SAND2014-19657C

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Sandia National Laboratories

Local-Nonlocal Coupling for Modeling Fracture

ASME 2014 International Mechanical Engineering Congress & Exposition

17 November 2014

David Littlewood
Stewart Silling
Pablo Seleson

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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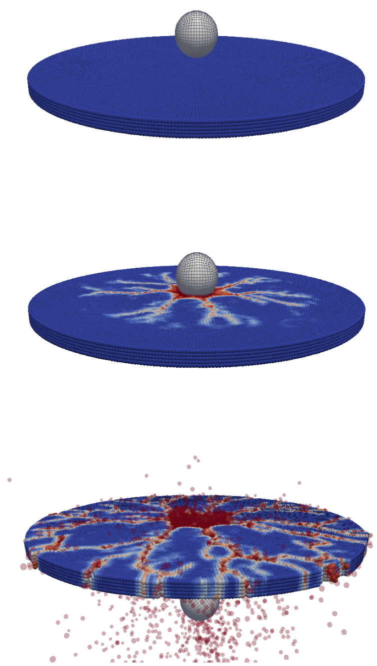
Local-Nonlocal Coupling for Integrated Fracture Modeling

PERIDYNAMICS OFFERS PROMISE FOR MODELING PERVASIVE MATERIAL FAILURE

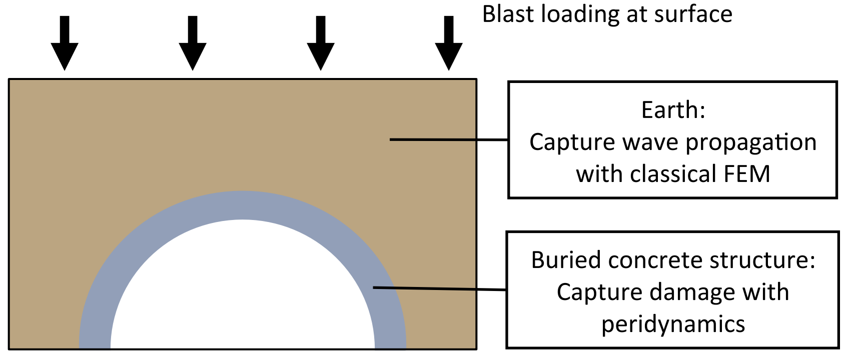
- Potential to enable rigorous simulation of failure and fracture
- Directly applicable to Sandia's national security missions



WE SEEK INTEGRATION WITH CLASSICAL FINITE-ELEMENT APPROCHES

- Integration with existing FEM codes provides a delivery mechanism to DOE and DoD analysts
- "Best of both worlds" through combined classical FEM and peridynamic simulations

Vision
Apply peridynamics in regions susceptible to material failure

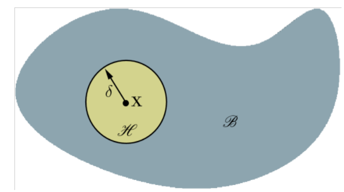


Peridynamic Theory of Solid Mechanics

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

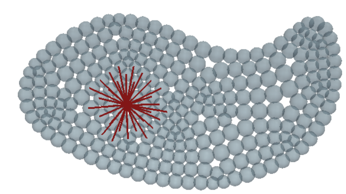
- Peridynamics is a nonlocal extension of continuum mechanics
- Remains valid in presence of discontinuities, including cracks
- Balance of linear momentum is based on an integral equation

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



- Peridynamic bonds connect any two material points that interact directly
- Peridynamic forces are determined by force states acting on bonds
- A peridynamic body may be discretized by a finite number of elements

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



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.

S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures*, 83:1526-1535, 2005.

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

Focus Areas under Local-Nonlocal Coupling Effort

- ★ Variable nonlocal length scale for peridynamic models
  - Novel *partial stress* formulation supports a variable peridynamic horizon
  - Reducing the peridynamic horizon in the vicinity of local-nonlocal interfaces improves mathematical consistency and provides a mechanism for integration with FEM

- Blending-based coupling approach
  - Derived specifically for the coupling of peridynamics and classical continuum mechanics
  - Coupling term specific to local-nonlocal interfaces mitigates ghost forces

- ★ Software framework for prototype implementation, verification, and testing
  - *Peridigm* and *Albany/LCM* codes directly coupled for combined peridynamic / classical finite element simulations

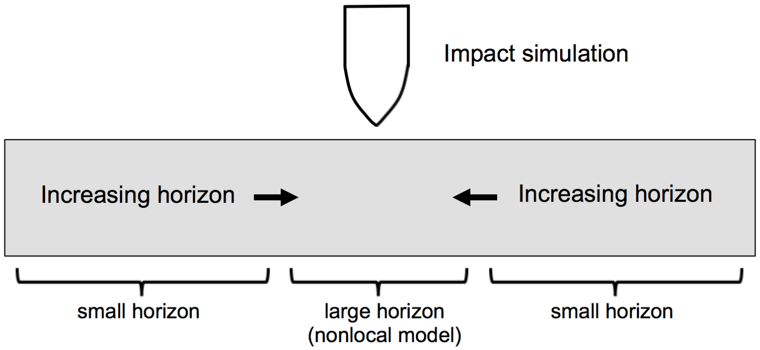
- Innovations for improved model agreement at local-nonlocal interfaces
  - Position-Aware Linear Solid (PALS) constitutive model
  - Improved quadrature for meshfree peridynamic discretizations

Variable Nonlocal Length Scale

Employ a variable peridynamic horizon to better facilitate local-nonlocal coupling in combined peridynamic / classical FEM simulations

MOTIVATION

- A variable horizon provides a smooth transition from a nonlocal model to a local model



CHALLENGE

- How can we vary the peridynamic horizon without introducing artifacts?

Variable Nonlocal Length Scale

DO CURRENT PERIDYNAMIC MODELS SUPPORT A VARIABLE LENGTH SCALE?

- No, standard peridynamic constitutive laws have very limited support for a variable length scale
  - A linearly varying horizon can be supported under certain conditions
  - Difficulties persist at transition from a constant horizon to a varying horizon

PATH FORWARD

- Develop an alternative formulation that mitigates spurious artifacts in the presence of a variable nonlocal length scale
- Target one-dimensional patch tests (expose spurious artifacts, if any)
  - Linear displacement field must be equilibrated
  - Quadratic displacement field must produce constant acceleration

Peridynamic Partial Stress Formulation

$$\nu_o(\mathbf{x}) := \int_{\mathcal{H}} \underline{\mathbf{T}}[\mathbf{x}]\langle\xi\rangle \otimes \xi \, dV_{\mathbf{x}'}$$

- Guaranteed to pass the linear patch test (even with a varying horizon)
- Partial stress and full peridynamic stress[2] are equal if the force state T[x] is independent of x
  - Example: homogeneous body under homogeneous deformation
  - Result suggests that partial stress is a good approximation of the full peridynamic stress under smooth deformation
- Partial stress formulation is not a good candidate for modeling material failure
- Provides a natural transition between the full peridynamic formulation and a classical stress-strain formulation (hybrid approach)

[1] Silling, S., and Seleson, P., Variable Length Scale in a Peridynamic Body, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, June 12, 2013.

[2] Lehoucq, R.B., and Silling, S.A. Force flux and the peridynamic stress tensor, Journal of the Mechanics and Physics of Solids, 56:1566-1577, 2008.

Application of Partial Stress within Peridynamics Framework

INTERNAL FORCE CALCULATION REQUIRES DIVERGENCE OPERATOR

- Internal force evaluated as divergence of partial stress

$$\mathbf{L}(\mathbf{x}) = \nabla \cdot \nu(\mathbf{x}) = \mathrm{Tr}(\nabla \nu(\mathbf{x}))$$

$$\nabla \nu(\mathbf{x}) = \int_{\mathcal{H}} \underline{\omega}\langle \xi \rangle \{\nu(\mathbf{x}') - \nu(\mathbf{x})\} \otimes \xi \, dV_{\mathbf{x}'} \; \mathbf{K}^{-1}$$

- The partial stress can be applied within the meshless approach of Silling and Askari [1]

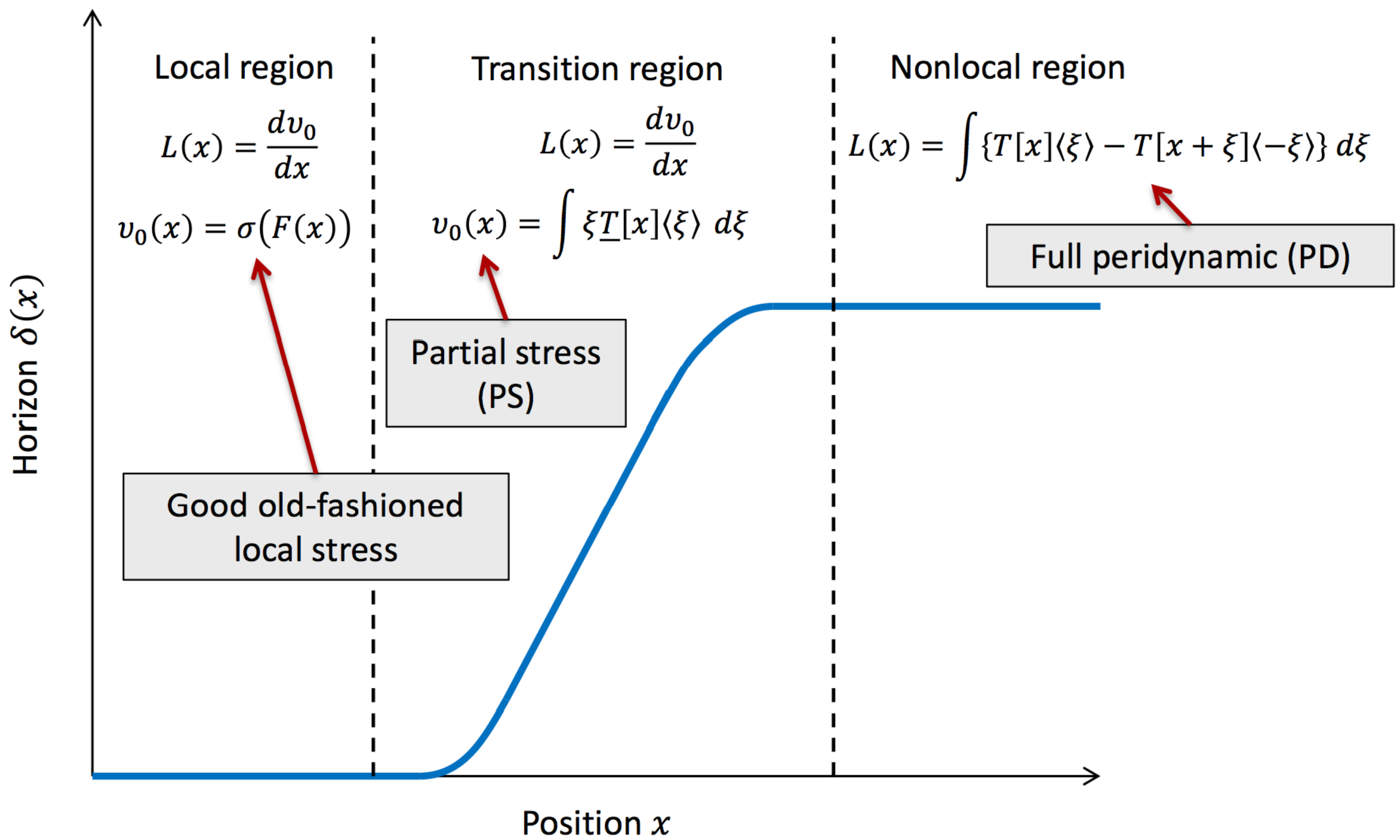
$$\nabla \cdot \nu(\mathbf{x}) = \mathrm{Tr}\left(\left(\sum_{n=1}^{N} \underline{\omega}\langle \xi^n \rangle \{\nu(\mathbf{x}^n) - \nu(\mathbf{x})\} \otimes \xi^n \, \Delta V^n \right) \mathbf{K}^{-1} \right)$$

★ The partial stress can also be applied within a standard finite-element scheme

[1] S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures*, 83:1526-1535, 2005.

Utilize the Partial Stress Formulation in a Transition Region

ALTER THE PERIDYNAMIC HORIZON WITHIN A BODY TO APPLY NONLOCALITY ONLY WHERE NEEDED



[Courtesy Stewart Silling]

Patch Tests for Partial Stress Formulation

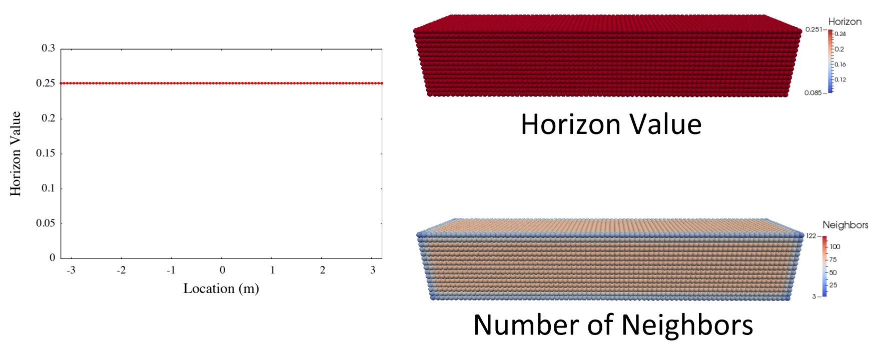
SUBJECT RECTANGULAR BAR TO PRESCRIBED DISPLACEMENT FIELDS

- Examine response under linear and quadratic displacement fields
- Investigate standard formulation with both constant and varying peridynamic horizon
- Investigate partial stress formulation with both constant and varying peridynamic horizon

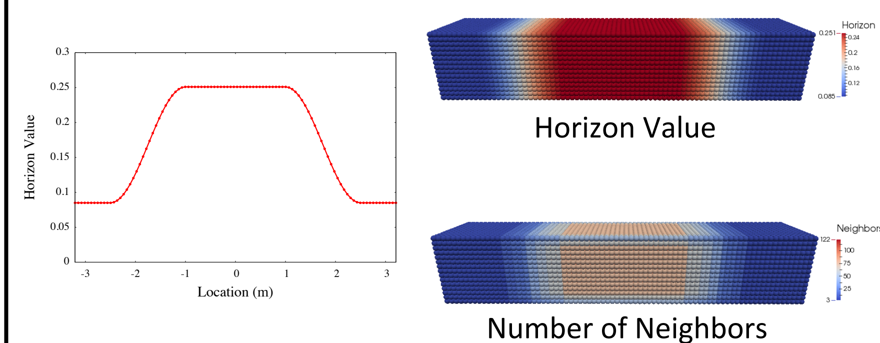
Elastic Correspondence Material Model

Density	7.8 g/cm^3
Young's Modulus	200.0 GPa
Poisson's Ratio	0.0
Stability Coefficient	0.0

Constant Horizon



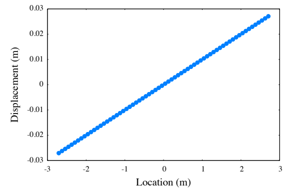
Varying Horizon



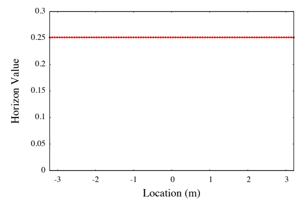
Patch Test: Prescribed Linear Displacement

Test set-up

Prescribe linear displacement field



Constant horizon throughout bar

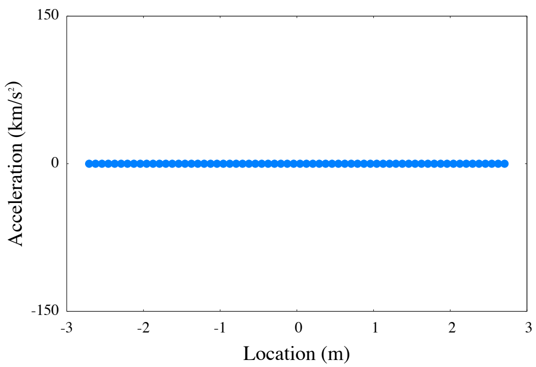


Can the standard model and the partial-stress model recover the expected zero acceleration?

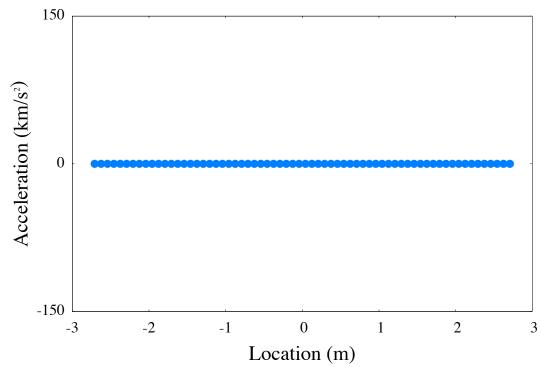
Both models produce the expected result when the horizon is **constant**

Test Results: Acceleration over the length of the bar

Standard material model



Partial-stress formulation

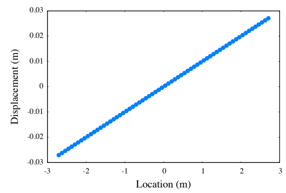


Note: nodes near ends of bar excluded from plots

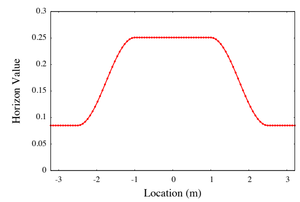
Patch Test: Prescribed Linear Displacement

Test set-up

Prescribe linear displacement field



Variable horizon

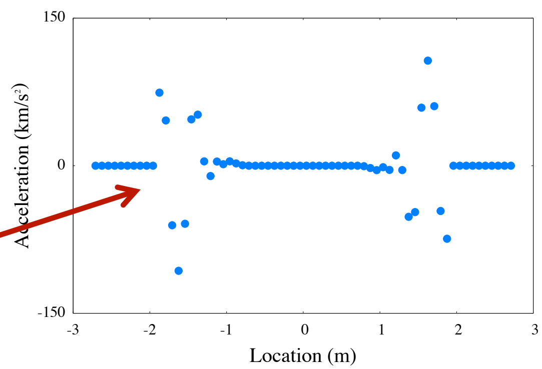


Can the standard model and the partial-stress model recover the expected zero acceleration?

Only the **partial stress** formulation produce the expected result when the horizon is **varying**

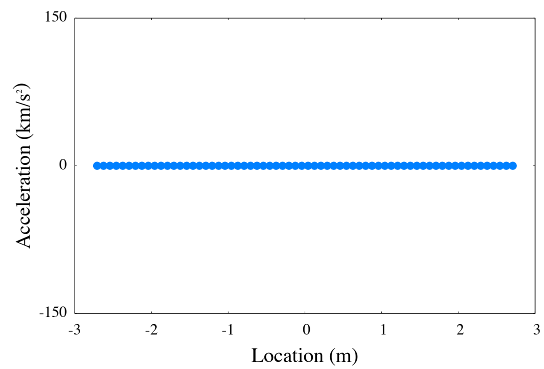
Test Results: Acceleration over the length of the bar

Standard material model



Spurious "ghost forces" present in standard formulation

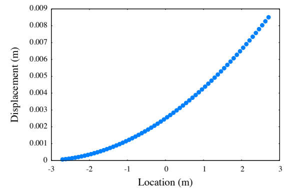
Partial-stress formulation



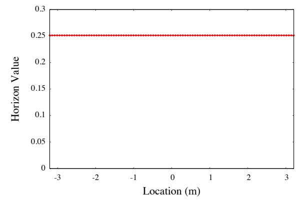
Patch Test: Prescribed Quadratic Displacement

Test set-up

Prescribe quadratic displacement field



Constant horizon throughout bar

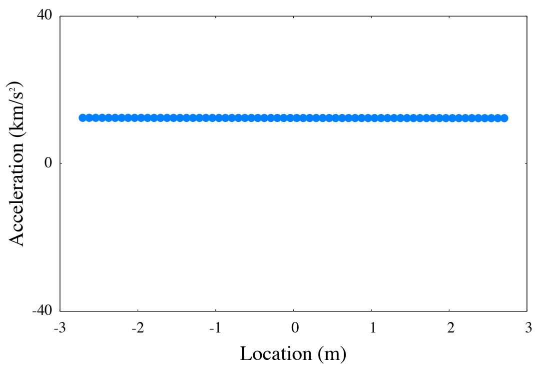


Can the standard model and the partial-stress model recover the expected constant acceleration profile?

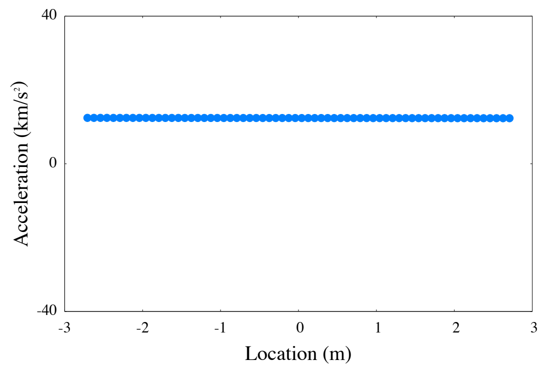
Both models produce the expected result when the horizon is **constant**

Test Results: Acceleration over the length of the bar

Standard material model



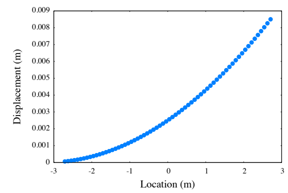
Partial-stress formulation



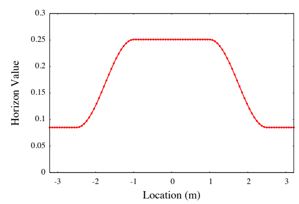
Patch Test: Prescribed Quadratic Displacement

Test set-up

Prescribe quadratic displacement field



Variable horizon

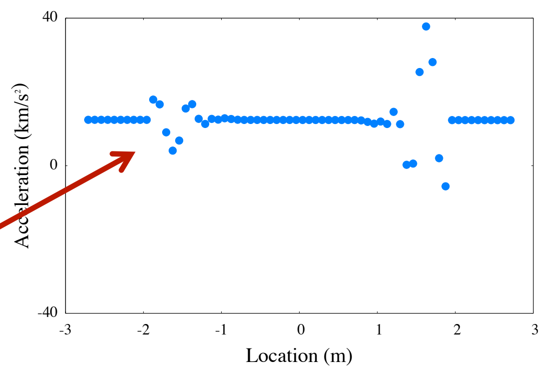


Can the standard model and the partial-stress model recover the expected constant acceleration?

Only the **partial stress** formulation produce the expected result when the horizon is **varying**

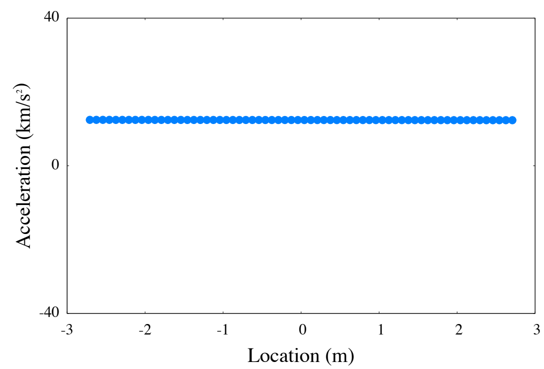
Test Results: Acceleration over the length of the bar

Standard material model



Spurious "ghost forces" present in standard formulation

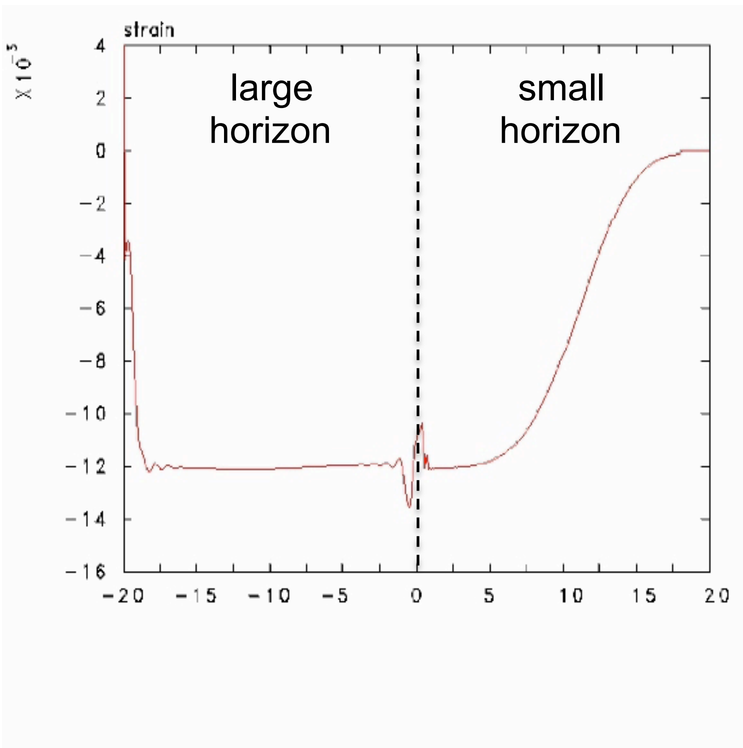
Partial-stress formulation



Wave Propagation through Region of Varying Horizon

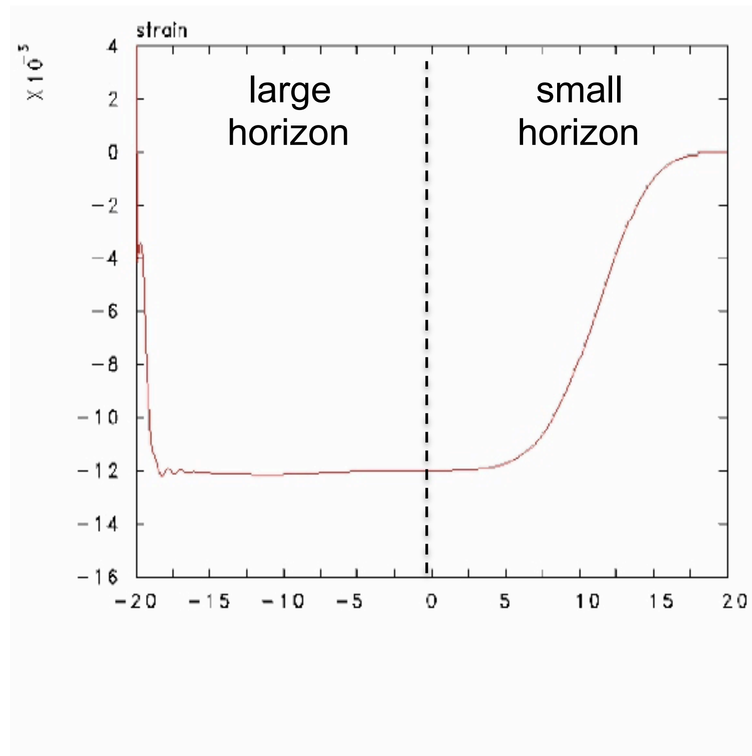
Standard peridynamic model

Numerical artifacts present at transition from large horizon to small horizon



Partial-stress approach

Greatly reduces artifacts, enables smooth transition between large and small horizons



[1] Silling, S., and Seleson, P., Variable Length Scale in a Peridynamic Body, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, June 12, 2013.

What about Performance?

USE OF A VARIABLE HORIZON IMPACTS PERFORMANCE IN SEVERAL WAYS

- Use of a variable horizon can reduce neighborhood size
  - Less computational cost per internal force evaluation
  - Reduces number of unknowns in stiffness matrix for implicit time integration
- Use of a variable horizon can reduce the critical time step
  - Critical time step is strongly dependent on the horizon [1, 2]
  - Smaller time step results in more total steps to solution for explicit transient dynamic simulations
  - Important note: the critical time step for analyses combining peridynamics and classical finite analysis is generally determine by the classical finite elements

Total Number of Bonds
(equal to number of nonzeros in stiffness matrix)

Constant Horizon	92.6 million
Varying Horizon	46.5 million

Stable Time Step [1, 2]
(explicit transient dynamics)

Constant Horizon	2.03e-5 sec.
Varying Horizon	7.15e-6 sec.

[1] S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures*, 83:1526-1535, 2005.

[2] Littlewood, D.J, Thomas, J.D., and Shelton, T.R. Estimation of the Critical Time Step for Peridynamic Models. SIAM Conference on the Mathematical Aspects of Material Science, Philadelphia, Pennsylvania, June 9-12, 2013.

The *Peridigm* Computational Peridynamics Code

Sandia National Laboratories

WHAT IS PERIDIGM?

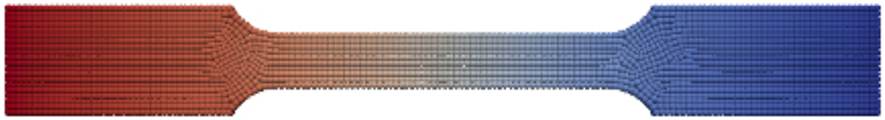
- Open-source software developed at Sandia National Laboratories
- C++ code based on Sandia's *Trilinos* project
- Platform for multi-physics peridynamic simulations
- Capabilities:
  - State-based constitutive models
  - Implicit and explicit time integration
  - Contact for transient dynamics
  - Large-scale parallel simulations
- Compatible with pre- and post-processing tools
  - Cubit mesh generation
  - Paraview visualization tools
  - SEACAS utilities
- Designed for extensibility

Peridigm

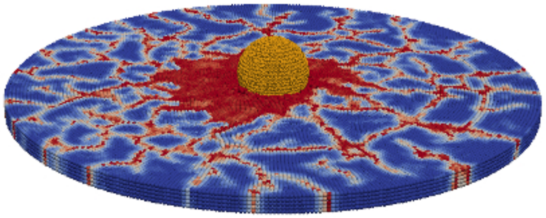
Trilinos

M.L. Parks, D.J. Littlewood, J.A. Mitchell, and S.A. Silling, Peridigm Users' Guide v1.0.0. Sandia Report SAND2012-7800, 2012.

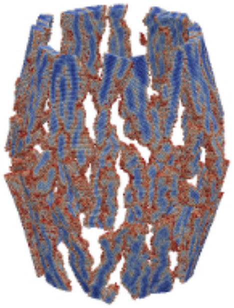
The *Peridigm* Meshfree Peridynamics Code



Quasi-statics (implicit time integration)



Contact

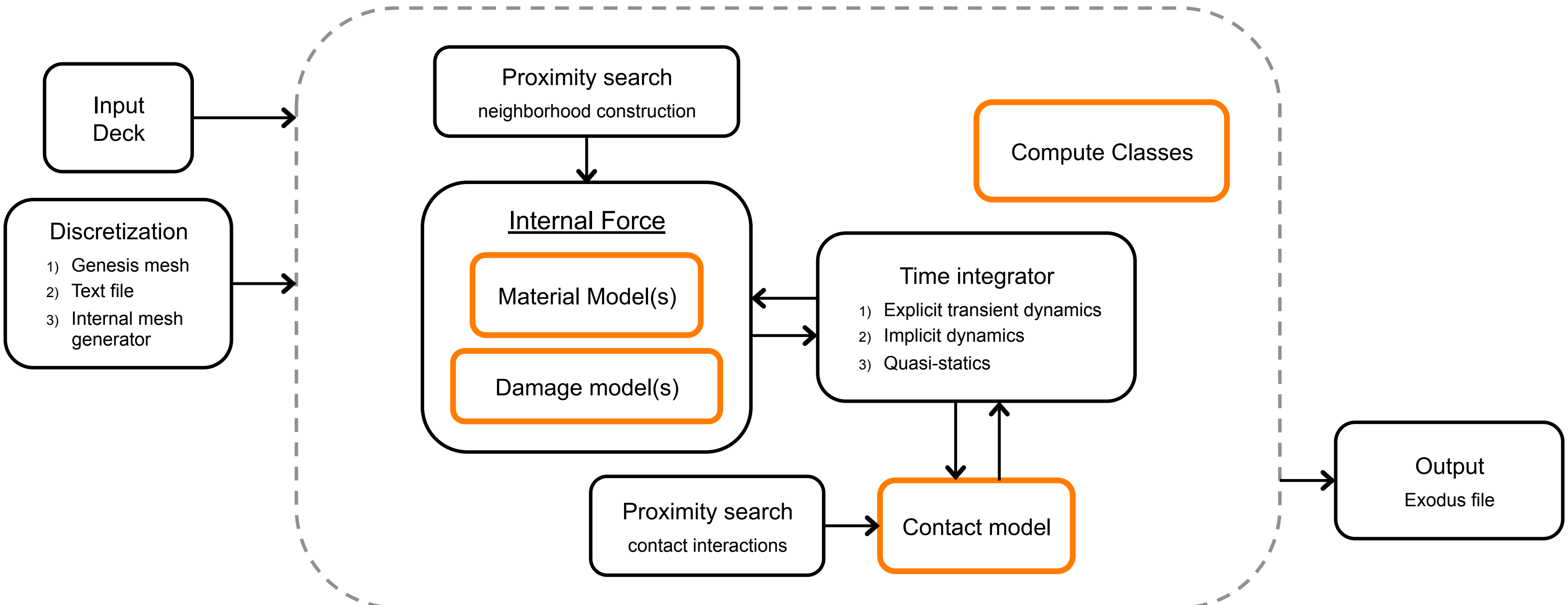


Explicit transient dynamics,
material failure

Peridigm Code Architecture

DESIGN GOALS:

- State-based peridynamics
- Explicit and Implicit time integration
- Contact
- Massively parallel
- Performance
- Extensibility



Orange denotes extensible components

The *Albany* Finite-Element Code

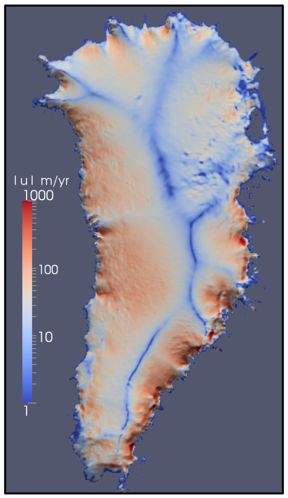
WHAT IS ALBANY?

- Open-source software developed at Sandia National Laboratories
- C++ code based on Sandia's *Trilinos* project
- Platform for multi-physics simulations
- Compatible with pre- and post-processing tools
  - Cubit mesh generation
  - Paraview visualization tools
  - SEACAS utilities
- Designed for extensibility
- Currently being applied to a wide variety of modeling efforts

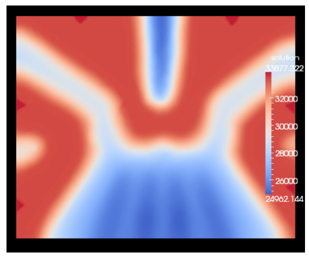
Mesh Tools	Linear Solvers	Analysis Tools	Software Quality
Partitioning	Iterative Solvers	Nonlinear Solver	Version Control
Load Balancing	Direct Solvers	Time Integration	Regression Testing
Adaptivity	Eigen Solver	Stability Analysis	Build System
Remeshing	Preconditioners	Optimization	Verification Tests
Grid Transfers	Multi-Level Algs	UQ Algorithms	Continuous Integration

The *Albany* Finite-Element Code

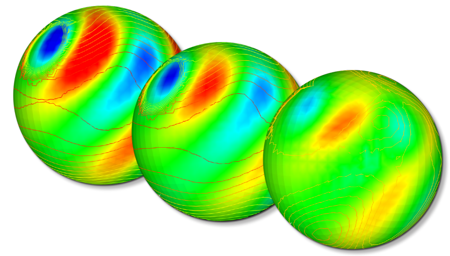
ALBANY IS A COMPONENT-BASED CODE WITH BROAD APPLICATIONS



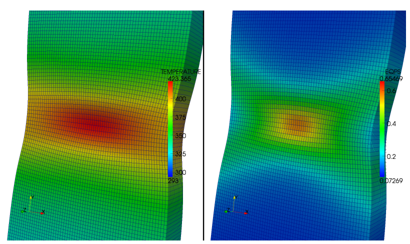
Ice Sheets



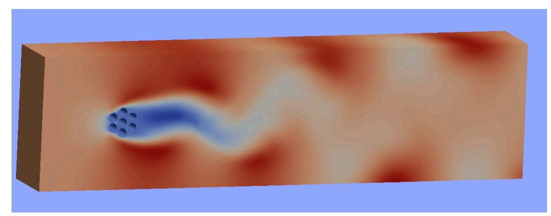
Quantum Devices



Atmosphere Dynamics



Computational Mechanics



Incompressible Flow

Peridigm-Albany Coupling for Algorithm Development

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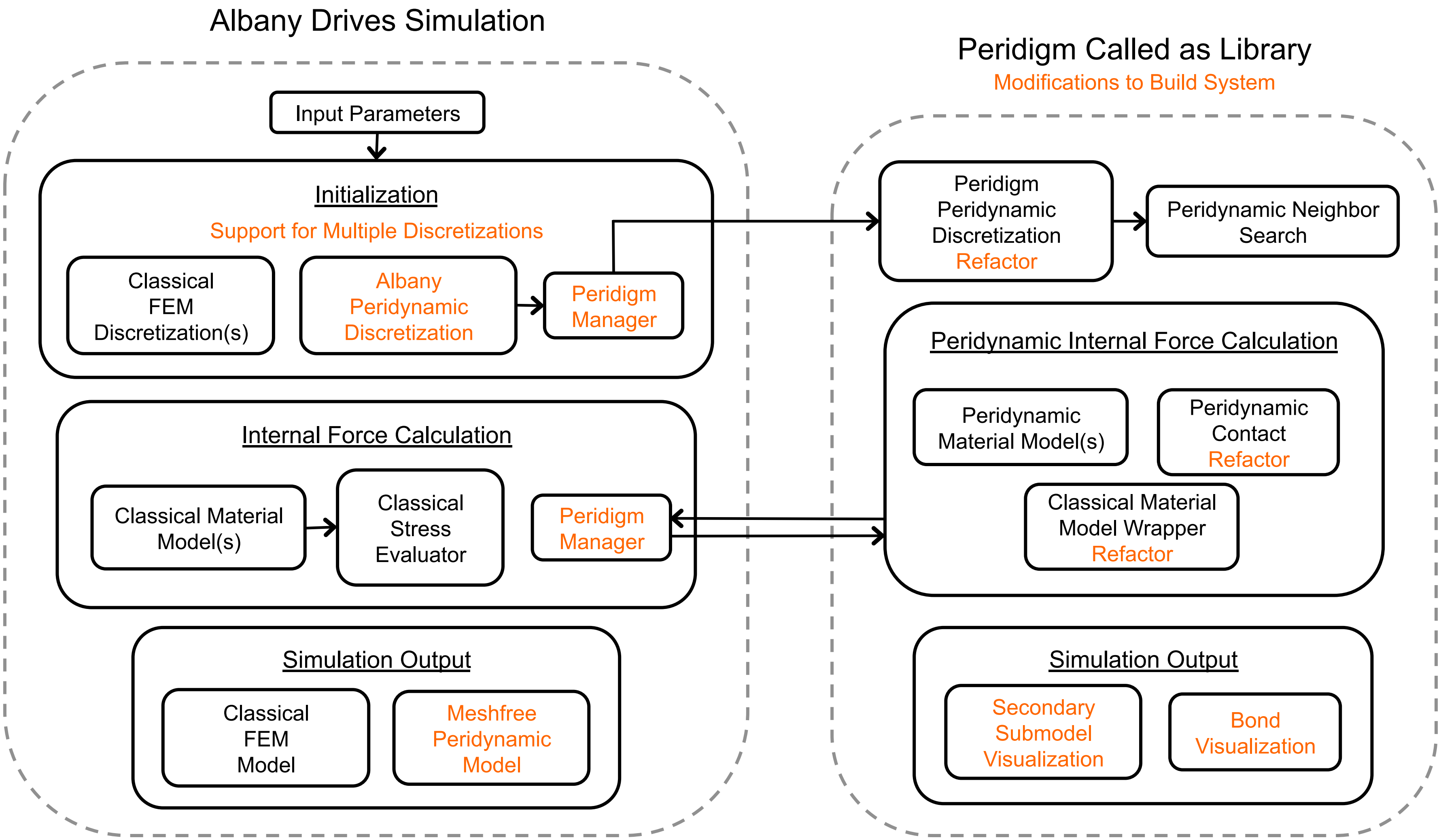
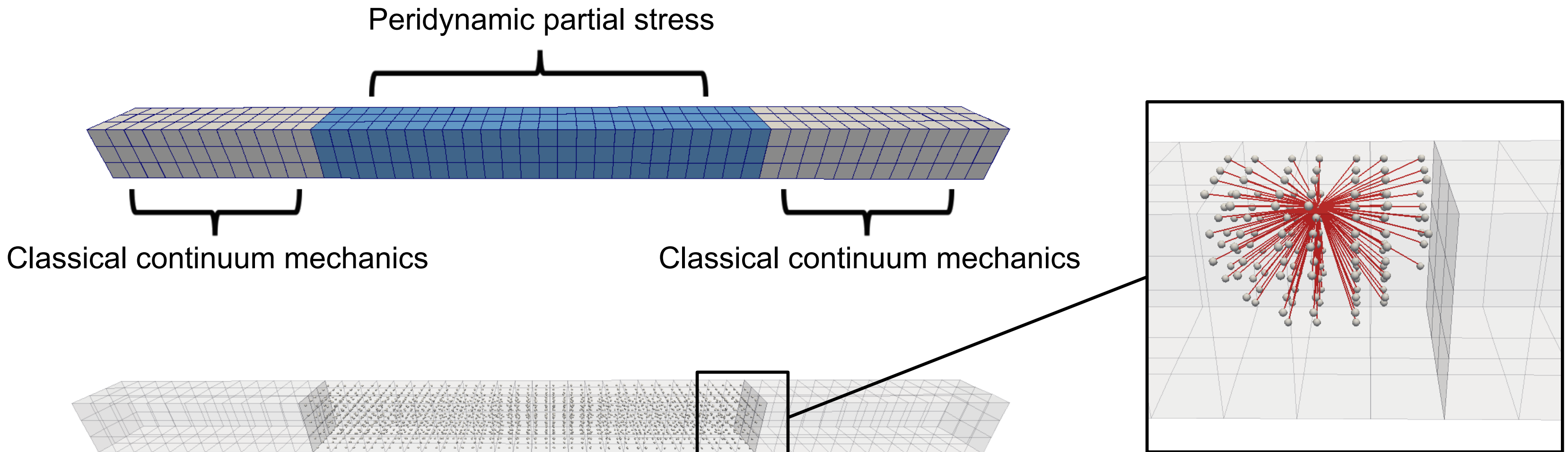
TRILINOS-BASED CODES ENABLE RAPID PROTOTYPE DEVELOPMENT

Orange: Specific to code coupling effort



A Prototype of the Partial Stress Formulation has been Implemented in Coupled *Albany-Peridigm* Code

- Software infrastructure in place for strongly coupled simulations
- Meshfree peridynamic models, peridynamic partial stress, and classical continuum mechanics (FEM) within single executable
- Partial stress utilized for transition between classical continuum mechanics (local model) and peridynamics (nonlocal model)



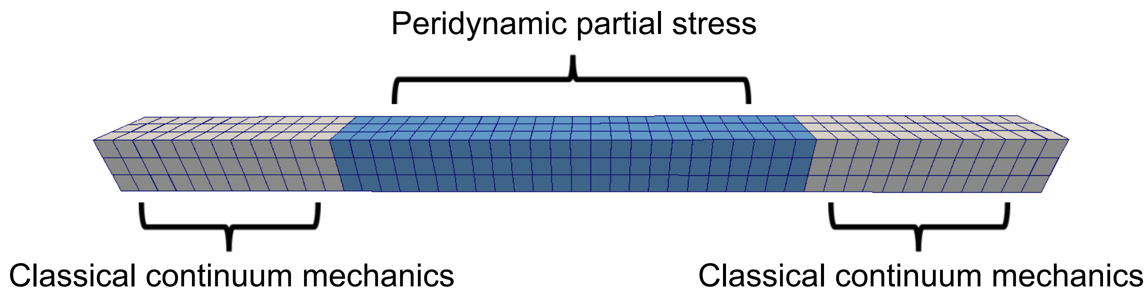
Peridynamic (*Peridigm*) material points located at FEM (*Albany*) quadrature points

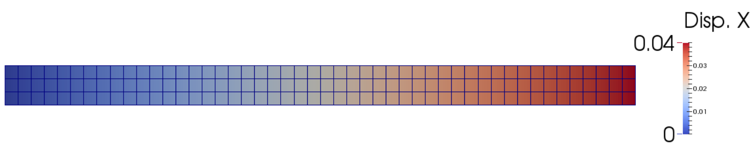
Nonlocal peridynamic interactions (bonds) occur across multiple FEM elements

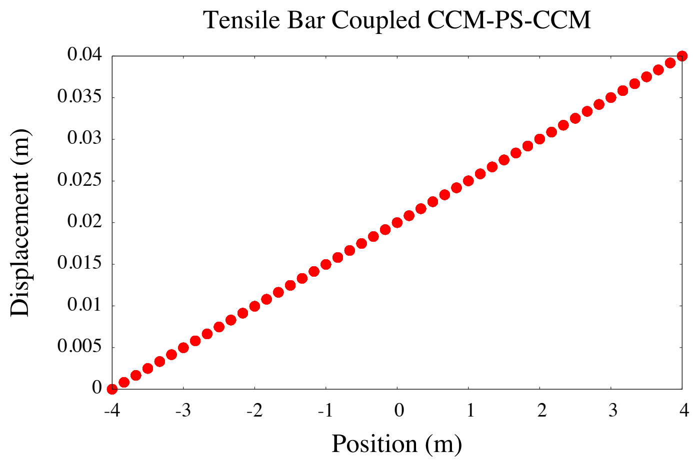
Demonstration Calculation

LINEAR PATCH TEST

- Coupling of classical continuum mechanics and peridynamic partial stress
- Local boundary conditions applied to areas at ends of bar (prescribed displacement)
- Implicit *Albany* solver (statics)



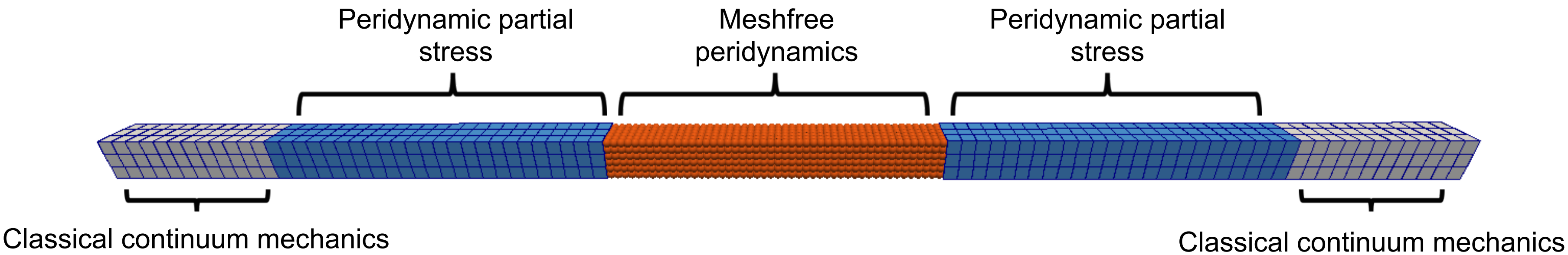


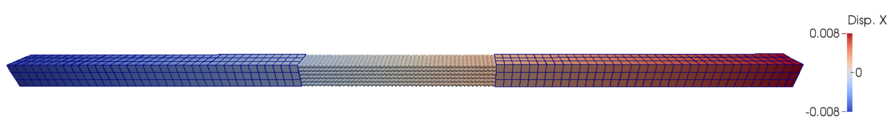


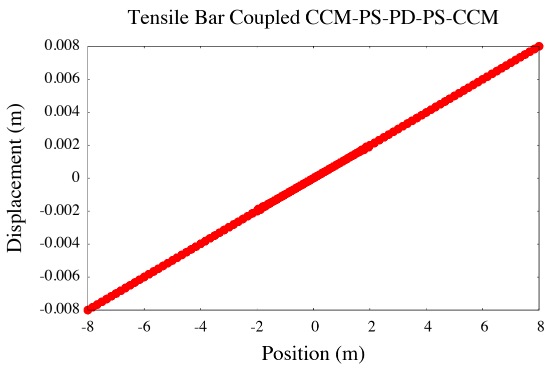
Demonstration Calculation

LINEAR PATCH TEST

- Coupling of classical continuum mechanics, peridynamic partial stress, and standard meshfree peridynamics
- Local boundary conditions applied to areas at ends of bar (prescribed displacement)
- Implicit *Albany* solver (statics)
- Interface between partial stress and meshfree peridynamics is a work in progress







Questions?

David Littlewood

djlittl@sandia.gov

http://peridigm.sandia.gov

Constitutive Models for Peridynamics

Sandia National Laboratories

MATERIAL MODEL FORMULATION STRONGLY AFFECTS CRITICAL TIME STEP

- Presence of multiple length scales differs from the classical (local) approach
- Complex deformation modes possible within a nonlocal neighborhood
- Material failure through the breaking of bonds may alter the stable time step

Microelastic Material [1]

- Bond-based constitutive model
- Pairwise forces are a function of bond stretch

$$s = \frac{y - x}{x}$$

- Magnitude of pairwise force density given by

$$\underline{t} = \frac{18k}{\pi\delta^4} s$$

Linear Peridynamic Solid [2]

- State-based constitutive model
- Deformation decomposed into deviatoric and dilatational components

$$\theta = \frac{3}{m}\int_{\mathcal{H}} (\underline{\omega}\,\underline{x}) \cdot \underline{e}\, dV \qquad \underline{e}^d = \underline{e} - \frac{\theta\,\underline{x}}{3}$$

- Magnitude of pairwise force density given by

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

Definitions

$\underline{x}$	bond vector
x	initial bond length
y	deformed bond length
s	bond stretch
$\underline{e}$	bond extension
$\underline{e}^d$	deviatoric bond extension
$\underline{\omega}$	influence function
V	volume
$\mathcal{H}$	neighborhod
m	weighted volume
θ	dilatation
δ	horizon
k	bulk modulus
μ	shear modulus
$\underline{t}$	pairwise force density

1. 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.
2. S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.

Classical Material Models Can Be Applied in Peridynamics

WRAPPER APPROACH RESULTS IN A NON-ORDINARY STATE-BASED MATERIAL MODEL [1]

- Approximate deformation gradient based on initial and current locations of material points in family

Approximate Deformation Gradient

$$\bar{\mathbf{F}} = \left(\underline{\mathbf{Y}} * \underline{\mathbf{X}}\right) \mathbf{K}^{-1}$$

Shape Tensor

$$\mathbf{K} = \underline{\mathbf{X}} * \underline{\mathbf{X}}$$

Definitions

$\mathbf{X}$	reference position vector state
$\mathbf{Y}$	deformation vector state
$\mathbf{K}$	shape tensor
$\bar{\mathbf{F}}$	approximate deformation gradient
ξ	bond
$\underline{\omega}$	influence function
σ	Piola stress

- Kinematic data passed to classical material model
- Classical material model computes stress
- Stress converted to pairwise force density

$$\underline{\mathbf{T}}\left\langle \xi \right\rangle = \underline{\omega}\left\langle \xi \right\rangle \, \sigma \mathbf{K}^{-1} \xi$$

- Suppression of zero-energy modes (optional) [2]

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

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MATERIAL MODELS

- Linear peridynamic solid [1]
- Elastic-perfectly-plastic [2]
- Elastic-plastic with isotropic hardening [3]
- Viscoelastic [4]
- Thermoelastic (thermal strains)

DAMAGE MODELS

- Critical stretch [5]

CONTACT MODELS

- Short-range force model [5]
- Short-range force model with friction

COMPUTE CLASSES

- Output of any node or element variable
- Per-block quantities (min, max, sum)
- Energy (kinetic, stored elastic)
- Neighborhood statistics (horizon, number of neighbors)
- Approximate deformation gradient [1]
- Many others…

1. S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.
2. J.A. Mitchell. A nonlocal, ordinary, state-based plasticity model for peridynamics. Sandia Report SAND2011-3166, 2011.
3. J.T. Foster, D.J. Littlewood, J.A. Mitchell, and M.L. Parks. Implicit-time integration of an ordinary state-based peridynamic plasticity model with isotropic hardening. ASME International Mechanical Engineering Congress and Exposition, Houston, Texas, November 9-15, 2012.
4. J.A. Mitchell. A non-local, ordinary-state-based viscoelasticity model for peridynamics, Sandia Report SAND2011-8064, 2011.
5. Silling, S.A. and Askari, E. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures* 83:1526-1535, 2005.

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AVAILABLE INTEGRATION SCHEMES

- Explicit dynamics: Velocity-Verlet (leapfrog) time integrator
- Implicit dynamics: Newmark-beta
- Quasi-statics: Nonlinear solver with modified Newton approach or Matrix-Free Newton Krylov approach
- Wide variety of linear solvers available via *Trilinos* software packages

CONSTRUCTION OF THE TANGENT MATRIX

- Three options for construction of the tangent matrix:
  - User-supplied tangent
  - Finite-difference scheme
  - *Automatic differentiation* via the *Trilinos Sacado* package
- Finite-difference scheme operates directly on internal-force calculation
  - No additional development required by material model developer
- Automatic differentiation approach requires C++ templates and (minor) extension of material model