SAND2012-8932P

Strong Local-Nonlocal Coupling for Integrated Fracture Modeling

LDRD FY13-FY15

David Littlewood

Albany Developers Meeting
2 October 2012

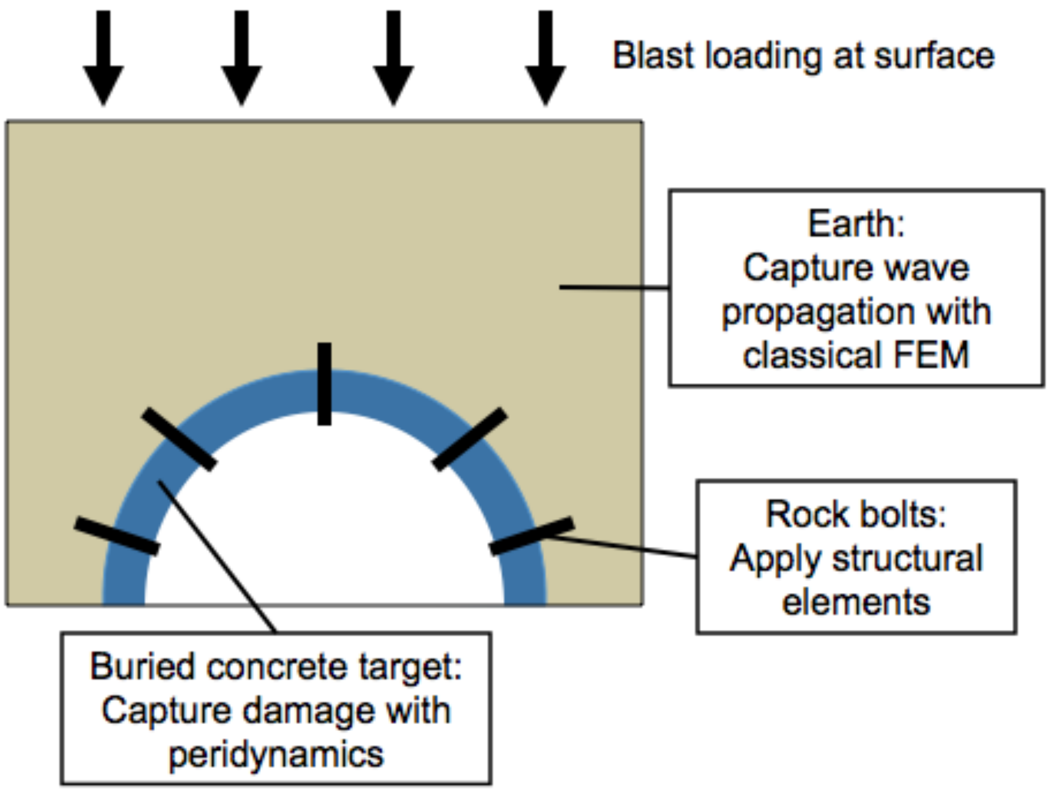
Goal: Direct Coupling of Peridynamics and Classical FEM

DRIVER

- Provide an integrated fracture modeling capability to the DOE and DoD

IMPACT

- Advance state of the art in computational simulation of material failure and fracture
- Integrated fracture modeling capability directly applicable to Sandia's mission



Vision
Apply peridynamics in regions susceptible to material failure

Local-Nonlocal Coupling for Integrated Fracture Modeling

APPROACH

- Fully integrate *peridynamics* with *classical finite-element models*
  - Mathematical foundations for local-nonlocal coupling
  - Algorithm and software prototyping
  - Initial validation against experimental data
  - Implementation in *Sierra/SolidMechanics*

TEAM

- Expertise: mathematics, mechanics, scientific computing, engineering analysis
- Direct line of sight from mathematical foundations to deployment

<u>Team Members</u>

David Littlewood (1444)
Michael Parks (1444)
Jakob Ostien (8256)
Stewart Silling (1444)
Max Gunzburger (FSU)
Pablo Seleson (U. Texas)

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Peridynamics

WHAT IS PERIDYNAMICS?

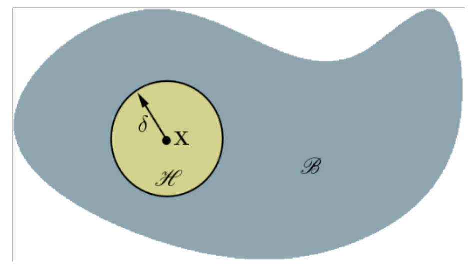
Peridynamics is a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles

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*:

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

The point X interacts directly with all points within its horizon



Increasing prominence of peridynamics

PERGAMON
Journal of the Mechanics and Physics of Solids
48 (2000) 175–209
JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS

Reformulation of elasticity theory for discontinuities and long-range forces

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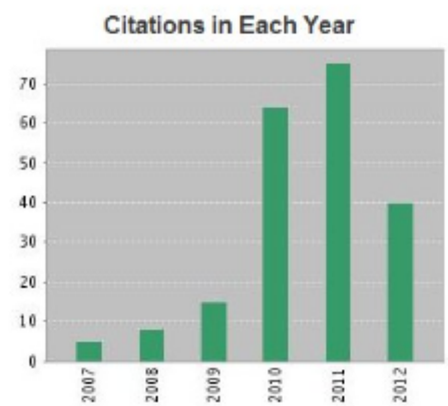
Received 2 October 1998; received in revised form 2 April 1999

Abstract

Some materials may naturally form discontinuities such as cracks as a result of deformation. As an aid to the modeling of such materials, a new framework for the basic equations of continuum mechanics, called the 'peridynamic' formulation, is proposed. The propagation of linear stress waves in the new theory is discussed, and wave dispersion relations are derived. Material stability and its connection with wave propagation is investigated. It is demonstrated by an example that the reformulated approach permits the solution of fracture problems using the same equations either on or off the crack surface or crack tip. This is an advantage for modeling problems in which the location of a crack is not known in advance.

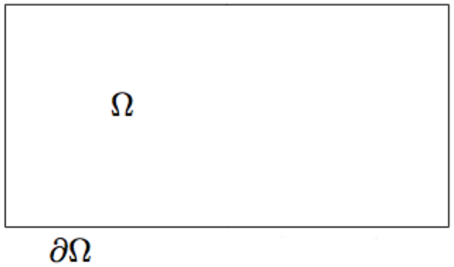
Keywords: Dynamics; Elastic material; Fracture; Stability and bifurcation; Stress waves



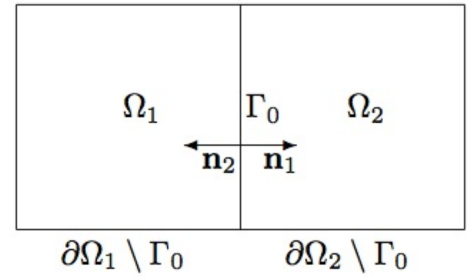
Local-Nonlocal Coupling: Domain Decomposition Approach

DOMAIN DECOMPOSITION FOR LOCAL MODELS

One Domain Problem



Equivalent Two Domain Problem



KEY POINTS

- For a given one-domain problem, an equivalent two-domain problem can be constructed
- Sub-domain problems are solved independently, subject to an additional set of *transmission conditions* (continuity & flux balance)
- Example: Transmission conditions for classical diffusion problem:

$$u_1(\mathbf{x},t) = u_2(\mathbf{x},t), \text{ on } \Gamma_0 \times (0,T).$$

$$(\mathbf{D}_1(\mathbf{x})\nabla u_1(\mathbf{x},t)) \cdot \mathbf{n}_1 = -(\mathbf{D}_2(\mathbf{x})\nabla u_2(\mathbf{x},t)) \cdot \mathbf{n}_2, \quad \text{on } \Gamma_0 \times (0,T).$$

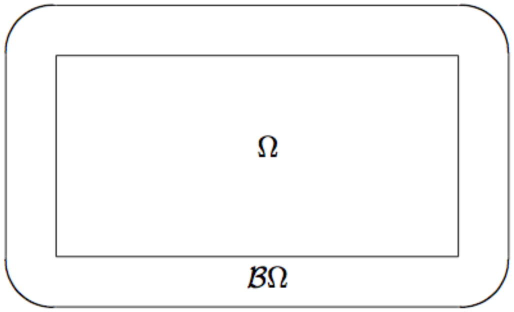
CAN DOMAIN DECOMPOSTION BE EXTENDED TO NONLOCAL MODELS?

- YES, domain decomposition for nonlocal diffusion has been developed by Seleson, Gunzburger, and Parks [*submitted for publication*, 2012]

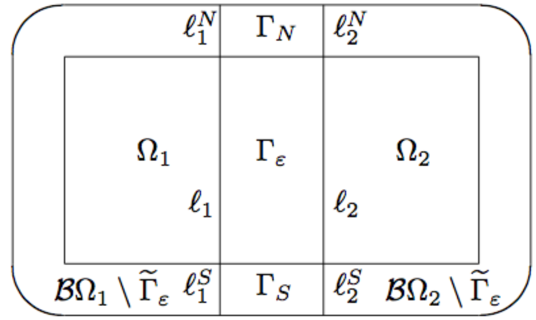
Local-Nonlocal Coupling: Domain Decomposition Approach

DOMAIN DECOMPOSITION FOR NONLOCAL MODELS

One Domain Problem



Equivalent Two Domain Problem



KEY POINTS

- Interface between domains is a boundary layer due to nonlocal interactions
- Transmission conditions must be derived for nonlocal models (continuity & flux balance)

$$u_1(\mathbf{x},t) = u_2(\mathbf{x},t), \text{ in } \Gamma_\varepsilon \times (0,T).$$

$$\frac{\partial u}{\partial t}(\mathbf{x},t) = \int_{\overline{\overline{\Omega}}} c_{\text{sym}}(\mathbf{x}',\mathbf{x})(u(\mathbf{x}',t) - u(\mathbf{x},t))\, dV_{\mathbf{x}'} + q(\mathbf{x},t), \text{ in } \Gamma_\varepsilon \times (0,T).$$

CAN DOMAIN DECOMPOSITION BE APPLIED TO LOCAL-NONLOCAL COUPLING?

- YES, local-nonlocal coupling is achieved by reducing the nonlocal length scale (peridynamic horizon) to zero within one of the domains
- Challenges remain for application to solid mechanics: Extension from scalar fields (*e.g.*, concentration) to vector fields (*e.g.*, displacements)

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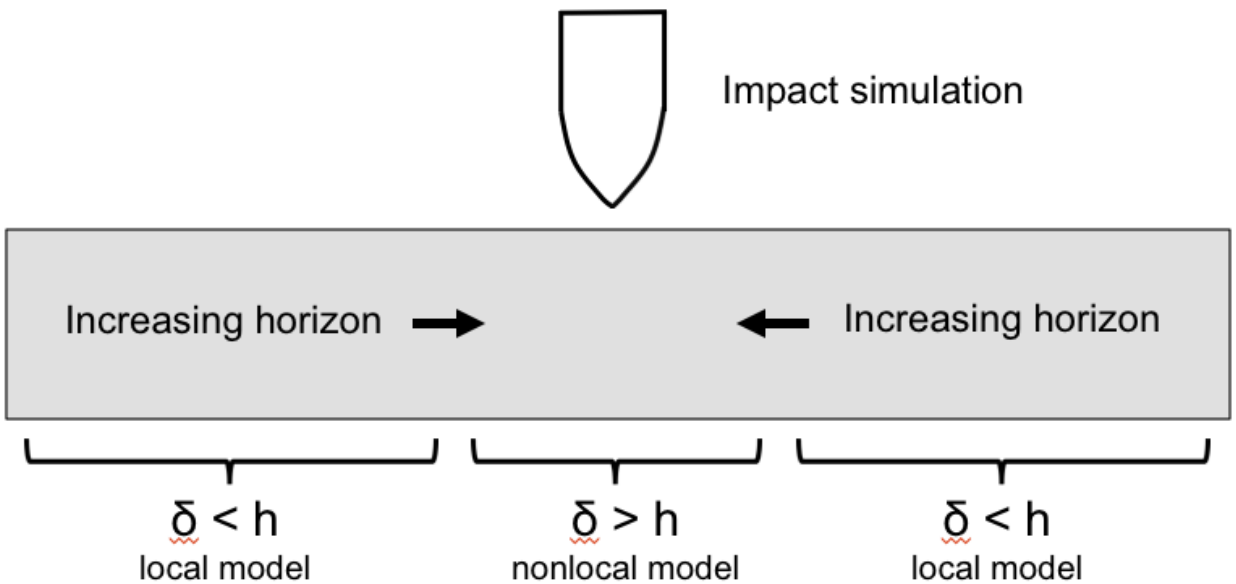
Implicit Local-Nonlocal Coupling

APPLY UNIFIED PERIDYNAMIC MODEL WITH A VARYING HORIZON

- Key point: Peridynamics converges to a local model as the horizon approaches zero
  - Horizon > mesh spacing produces a nonlocal model
  - Horizon < mesh spacing produces a local model
- Apply local-local coupling to peridynamics (horizon < mesh spacing) and classical FEM
- *Key challenge*: Current mesh-free discretization and quadrature rules do not support a horizon < mesh spacing
  - Higher-order peridynamic quadrature must be developed
  - Current quadrature work: Gunzburger, and Bond and Lehoucq



S.A. Silling and R.B. Lehoucq, Convergence of peridynamics to classical elasticity theory, *Journal of Elasticity*, 93 (1), pp. 13-37, 2008.

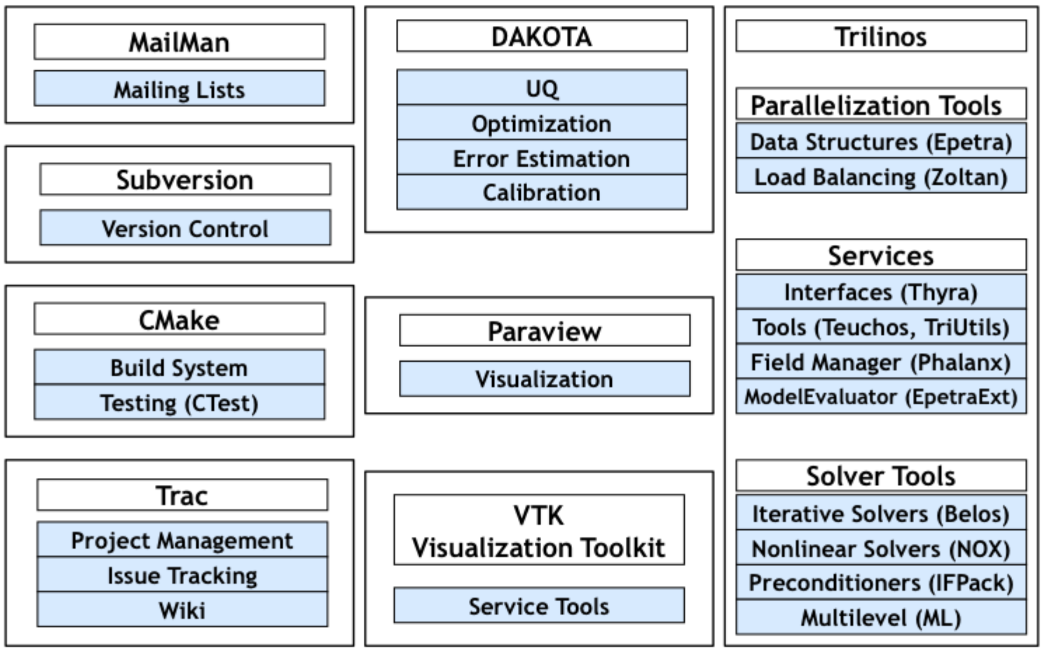
Algorithm Development and Software Prototyping

VET ALGORITHMS IN AN OPEN-SOURCE, COLLABORATIVE SOFTWARE FRAMEWORK

- Candidate algorithms for local-nonlocal coupling
- Higher-order peridynamic quadrature
- Algorithm design for compatibility with production analysis code
- Platform for initial model validation

PROTOTYPE DEVELOPMENT

- *Peridigm* peridynamics code [Parks, Littlewood, Mitchell]
- *Albany/*LCM classical finite-element code [Salinger, Ostien]
- Trilinos agile components
  - Rapid prototype development
  - Feedback mechanism to Trilinos developers

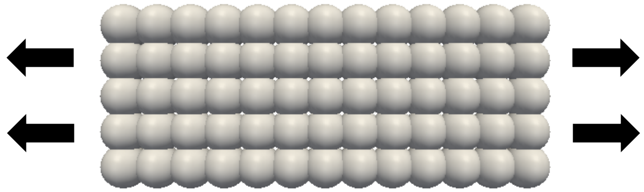


M. Parks, D. Littlewood, A. Salinger, and J. Mitchell, *Peridigm* Summary Report: Lessons Learned in Development with Agile Components, SAND2011-7045.

Prototyping in *Albany*/LCM and *Peridigm*

PERIDIGM SIMULATIONS USING CLASSICAL MATERIAL MODELS

- Non-ordinary state-based peridynamics
  1. *Peridigm* computes approximate deformation gradient
  2. Kinematic data passed to material model in *Albany*
  3. *Peridigm* converts stresses to pairwise peridynamic forces



Initial milestones: pure peridynamic simulations

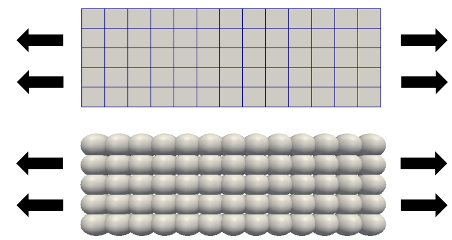
DRIVE PERIDYNAMICS SIMULATION FROM ALBANY

- Wrap *Peridigm* in a `PHX::Evaluator`
  - Internal force / Jacobian
  - Implicit / explicit time integration
  - File I/O, conversion to sphere elements
  - Contact

Prototyping in *Albany*/LCM and *Peridigm*

COMBINED PERIDYNAMICS / CLASSICAL FEM SIMULATIONS

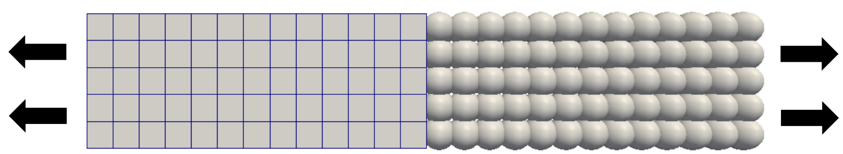
- Drive simulations from *Albany*
- Independent blocks for peridynamics and classical FEM



Combined simulation

COUPLED PERIDYNAMICS / CLASSICAL FEM SIMULATIONS

- Drive simulations from *Albany*
- Mesh tying couples the peridynamic and classical-FEM portions of the simulation
  - Multi-point constraints provide quickest path to (lousy) coupled simulation
  - Create framework for implementation of coupling algorithms



Coupled simulation

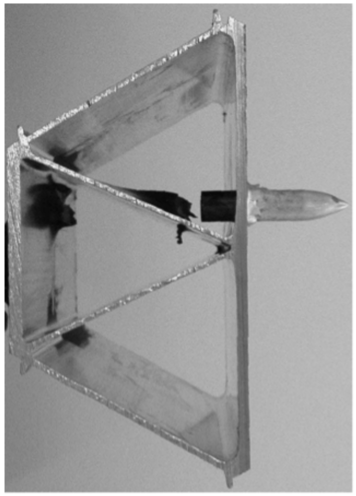
HIGHER-ORDER QUADRATURE FOR PERIDYNAMICS IN PERIDIGM

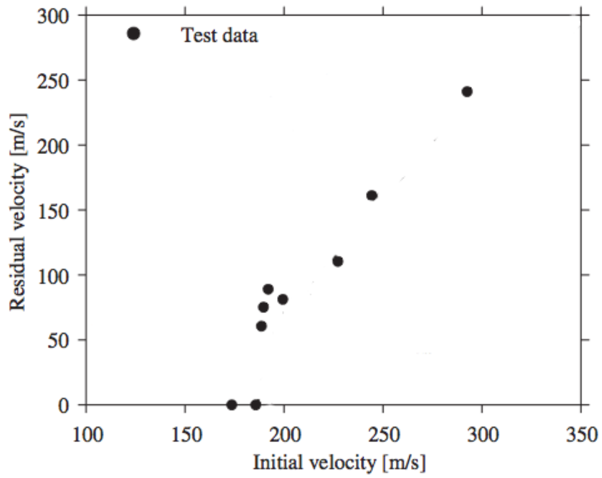
- Mathematical formulations must be extended to three dimensions
- Payoff: Increased accuracy and improved convergence rates
- Payoff: Allows for peridynamic horizon that is smaller than the element size
  - Natural path to local-nonlocal coupling

Initial Model Validation

PERFORATION OF ALUMINUM PANELS

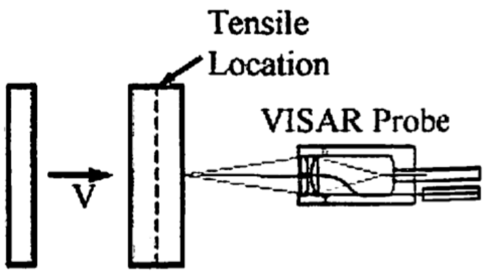
- Perforation of extruded AA6005-T6 panels by steel projectiles [Borvik, *et. al*, 2005]
- Validate exit velocities against experimental measurements
- Qualitative evaluation of localization and damage patterns

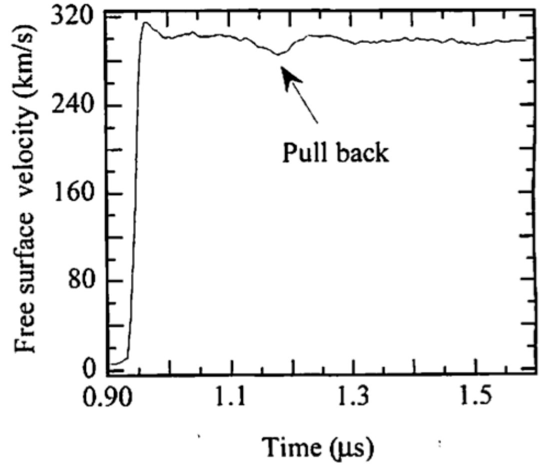




SPALLATION OF SILICON CARBIDE

- Spall in shock-loaded silicon carbide [Dandekar, 2004]
- Validate free-surface velocities against experimental data





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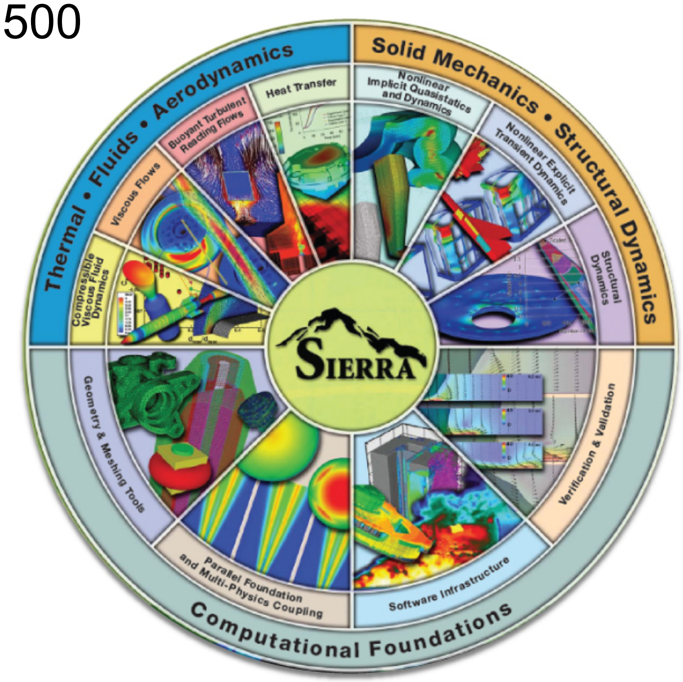
Implementation in Sierra/SolidMechanics

DEPLOYMENT TO THE DOE AND DOD

- Sierra is the engineering mechanics simulation code suite supporting the nation's nuclear weapons mission, as well as other customers
- Leverage existing implementation of peridynamics in *Sierra/SM* [Littlewood, *Sierra/SM* team]
- Strengthen collaboration between 1400, 8200, and 1500



MEASURES OF SUCCESS

- Performance in validation experiments
- Range of applicability
  - Hexahedron elements (focus is here)
  - Tetrahedron elements, structural elements
  - RKPM
- Impact on code complexity, performance, and maintainability

IMPACT

- Failure modeling capability of direct relevance to Sandia's national security missions

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Questions?

Strong Local-Nonlocal Coupling for Integrated Fracture Modeling

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Multiphysics Simulation Technologies (Org. 1444)

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