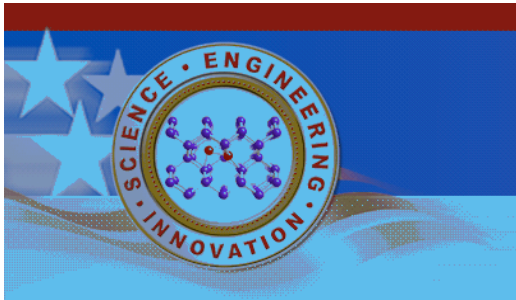

Peridynamics as a Rigorous Coarse-Graining of Atomistics for Multiscale Materials Design

PI:Rich Lehoucq (1414), PM:John Aidun (1435), Stephen Foiles (1814), Mike Parks (1414), Mark Sears (1435), Stewart Silling (1435)

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories

Peridynamics (Silling 2000)

- ***Motivation:*** **Continuum theory for discontinuous deformation**
- ***Impact:*** **3D material failure simulations**
- ***Key:*** **nonlocal model of force**

PERGAMON

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Reformulation of elasticity theory for discontinuities and long-range forces

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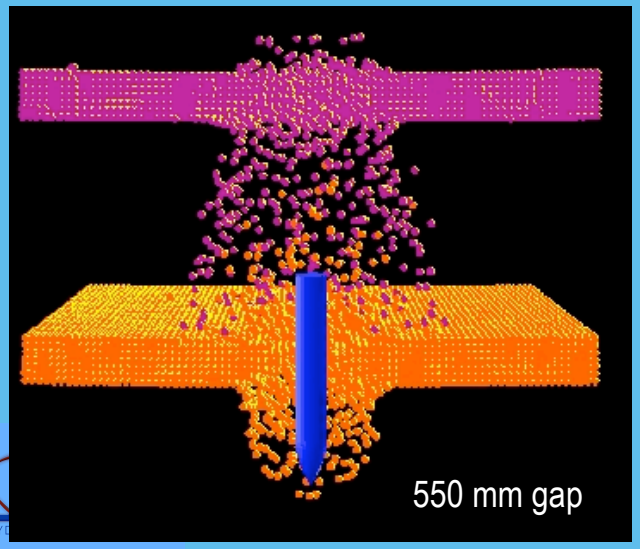
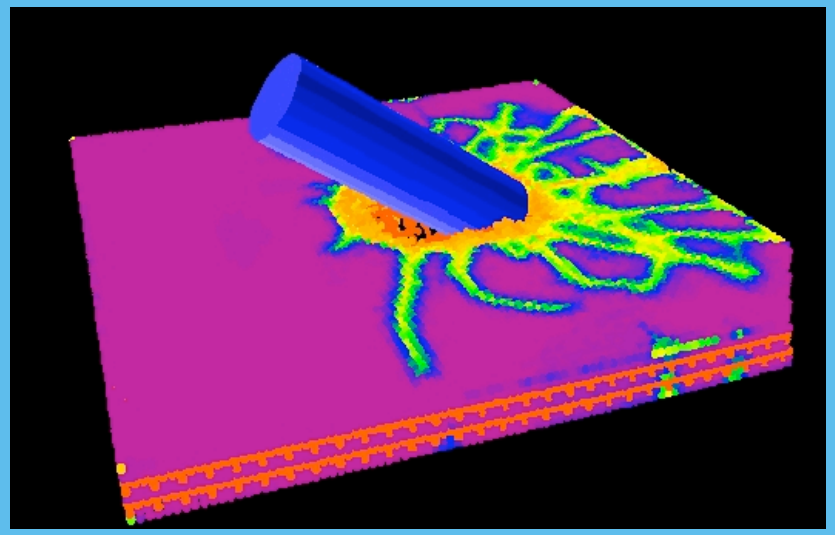


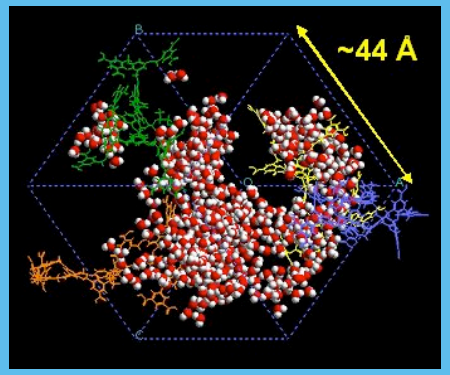


Question: What is the relationship between molecular dynamics and peridynamics?

$$\rho\ddot{u} = \int k(x', x)dx' + b$$

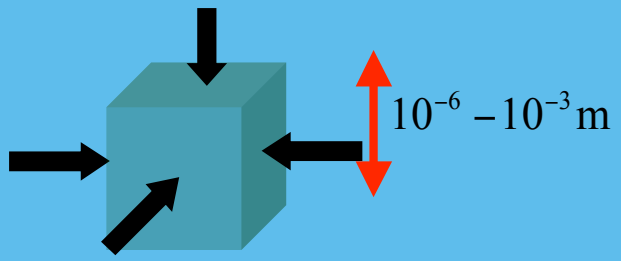
Mesoscopic or an intermediate scale

Molecular, or atomistic regime



$$m_i\ddot{y}_i = f_i^{\text{int}} + f_i^{\text{ext}}$$

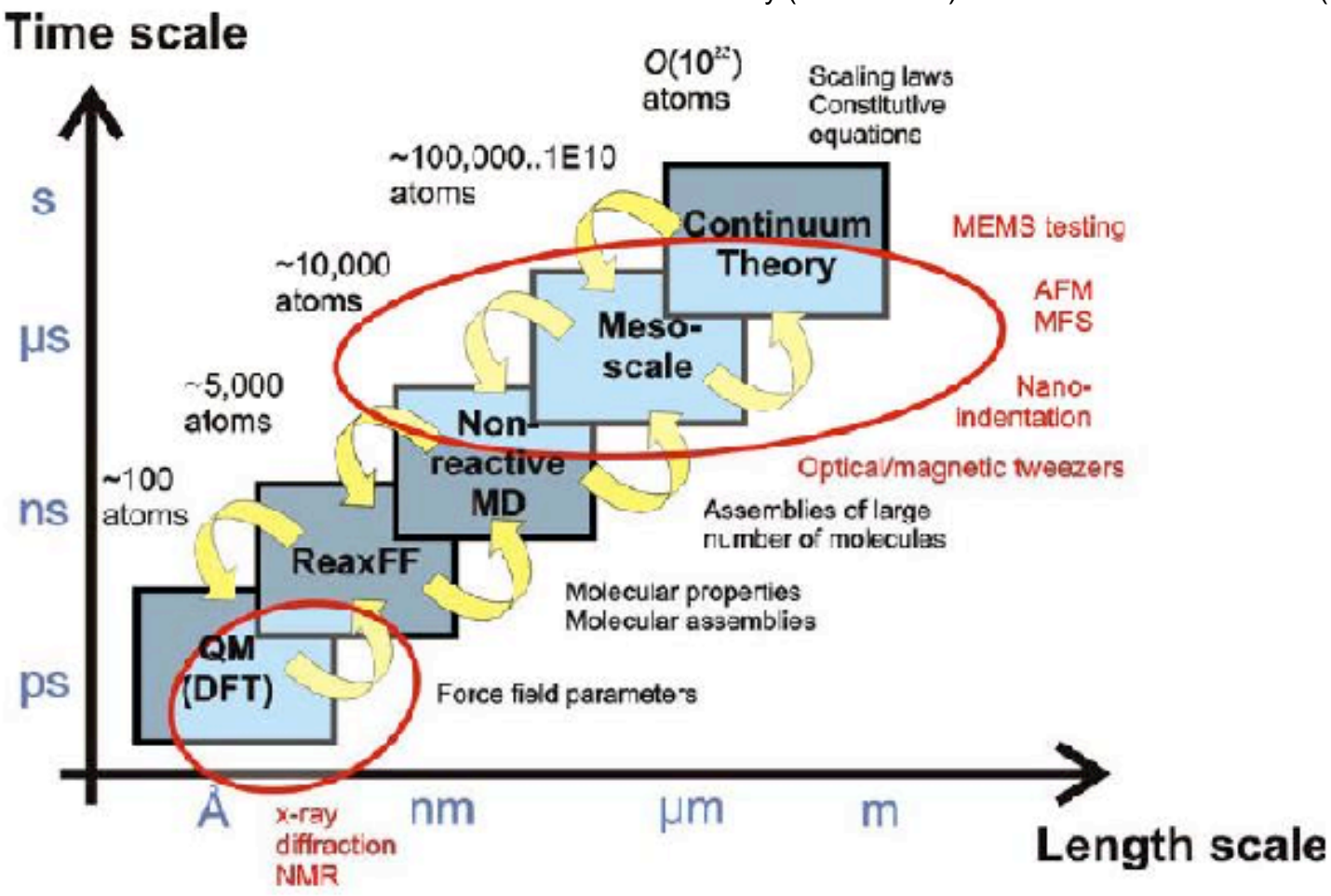
Traditional engineering length scale



$$\rho\ddot{u} = \text{div}\sigma + b$$

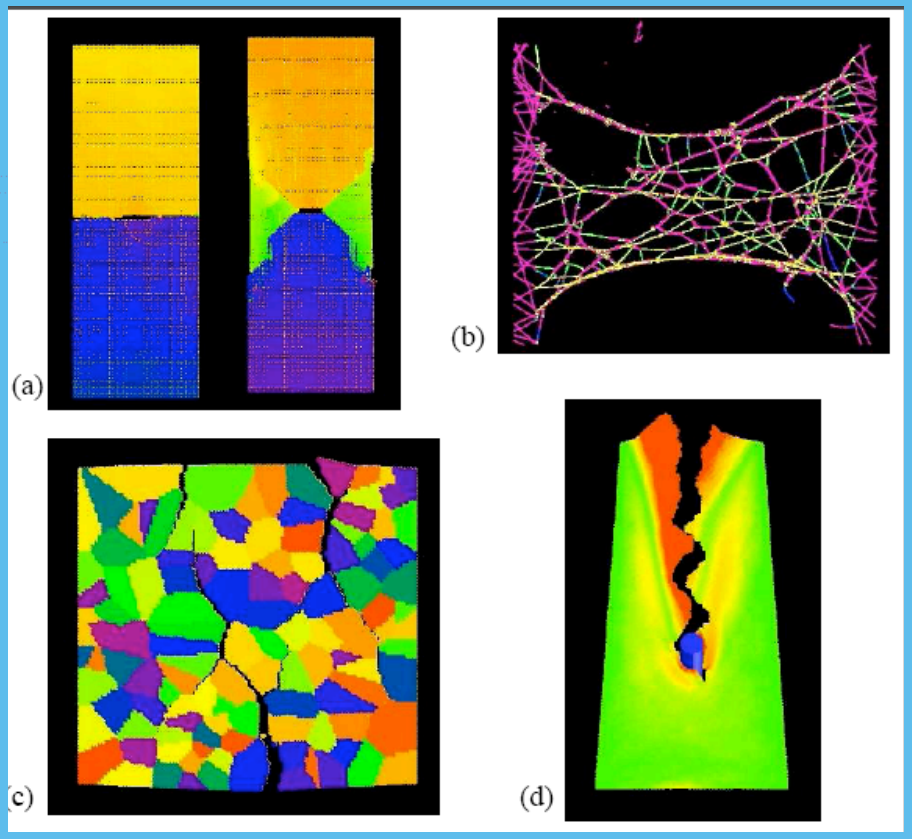
Purview of peridynamics is the mesoscopic regime

Courtesy (via the web) Professor Marcus Buehler (MIT)



Peridynamic applications

Cracking in a notched graphite/epoxy composite laminate (joint with Boeing)



Stretching and failure of initially square nanofiber network (Bobaru)

Dynamic fracture in a polycrystal (Bobaru and Silling)

Oscillatory crack path in a thin membrane (Bobaru and Silling)

Simulations performed with EMU Fortran 90 code (Silling)

Statistical mechanical foundations

The Statistical Mechanical Foundations of Peridynamics

I. Mass and Momentum Conservation Laws

SAND 2009-0971J, under revision for PRE

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(Dated: March 5, 2009)

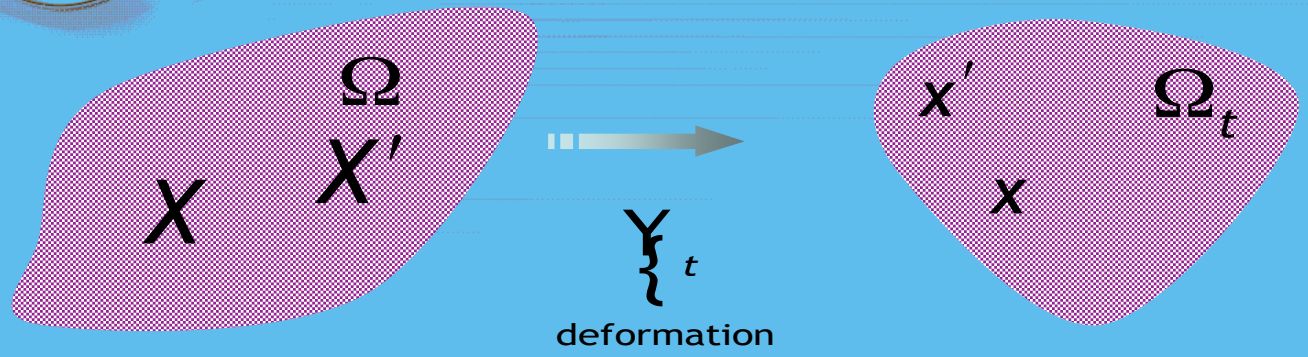
- Peridynamics has a statistical mechanical foundation—it lies at the mesoscopic regime
- Justifies our claim that peridynamics is a rigorous coarse-graining of atomistics, or molecular mechanics

Recipe for generating balance equations

- Express densities (mass, momentum, force, energy) as phase space (statistical) expectation
- Using Liouville's equation, compute the rate of change of this expectation
- Much tedious manipulation results in the balances of mass, momentum (peridynamic) and energy (peridynamic)
- Force and heat flux are nonlocal quantities

Question: What about constitutive relationships? What do we replace stress-strain relationships with?

Deformation



$$x = \Psi_t(X), \quad x' = \Psi_t(X')$$

$$\Phi(x, x') := x' - x = \Psi_t(X') - \Psi_t(X)$$

$$\approx \underbrace{\nabla \Psi_t(X)}_{\text{Deformation gradient}} \left(X' - X\right)$$

Constitutive relation

Question: What about constitutive relationships? (What do we replace stress-strain relationships with?)

$$\mathrm{div}\sigma(x) = \mathrm{div}\sigma(\mathrm{grad}\Psi(x))$$

Answer: Map Φ(x,x') to force density (via an integral operator)

$$\int k(x', x)dx' = \int k(\Psi(x, x'))dx'$$

Nonlocal because points x'≠x are involved

The goal of the coarse-graining of atomistics into peridynamics is to provide a basis for approximating constitutive relationships at the mesoscopic scale

LAMMPS and molecular dynamics

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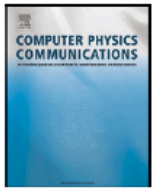


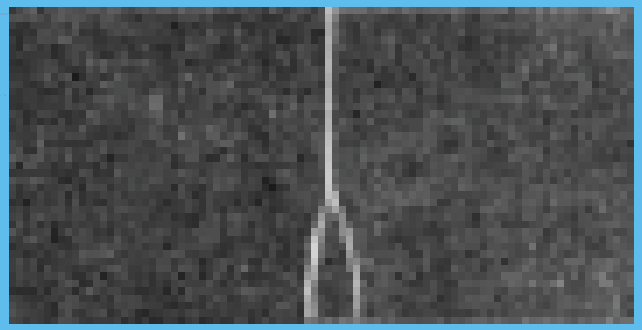
Implementing peridynamics within a molecular dynamics code

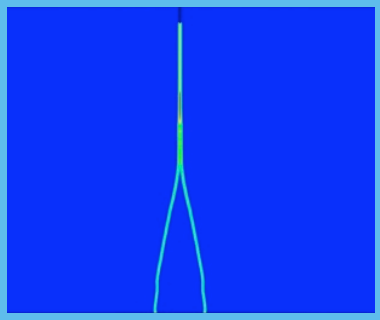
Michael L. Parks [a,*,1], Richard B. Lehoucq [a,1], Steven J. Plimpton [b,1], Stewart A. Silling [c,1]

- Implemented within LAMMPS (SNL mpp molecular dynamic code)
- Provide a software platform for experimentation
- Enable molecular dynamic users access to a continuum mechanics capability for mesoscopic computing
- Provide continuum mechanicians a molecular mechanics capability

3D dynamic brittle fracture in glass simulations

Physical experiment: S F. Bowden, J. Brunton, J. Field, and A. Heyes, *Controlled fracture of brittle solids and interrup tion of electrical current*, Nature, 216, 42, pp.38-42, 1967





Summary

- Peridynamics is given a statistical mechanical foundation
- The theoretical basis for multiscale materials modeling has been established