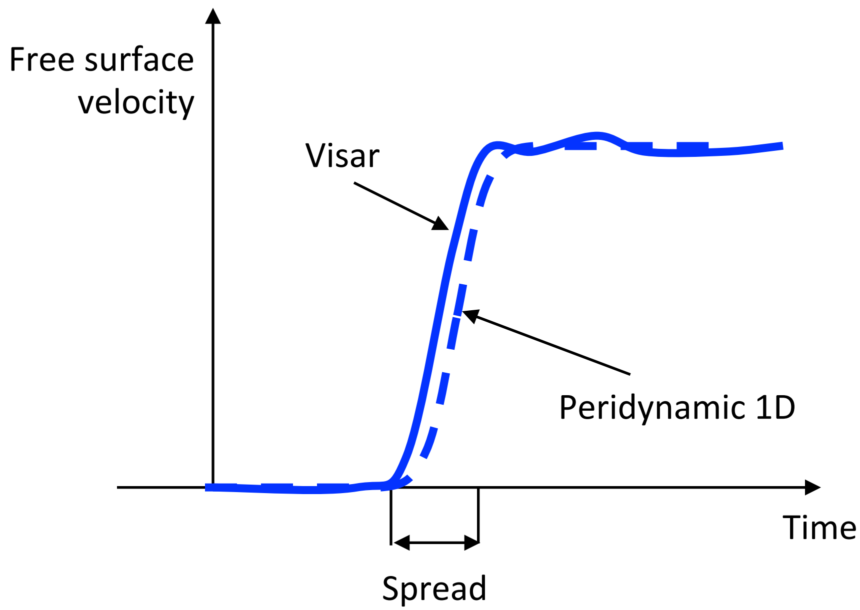
[Courtesy S. Silling]

Physical Interpretation of Peridynamic Horizon

PROPOSED EXPERIMENTAL METHOD FOR MEASURING THE PERIDYNAMIC HORIZON

- Measure how much a step wave spreads as it goes through a heterogeneous sample
- Fit the horizon in a peridynamic model to match observed spread





Local model would predict zero spread

[Courtesy S. Silling]

Peridynamics and Higher-Order Gradient Methods

- Local models contain no length scale

$$\ddot{u}(x) = au''(x)$$

- Higher-order gradients introduce length scale in a weak sense

$$\ddot{u}(x) = au''(x) + bu''''(x)$$

➡ Dimensional analysis shows that sqrt(b/a) has units of length

- Peridynamics is a (strongly) nonlocal model

Peridynamic model (nonlocal)

$$\rho\ddot{u}(x,t) = \int_{-\delta}^{\delta} \frac{c}{|\epsilon|}\left[u(x+\epsilon,t) - u(x,t)\right] d\epsilon$$

Taylor Series ↓

Higher-order gradient model (weakly nonlocal)

$$\rho\ddot{u}(x,t) = \mathrm{K}_a \left[\frac{\partial^2 u}{\partial x^2} + \frac{\delta^2}{24}\frac{\partial^4 u}{\partial x^4} + \frac{\delta^4}{1080}\frac{\partial^6 u}{\partial x^6} + \dots\right]$$

$\lim\ \delta \to 0$ ←

Local model

$$\rho\ddot{u}(x,t) = \mathrm{K}_a \frac{\partial^2 u}{\partial x^2}$$

S.A. Silling and R.B. Lehoucq, Convergence of peridynamics to classical elasticity theory, *Journal of Elasticity*, 93(1), 2008.

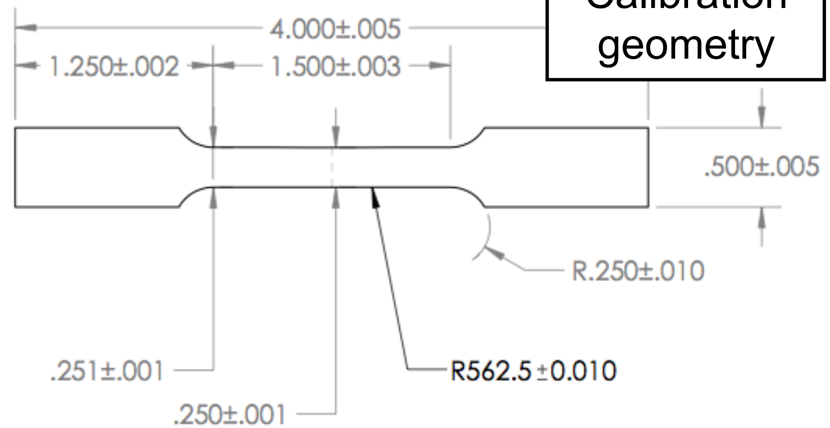
Pablo Seleson, Michael L. Parks, Max Gunzburger, and Richard B. Lehoucq. Peridynamics as an upscaling of molecular dynamics. *Multiscale Modeling and Simulation*, 8(1), 2009.

Necking Experiment

CAN A PERIDYNAMIC MODEL PREDICT LOCALIZATION?

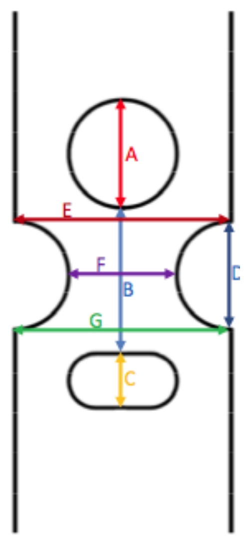
- Test setup:
  - 304L stainless steel (very ductile)
  - Quasi-static loading conditions
  - Standard tensile test results provided for calibration

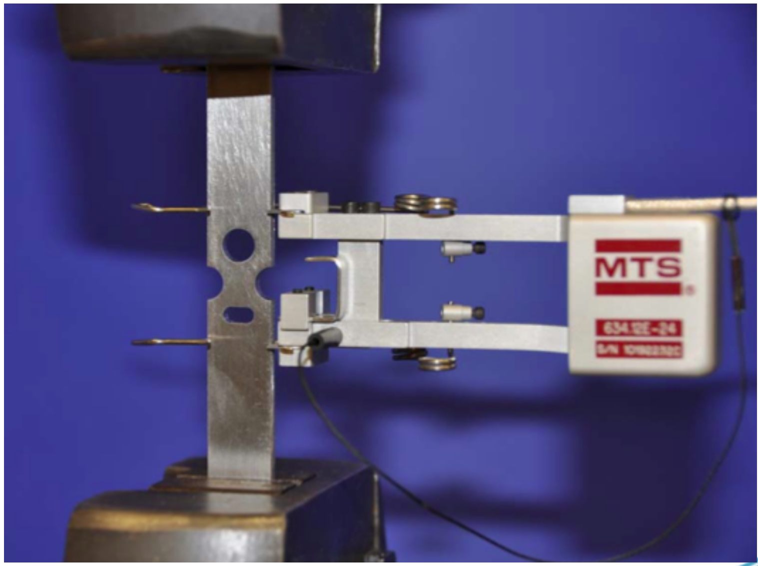
Calibration geometry



- Challenge:
  - Predict force and engineering strain at peak load
  - Predict engineering strain when force has dropped to 95% of peak load
  - Predict chord lengths when force has dropped to 95% of peak load

Test geometry

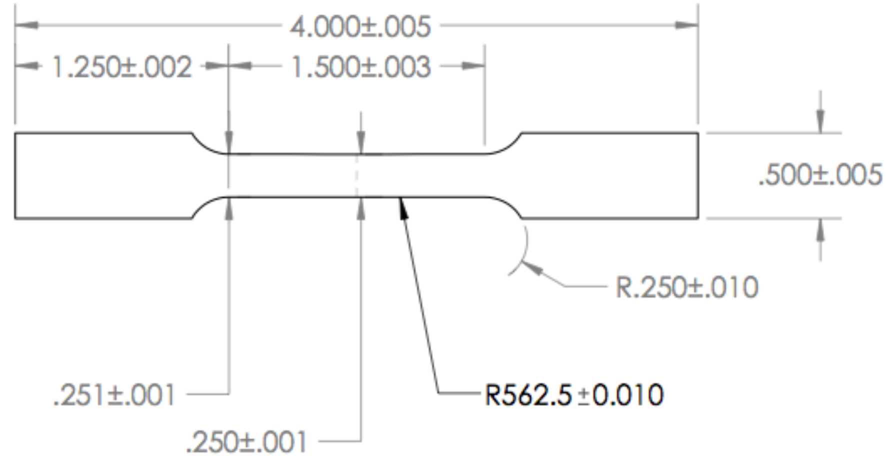


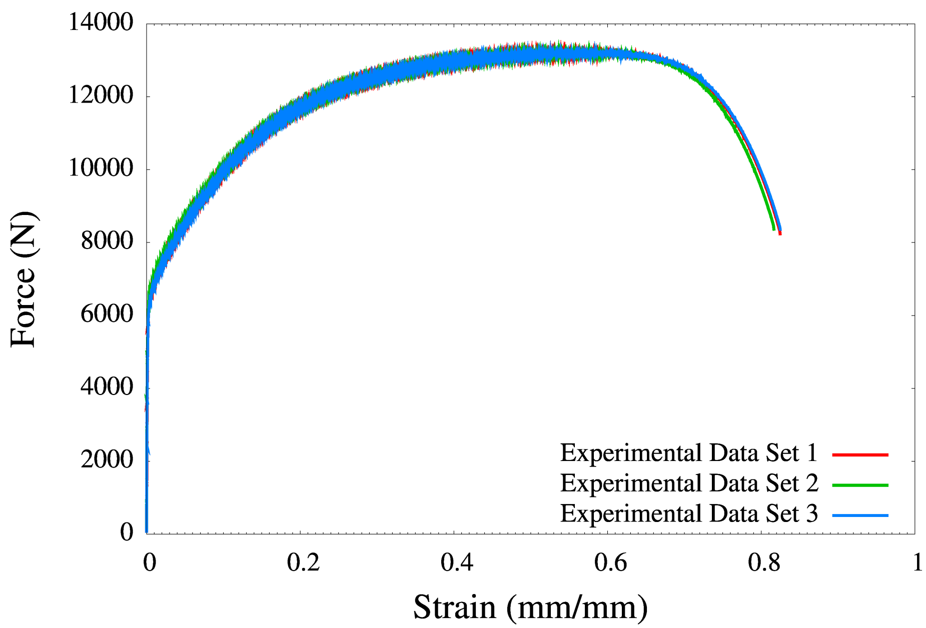


Necking Experiment: Calibration of Peridynamic Model

TENSILE TEST CALIBRATION DATA

- Force versus engineering strain
- Cross-sectional area at the point where the force dropped to 75% of peak load





<u>Cross-sectional Area</u>

Initial value: 0.0310 in^2

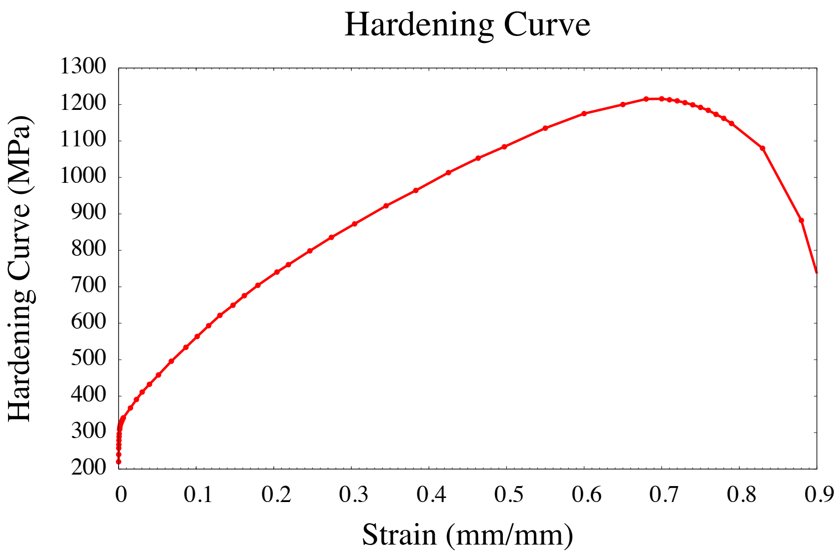
At 75% peak load: 0.0107 in^2

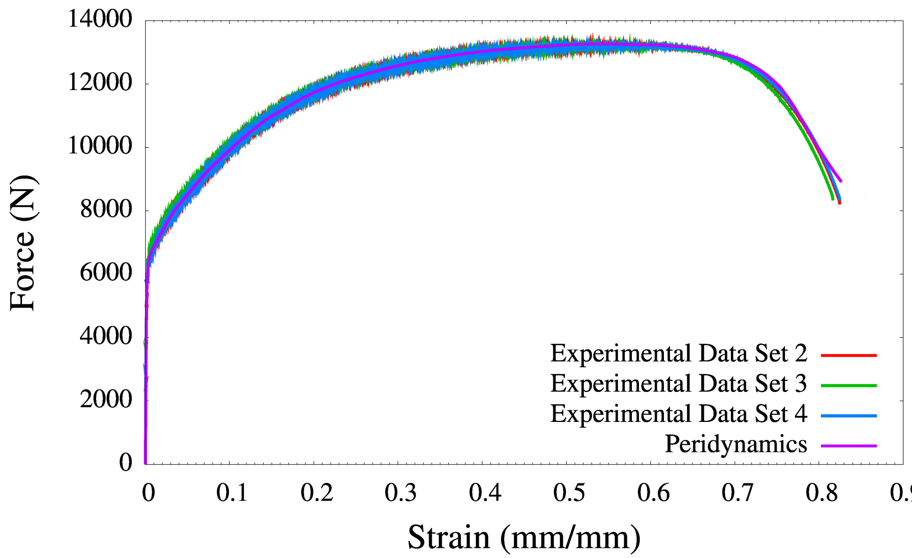
Necking Experiment: Calibration of Peridynamic Model

ELASTIC-PLASTIC MODEL WITH PIECEWISE LINEAR HARDENING CURVE

- Quasi-static simulations carried out with *Sierra/SolidMechanics*
- Initial calibration taken from classical finite-element model of tensile test (automated calibration tool)
- Hardening curve manually adjusted past ultimate tensile strength

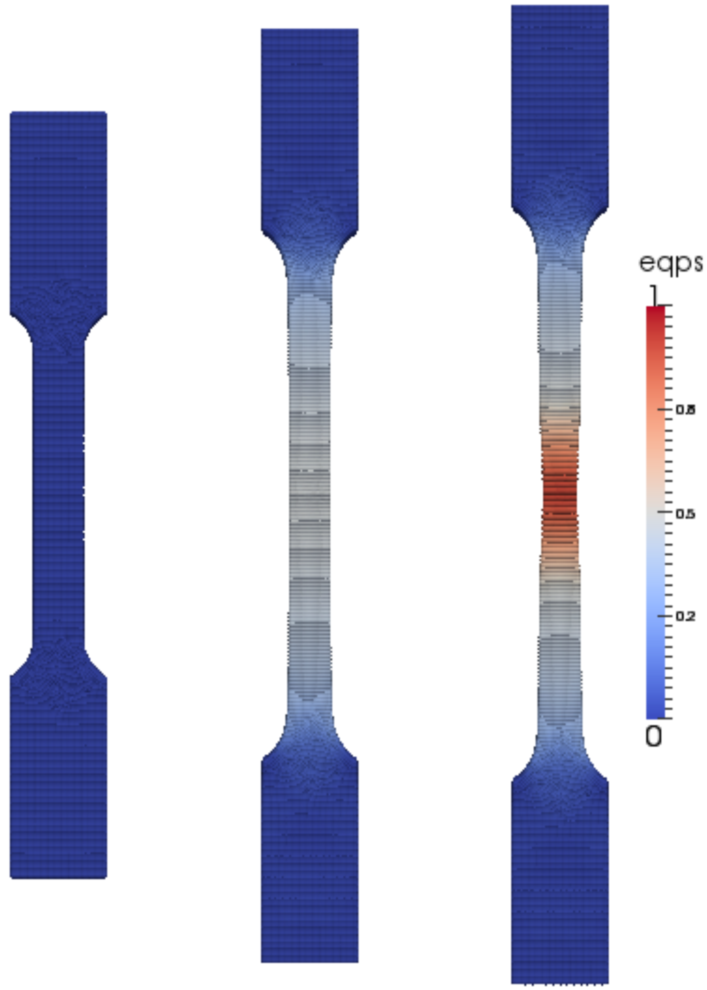
Young's Modulus	199.95e3 MPa
Poisson's Ratio	0.285
Yield Stress	220.0 MPa





Necking Experiment: Calibration of Peridynamic Model

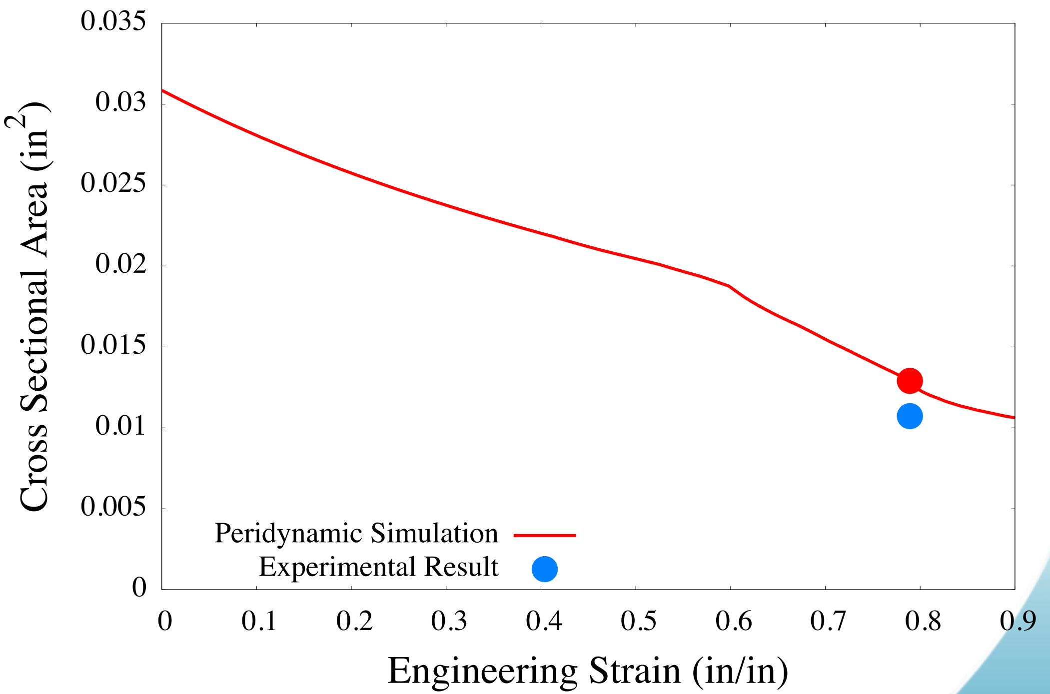
LOCALIZATION IN TENSILE TEST



Cross-sectional Area

Initial value: 0.031 in^2

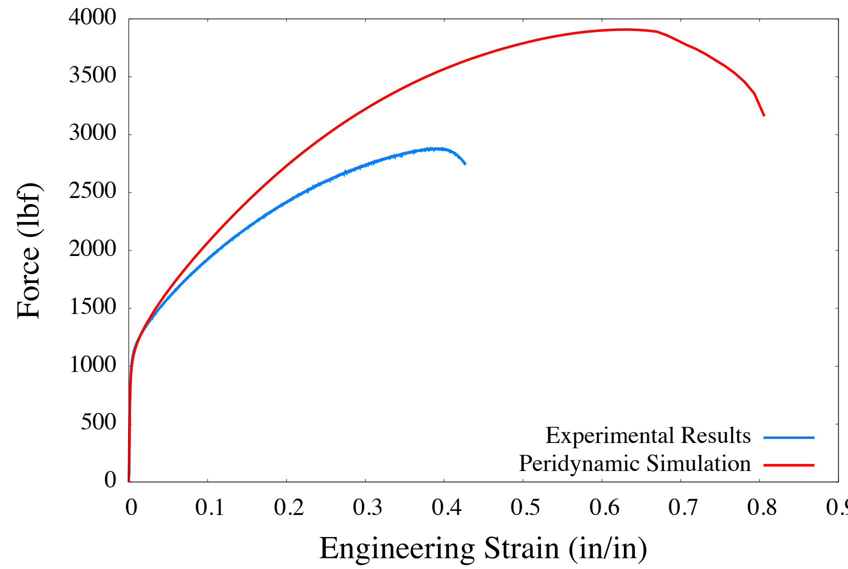
Simulation at 75% peak load: 0.0129 in^2

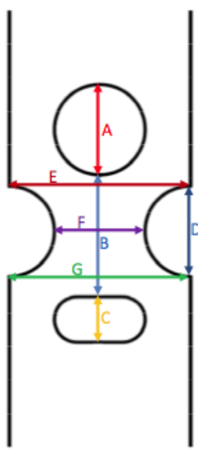


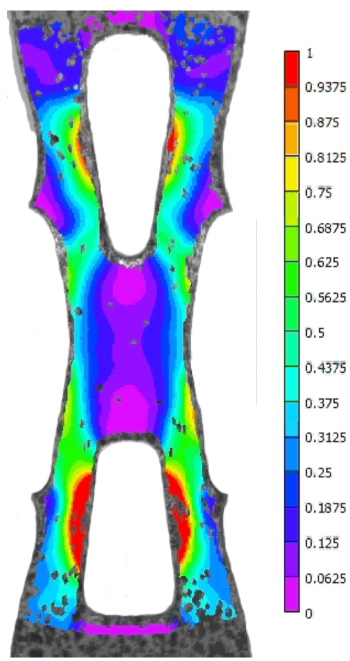
Necking Experiment: Test Geometry

DIRECT TRANSFER OF CALIBRATION PARAMETERS

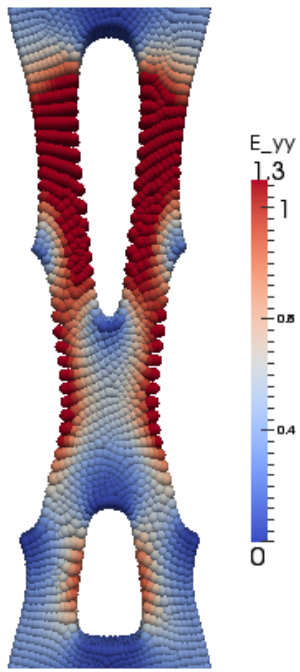
- Peridynamic horizon and mesh refinement were sufficient for calibration geometry but insufficient for test geometry
- Failed to predict response of test geometry



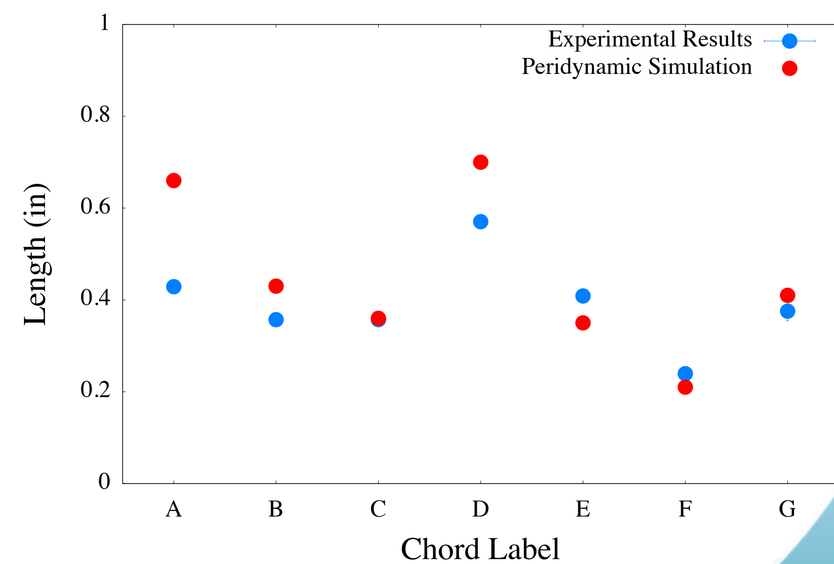




Experimental DIC image [Boyce]



Simulation result



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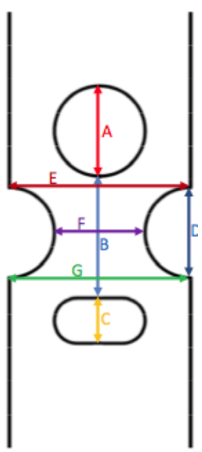
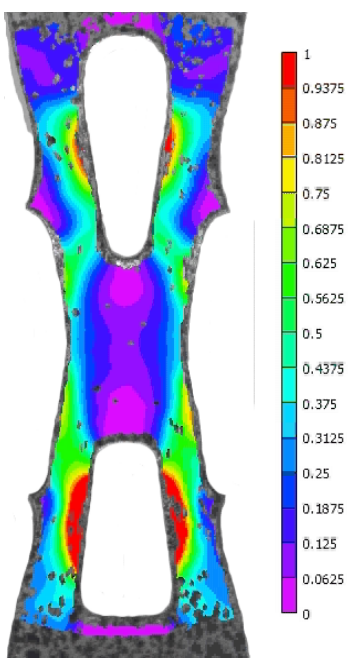
Necking Experiment: Test Geometry

REDUCTION OF PERIDYNAMIC HORIZON

- Peridynamic horizon reduced from 1.055 mm to 0.353 mm
- Mesh density increased from 189K elements to 1,507K elements
- Dramatically improved agreement between peridynamic model and experimental data





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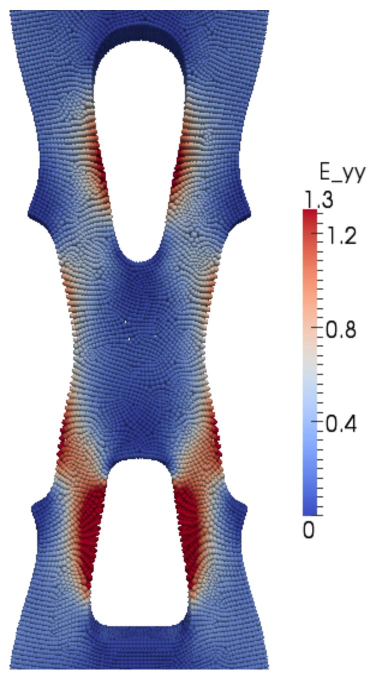
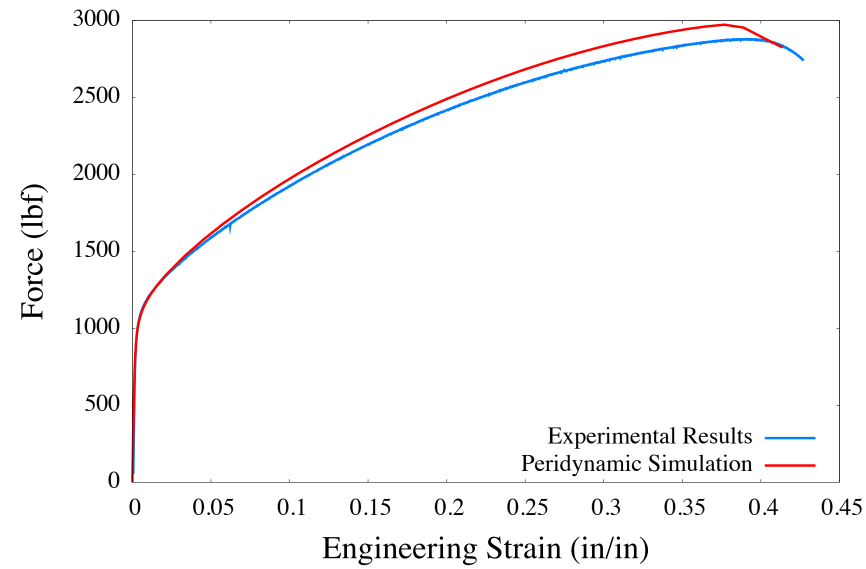
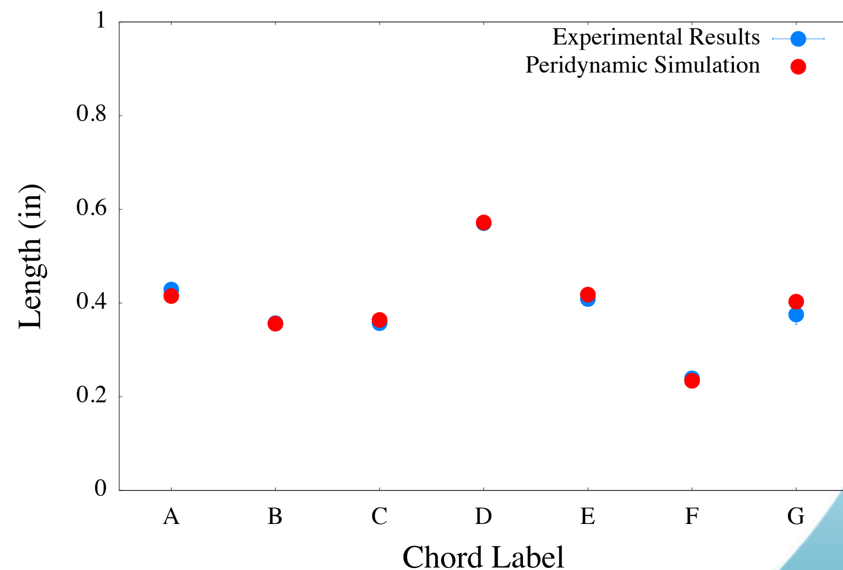


Simulation result





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Questions?

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RESOURCES

Advanced Simulation and Computing (ASC)

http://www.sandia.gov/asc/

Peridigm: A publicly-available peridynamics code

https://software.sandia.gov/trac/peridigm/