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# A Nonlocal Approach to Modeling Crack Nucleation in AA 7075-T651

ASME 2011 International Mechanical Engineering Congress and Exposition

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# Fatigue Failure of AA 7075-T651 in EA-6B Aircraft

**Goal:** Model the incubation, nucleation, and propagation stages of microstructurally small fatigue cracks in AA 7075-T651

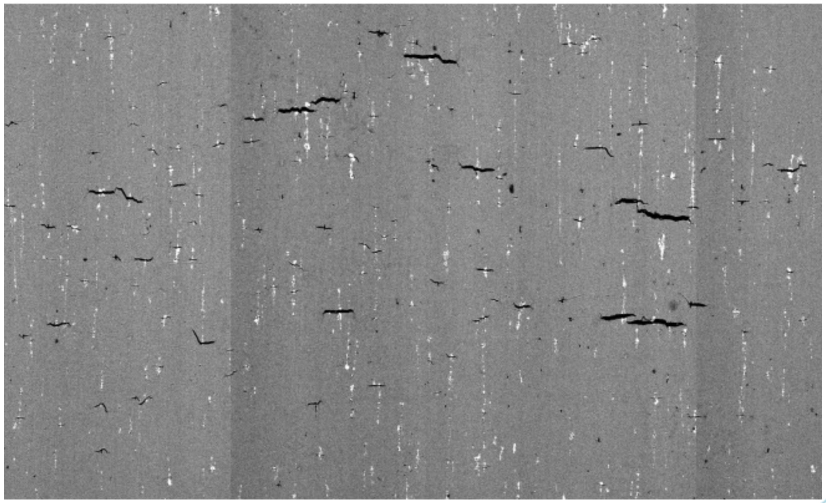
**Approach:** Focus on microstructure

**Prior work:** Structural Integrity Prognosis System (SIPS) Project

- Fatigue cracks observed to initiate primarily at cracked $Al_7Cu_2Fe$ particle inclusions
- The length of fatigue cracks is not observed to be a function of particle size

Fatigue damage in EA-6B wing panel

EA-6B



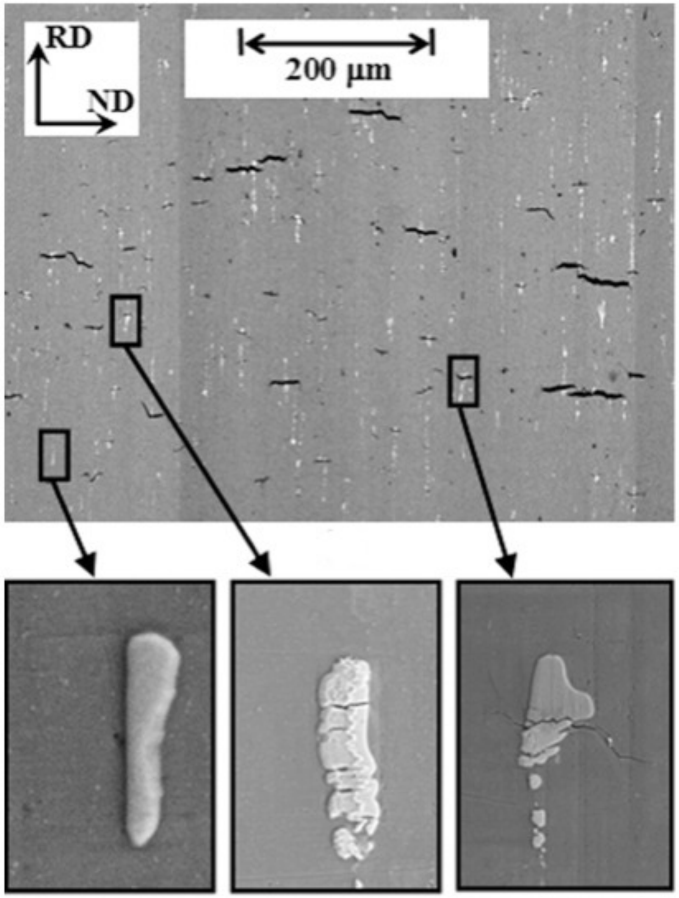
AA7075-T651 micrograph
[Anagnostou and Papazian]

# Why do some inclusions spawn matrix cracks, while others do not?

*IDENTIFY CONTRIBUTING GRAIN-SCALE MECHANISMS*

- Geometric factors
  - Particle shape
  - Lattice orientation of surrounding grain(s)
- Damage accumulation
  - Accumulation of dislocations facilitate failure mechanisms
- Loading
  - Combination of stress and dislocation buildup leads to crack nucleation into matrix material

Apply crystal plasticity material model with damage metrics to polycrystal RVE




Particle inclusions in AA 7075-T651 [Bozek, et al.]

J.E. Bozek, J.D. Hochhalter, M.G. Veilleux, M. Liu, G. Heber, S.D. Sintay, A.D. Rollett, D.J. Littlewood, A.M. Maniatty, H. Weiland, R.J. Christ Jr., J. Payne, G. Welsh, D.G. Harlow, P.A. Wawrzynek, and A.R. Ingraffea. A geometric approach to modeling microstructurally small fatigue crak formation: I. Probabilistic simulation of constituent particle cracking in AA 7075-T651. *Modelling and Simulation in materials Science and Engineering* 16 (2008).

# Crystal Plasticity Material Model

$$\mathbf{F} = \mathbf{F}^e\,\mathbf{F}^p$$

Elastic behavior governed by hyperelastic potential

$$\hat{\mathrm{W}} = \hat{\mathrm{W}}\left(\mathbf{F}^e\right) = \frac{1}{2}\mathbf{E}^e : \mathcal{L} : \mathbf{E}^e \qquad \hat{\mathbf{E}}^e = \frac{1}{2}\left(\mathbf{F}^{e^{\mathrm{T}}}\,\mathbf{F}^e - \mathbf{I}\right)$$

$$\hat{\mathbf{S}} = 2\frac{\partial \hat{W}}{\partial \mathbf{C}^e} = \mathcal{L} : \hat{\mathbf{E}}^e \qquad \sigma = \mathbf{F}^e\left(\frac{1}{\det\left(\mathbf{F}^e\right)}\mathbf{S}\right)\mathbf{F}^{e^{\mathrm{T}}}$$

Plastic response determined by crystallographic slip

$$\hat{\mathbf{L}}^p = \sum_{\alpha=1}^{12} \dot{\gamma}^\alpha\,\mathbf{P}^\alpha \qquad \dot{\gamma}^\alpha = \dot{\gamma}_o \frac{\tau^\alpha}{g^\alpha}\left|\frac{\tau^\alpha}{g^\alpha}\right|^{\frac{1}{m}-1}$$

$$\dot{g}^\alpha = G_o\left(\frac{g_s - g^\alpha}{g_s - g_o}\right)\sum_{\beta=1}^{12} 2\left|\mathbf{P}^\alpha_{\mathrm{sym}} : \mathbf{P}^\beta_{\mathrm{sym}}\right|\left|\dot{\gamma}^\beta\right|$$

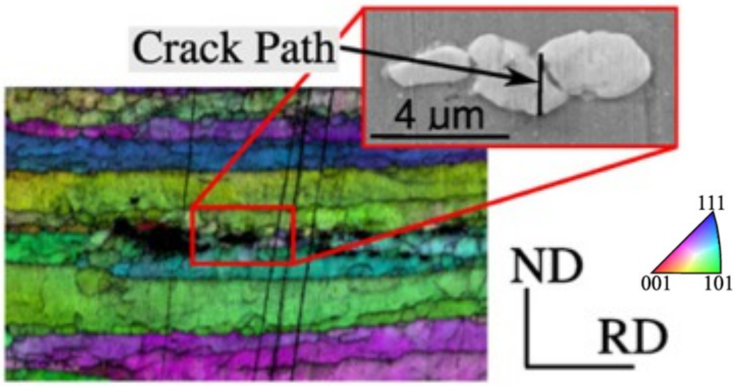
Damage metric is a function of stress and plastic slip

$$D_{\text{Fatemi Socie}} = \max_p \int_0^t \sum_{\alpha=0}^{3}\left|\dot{\gamma}^\alpha_p\right|\left(1 + k\frac{\langle \sigma_{np}\rangle}{g_o}\right)dt$$

Matous, K., and Maniatty, A. Finite element formulation for modelling large deformations in elasto-viscoplastic polycrystals. *International Journal for Numerical Methods in Engineering*, 60:2313-2333, 2004.

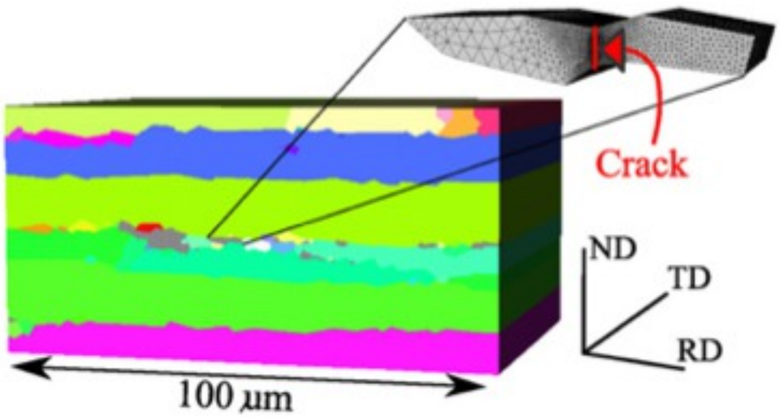
Fatemi, A., and Socie, D.F. A critical plane approach to multiaxial fatigue damage including out-of-phase loading. *Fatigue and Fracture of Engineering Materials and Structures*. 11:149-165, 1988.

# Construction of Finite Element Model from Experimental Data

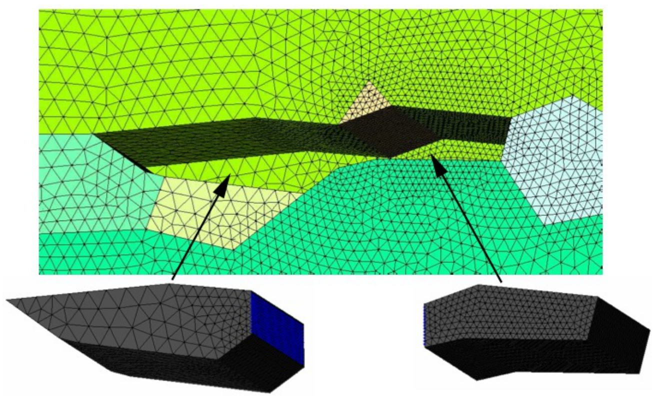



Experimental data

- Experimental data [Northrop-Grumman]
  - Grain boundaries
  - Lattice orientations
  - Particle geometry
- Computational Model
  - Explicit modeling of cracked particle inclusion
  - Extrusion in third dimension




Computational model



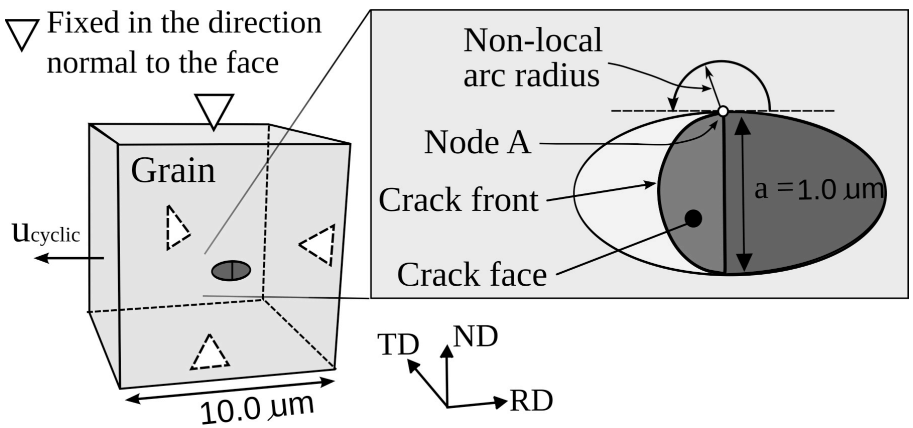
Mesh in vicinity of inclusion

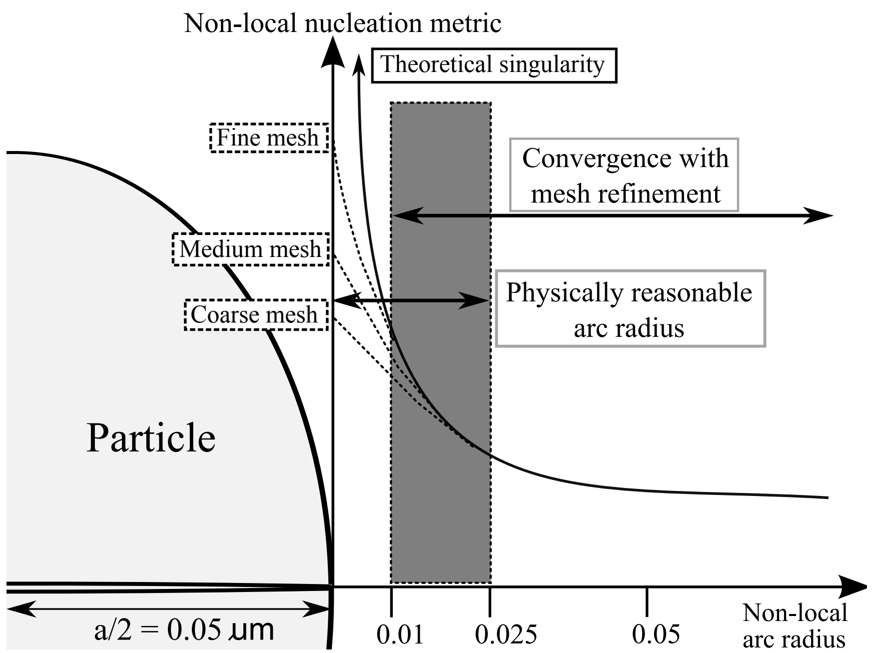

J.D. Hochhalter, D.J. Littlewood, R.J. Christ Jr., M.G. Veilleux, J. E. Bozek, A.R. Ingraffea, and A.M. Maniatty. A geometric approach to modeling microstructurally small fatigue crak formation: II. Physically based modeling of microstructure-dependent slip localization and actuation of the crack nucleation mechanism in AA 7075-T651. *Modelling and Simulation in materials Science and Engineering* 18 (2010).

# Nonlocal sampling approach in the vicinity of crack tip

Governing equations not well defined at crack tip,
Ad-hoc nonlocal approach applied to track damage

- Singularity at crack tip preclude mesh convergence
- Mitigate mesh dependence by sampling along nonlocal arc centered at crack tip

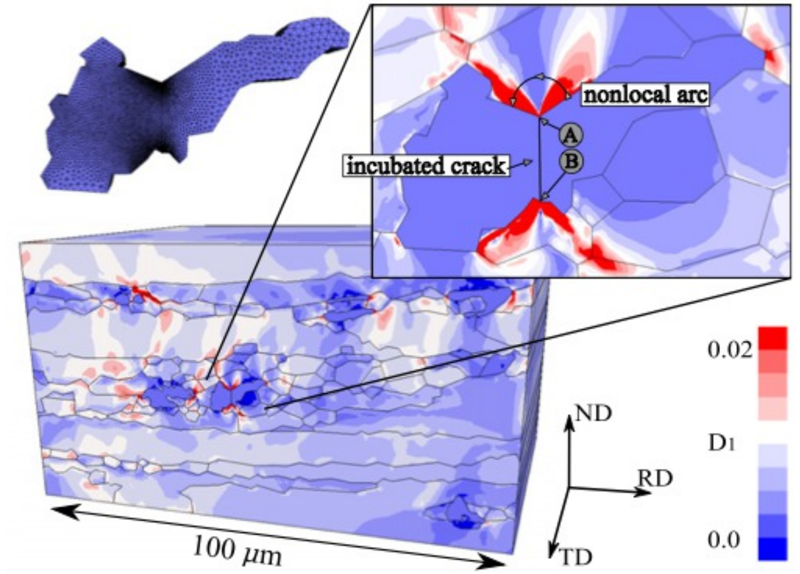



J.D. Hochhalter, D.J. Littlewood, R.J. Christ Jr., M.G. Veilleux, J. E. Bozek, A.R. Ingraffea, and A.M. Maniatty. A geometric approach to modeling microstructurally small fatigue crack formation: II. Physically based modeling of microstructure-dependent slip localization and actuation of the crack nucleation mechanism in AA 7075-T651. *Modelling and Simulation in materials Science and Engineering* 18 (2010).

# Results and Conclusions from SIPS Modeling

- Fatigue cracks nucleate when stress exceeds critical value
- Critical stress value is reduced with accumulated plastic slip
  - Accumulation of dislocations facilitate failure mechanisms




Damage metric contours in vicinity of cracked particle inclusion

Can we improve on nonlocal sampling approach?
YES, with peridynamics


J.D. Hochhalter, D.J. Littlewood, M.G. Veilleux, J. E. Bozek, A.M. Maniatty, A.D. Rollett, and A.R. Ingraffea. A geometric approach to modeling microstructurally small fatigue crack formation: III. Development of a semi-empirical model for nucleation. *Modelling and Simulation in materials Science and Engineering* 19 (2011).




Sandia National Laboratories

# Peridynamics

### *WHAT IS PERIDYNAMICS?*

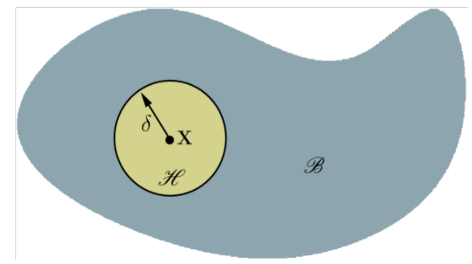
Peridynamics is a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles.

### *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*:

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

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*

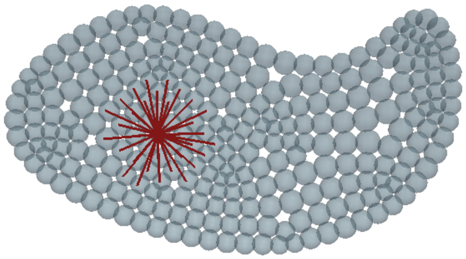
- Peridynamic *bonds* connect any two material points that interact directly.
- Peridynamic forces are determined by *force states* acting on bonds.

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

- Force states are determined by constitutive laws and are functions of the deformations of all points within a neighborhood.
- *Damage* 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.



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

# 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

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

Hourglass vector projected onto bond

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

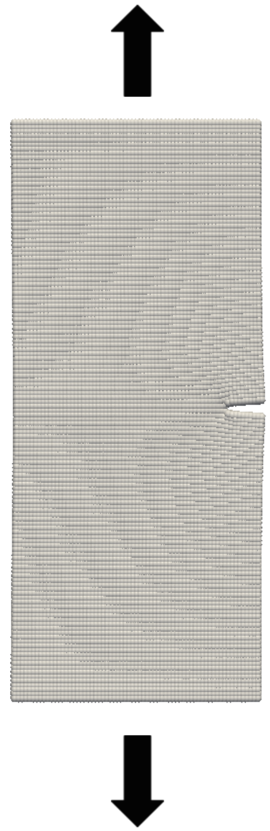
Hourglass force

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

# Verification:  Mesh Independent Plastic Zone

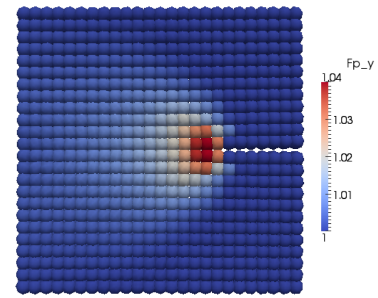
*NONLOCALITY YIELDS MESH CONVERGENCE AT CRACK TIP*

- 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

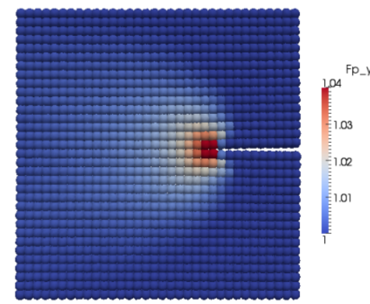


Pre-cracked specimen loaded in tension

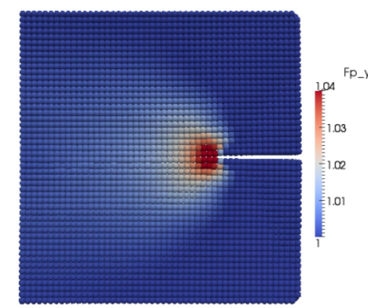
Coarse mesh




Medium mesh




Fine mesh




Component of plastic deformation gradient in loading direction

# Capability Demonstration: Baseline Model

*SIMULATION OF AN ELASTIC PARTICLE INCLUSION IN A SINGLE GRAIN*

- Single hard elastic inclusion embedded in single grain
- Tensile loading to 1% strain
- Compared simulations with two different grain orientations
- Compared simulations with two different particles: uncracked and cracked.

Crystal plasticity parameters

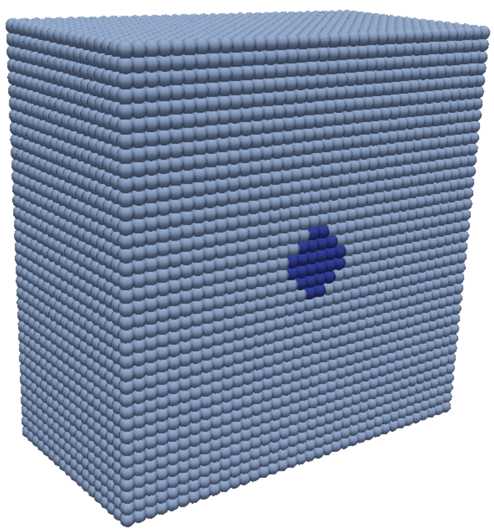
| Parameter | Value |
|---|---|
| $\rho$ | 2810.0 kg/m$^3$ |
| $\lambda$ | 60.9 GPa |
| $\mu$ | 28.3 GPa |
| $\eta$ | 5.1 GPa |
| $m$ | 0.005 |
| $g_o$ | 220.0 MPa |
| $\dot{\gamma}_o$ | 1.0 s$^{-1}$ |
| $G_0$ | 120.0 MPa |
| $g_{s_o}$ | 250.0 MPa |
| $\dot{\gamma}_s$ | 5.0e10 s$^{-1}$ |
| $\omega$ | 0.0 |

Elastic parameters

| Parameter | Value |
|---|---|
| $\rho$ | 2810.0 kg/m$^3$ |
| $\lambda$ | 66.99 GPa |
| $\mu$ | 31.13 GPa |
| $\eta$ | 0.0 GPa |

Lattice orientations

| | Euler Angles ($\phi_1$, $\Phi$, $\phi_2$) |
|---|---|
| Orientation A | (0.9738, 0.4322, -1.3822) |
| Orientation B | (1.9490, 0.8644, -2.120) |

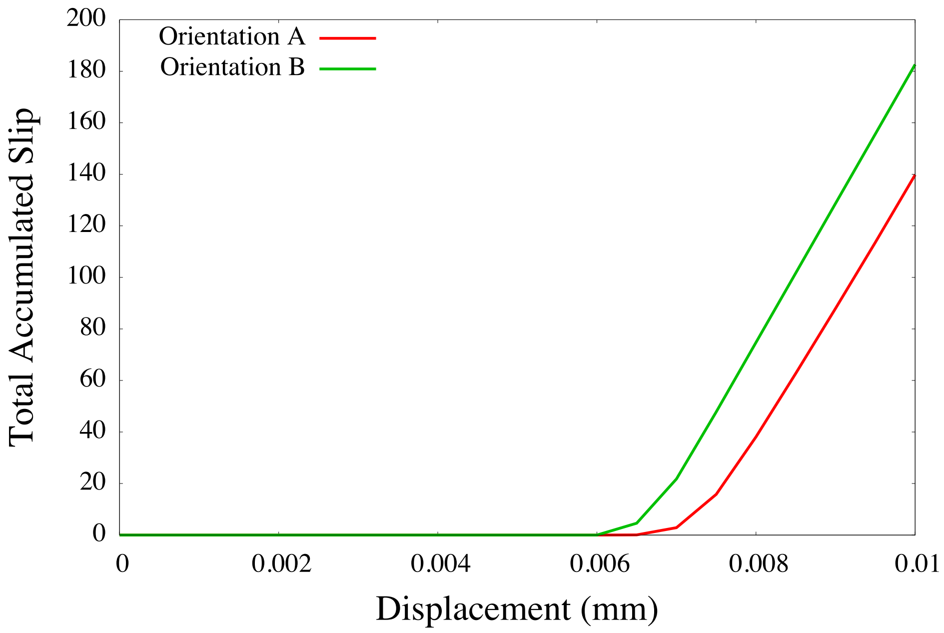


Model discretization

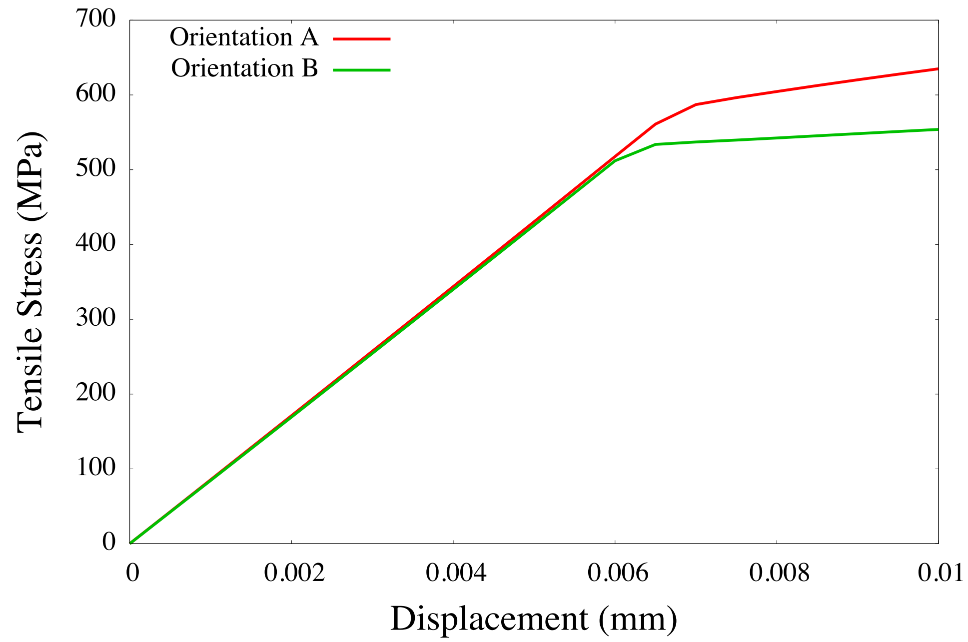
# Effects of Lattice Orientation: Plastic Slip and Stress

*MATERIAL RESPONSE IS A FUNCTION OF LATTICE ORIENTATION*

Total accumulated slip in crystal

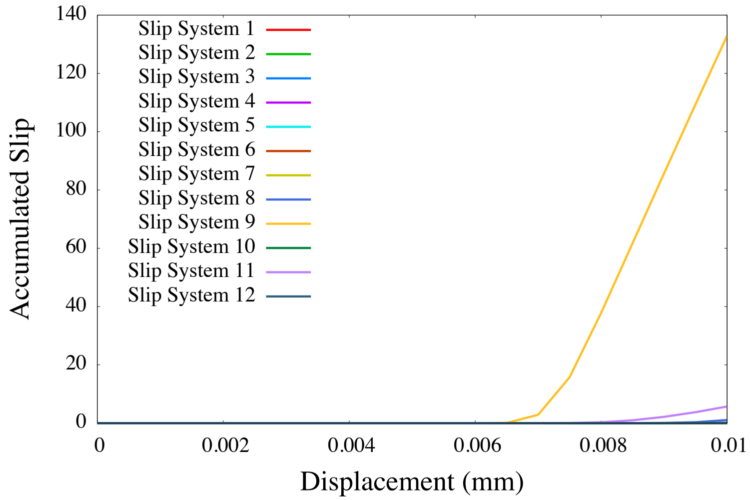



Tensile stress in particle inclusion

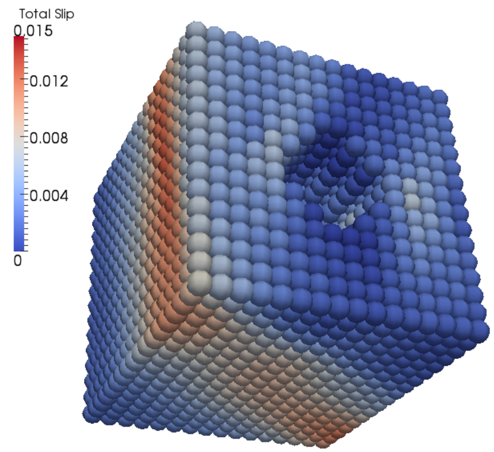


# Uncracked Particle: Plastic Slip and Stress

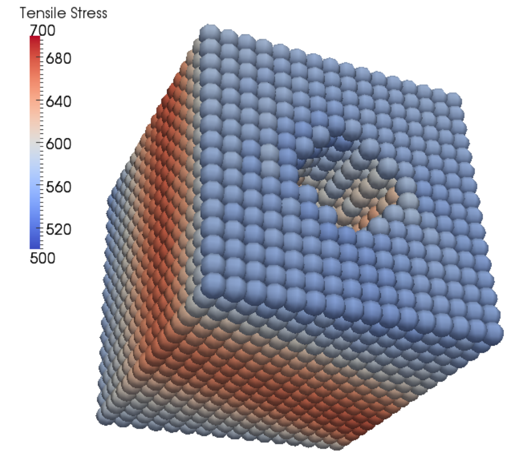
## Orientation A




Slip on individual slip systems

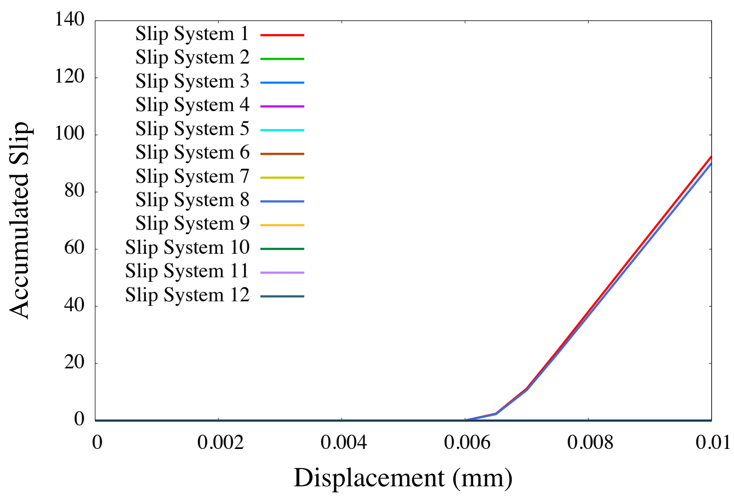



Total slip

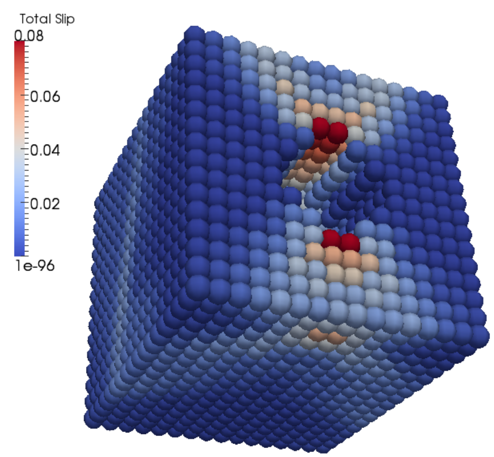



Tensile stress

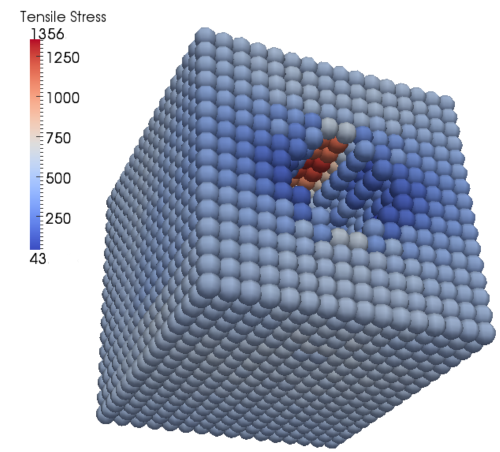
## Orientation B




Slip on individual slip systems



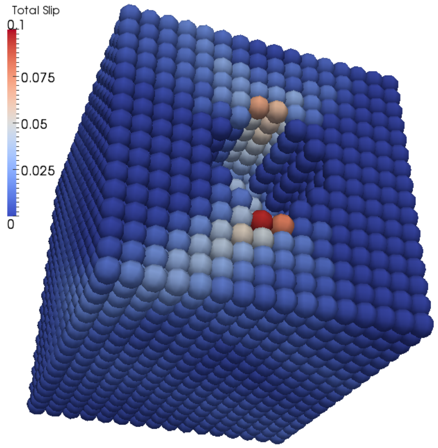

Total slip



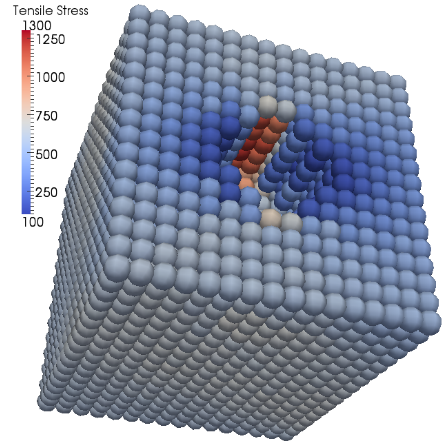

Tensile stress

# Cracked Particle: Plastic Slip, Stress, and Damage

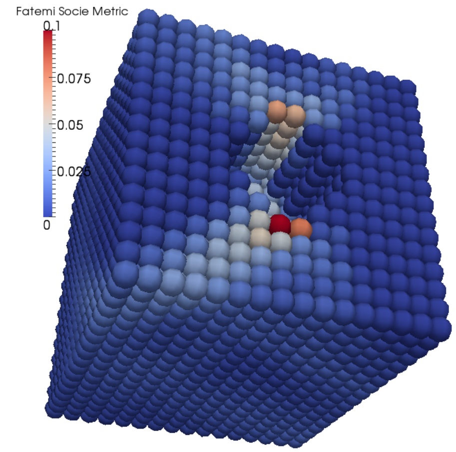
## Orientation A




Total slip

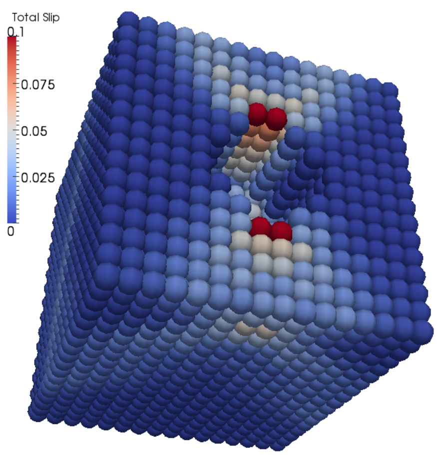



Tensile stress

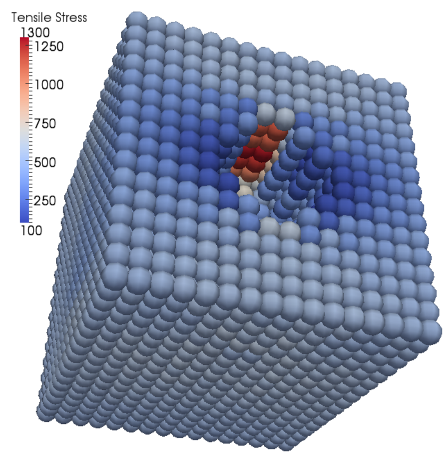



Fatemi-Socie damage metric

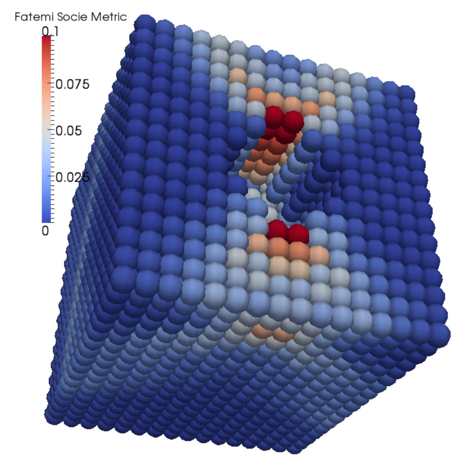
## Orientation B




Total slip




Tensile stress




Fatemi-Socie damage metric

# Summary

*WHAT HAS BEEN DONE?*

- Proposed peridynamics as a means to overcome limitations in classical continuum mechanics that restrict our ability to model crack nucleation in Al 7075-T651.
  - Peridynamics remains valid in the direct vicinity of a crack tip.
  - Peridynamics offers a natural means for crack nucleation and propagation.
- Proof-of-concept demonstration of crystal plasticity within peridynamic framework.

*WHAT IS THERE LEFT TO DO?*

- Extend peridynamic crystal plasticity to polycrystalline RVE models.
- Adaptation / calibration of damage models for use in nonlocal framework.
- Link damage models to peridynamic bond-breaking law.
- Validate nonlocal crystal plasticity against experimental observations.

David J. Littlewood. A nonlocal approach to modeling crack nucleation in AA 7075-T651. Proceedings of the ASME 2011 International Mechanical Engineering Congress and Exposition. Denver, Colorado, 2011.

# Extra Slides

# Peridynamics

*WHAT IS THE IMPACT?*

- Nonlocality
- Larger solution space (admits fracture)
- Length scales (multiscale material model)

*HOW DOES IT RELATE TO THE CLASSICAL THEORY?*

- Assuming u smooth, can re-write in terms of nonlocal stress tensor

$$\rho \ddot{u}(x,t) = \int_H \left( T[x,t]\langle x' - x \rangle - T[x',t]\langle x - x' \rangle \right) dV_{x'} + b(x,t)$$

$$= \nabla \cdot \nu(x,t) + b(x,t)$$

*Peridynamic stress tensor*

- If displacement smooth, convergence to classical elasticity in limit as $\delta \to 0$

$$\rho \ddot{u}(x,t) = \lim_{\delta \to 0} \int_H \left( T[x,t]\langle x' - x \rangle - T[x',t]\langle x - x' \rangle \right) dV_{x'} + b(x,t)$$

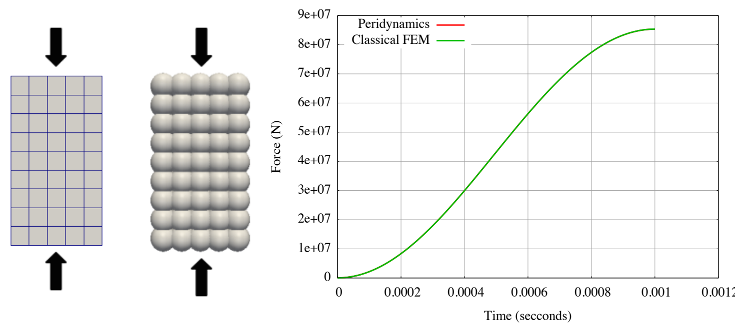
$$= \nabla \cdot P(x,t) + b(x,t)$$

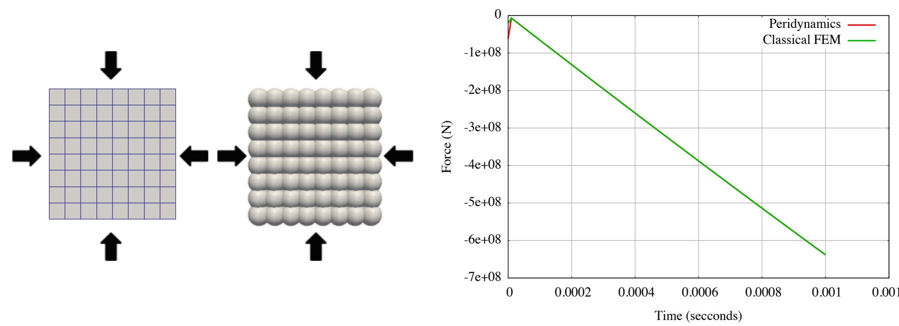
*Piola-Kirchhoff stress tensor*

# Verification: Patch tests

## Uniaxial and hydrostatic compression

- Tests constructed such that peridynamics and classical FEM should yield same result
- Simulation results verified for numerous material models

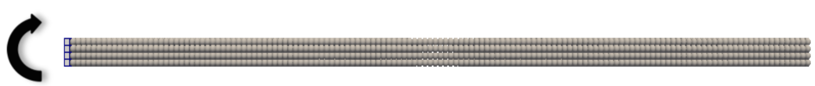


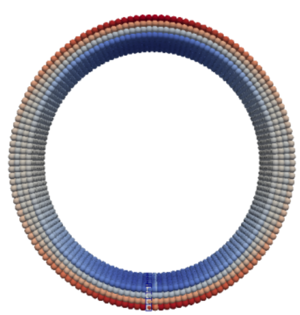

## Beam bending

- Test peridynamics with neo-Hookean material model against classical beam bending theory
- Simulation gives expected bending response and stress distribution

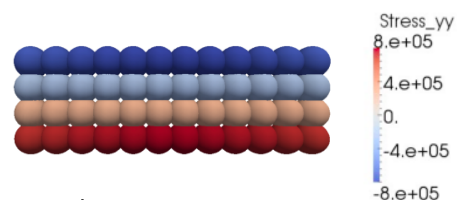
Applied rotation



Fixed support



Increased pure bending eventually produces circle




Linear stress distribution through cross section