

Computational Modeling of Nanostructures using the Peridynamic Model

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Summary

The theory of elasticity was developed by Navier and Cauchy in the 1820's, together with the associated concepts of stress and strain. Later generalized as the theory of continuum mechanics, material behavior is defined by stress vs. strain constitutive relations. However, in many situations involving nanostructures, size scales are so small that the assumptions of continuum mechanics are inapplicable. In addition, displacements may become discontinuous resulting in undefined strains. For many regimes, continuum mechanics fails to adequately describe mechanical behavior.

On the other hand, lattice theory, atomistics, and molecular dynamics, while physically appealing, are often too computationally expensive to simulate important problems in micro- and nanostructures.

The peridynamic (near-force) model, developed by Silling and his colleagues [1, 2] over the past decade, presents a radical departure from both the theory of continuum mechanics and lattice theory. In the peridynamic model, displacements may be discontinuous. Continuum mechanics, atomistics, and fracture mechanics are all well-described by the peridynamic model.

I will present the theory of peridynamics, and several example problems, as well as potential applications of peridynamics to micro engineered mechanical systems and nanostructures.

References

1. Silling, S.A. (2000): Reformulation of Elasticity Theory for Discontinuous and Long-Range Forces, *J. Mech. Phys. Solids* 48, 175-209.
2. Silling, S.A.; Epton, M.; Weckner, O.; Xu, J.; Askari, E. (2007): Peridynamic States and Constitutive Modeling, *J. Elasticity*, Springer, 88:151-184.

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