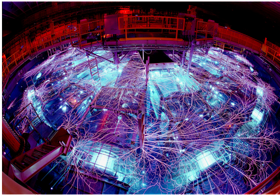
Laboratories

SAND2021-6324C



Constraints imposed by material stability for an anisotropic peridynamic model

SIAM Conference on Mathematical Aspects of Materials Science

Presenter: Jeremy Trageser (SNL)
Collaborator: Pablo Seleson (ORNL)

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND NO.

Outline

1. Goals
2. Classical linear elasticity
   - Symmetry classes
   - Material stability
3. Linear bond-based peridynamics
   - Symmetry classes
   - Material stability
   - Comparison of local and nonlocal
4. Future work
5. Conclusions and acknowledgments

Goals

Sandia National Laboratories

- Explore material stability conditions for an anisotropic linear peridynamic model.
- Develop conditions on the elasticity tensor which guarantee material stability in the peridynamic model.
- Compare material stability conditions between peridynamics and the local theory.

Classical Linear Elasticity

In linear elasticity stresses and strains are related via a generalized Hooke's Law:

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl} \tag{1}$$

$\boldsymbol{\sigma}$: stress tensor, ϵ: strain tensor, $\mathbb{C}$: elasticity tensor.
$\mathbb{C}$ has the following symmetries:

$$\text{Minor Symmetries}: \quad C_{ijkl} = C_{jikl} = C_{ijlk}$$

$$\text{Major Symmetry}: \quad C_{ijkl} = C_{klij}$$

Classical equation of motion:

$$\rho(\mathbf{x})\ddot{u}_i(\mathbf{x},t) = \frac{\partial}{\partial x_j}\sigma_{ij}(\mathbf{x},t) + b_i(\mathbf{x},t) = C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l}(\mathbf{x},t) + b_i(\mathbf{x},t)$$

ρ: mass density, $\mathbf{u}$: displacement, and $\mathbf{b}$: body force density.

Cauchy's Relations

- Term coined by Love in [1].
- Derived from a molecular description of materials assuming central forces between pairs of molecules.
- In two dimensions it is single relation between the elasticity constants in the elasticity tensor which forces $\mathbb{C}$ to be completely symmetric:

$$C_{1212} = C_{1122}$$

- Reduces the number of independent constants in $\mathbb{C}$ from 6 to 5.
- Determined to be invalid for the majority of materials.

[1] A. E. H. Love. *A Treatise on the Mathematical Theory of Elasticity, Volume I*. Cambridge University Press, 1892.

Symmetry Classes of $\mathbb{C}$

Definition

An orthogonal transformation $\mathbf{Q}$ between bases $\mathbf{e}$ and $\mathbf{e}'$ is called a symmetry transformation of the elasticity tensor $\mathbb{C}$ if

$$C_{ijkl} = Q_{ip}Q_{jq}Q_{kr}Q_{ls}C_{pqrs}. \quad (2)$$

Proposition

The set of symmetry transformations of $\mathbb{C}$ forms a group which we call a symmetry group of $\mathbb{C}$.

Definition

The symmetry class of $\mathbb{C}$ is the set of symmetry groups of $\mathbb{C}$ which are equivalent up to a change in orientation.

Theorem

There are exactly four symmetry classes of the elasticity tensor in two dimensions: oblique, rectangular, cubic, and isotropic [1].

[1] He, Q.C., Zheng, Q.S.: On the symmetries of 2D elastic and hyperelastic tensors. Journal of Elasticity 43(3), 203–225(1996).

The Symmetry Classes of 2D Linear Elasticity

Symmetry Class	Elasticity Tensor	Elasticity Tensor (Cauchy's relation imposed)
Oblique	$\begin{bmatrix} C_{11} & C_{12} & C_{16} \\ C_{12} & C_{22} & C_{26} \\ C_{16} & C_{26} & C_{66} \end{bmatrix}$	$\begin{bmatrix} C_{11} & C_{12} & C_{16} \\ C_{12} & C_{22} & C_{26} \\ C_{16} & C_{26} & C_{12} \end{bmatrix}$
Rectangular	$\begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{66} \end{bmatrix}$	$\begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{12} \end{bmatrix}$
Square	$\begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & C_{66} \end{bmatrix}$	$\begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & C_{12} \end{bmatrix}$
Isotropic	$\begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & \frac{C_{11}-C_{12}}{2} \end{bmatrix}$	$\begin{bmatrix} C_{11} & \frac{1}{3}C_{11} & 0 \\ \frac{1}{3}C_{11} & C_{11} & 0 \\ 0 & 0 & \frac{1}{3}C_{11} \end{bmatrix}$

Stability in Classical Linear Elasticity

Strain energy density:

$$W = \frac{1}{2} C_{ij} \varepsilon_i \varepsilon_j. \tag{3}$$

In the absence of external loads, the condition for material stability is:

$$W > 0, \quad \forall \boldsymbol{\varepsilon} \neq \mathbf{0}.$$

The quadratic form (3) is positive if and only if the elasticity matrix **C** is positive definite.

Theorem (Sylvester's criterion)

A symmetric matrix is positive definite if and only if its leading principal minors are positive.

Elastic Stability Criteria in 2D Linear Elasticity

Symmetry Class	Elastic Stability Criteria
Oblique	$C_{11} > 0, C_{11}C_{22} > C_{12}^2, \det(\mathbf{C}_{\text{obl}}) > 0$
Rectangular	$C_{11} > 0, C_{66} > 0, C_{11}C_{22} > C_{12}^2$
Square	$C_{11} > \lvert C_{12}\rvert, C_{66} > 0$
Isotropic	$C_{11} > \lvert C_{12}\rvert$

Table 1: Without Cauchy's relation imposed.

Symmetry Class	Elastic Stability Criteria
Oblique	$C_{11} > 0, C_{11}C_{22} > C_{12}^2, \det(\tilde{\mathbf{C}}_{\text{obl}}) > 0$
Rectangular	$C_{11} > 0, C_{12} > 0, C_{11}C_{22} > C_{12}^2$
Square	$C_{11} > C_{12} > 0$
Isotropic	$C_{11} > 0$

Table 2: With Cauchy's relation imposed

Linear Bond-Based Peridynamic Equation of Motion

Given a pairwise equilibrated reference configuration, the linear bond-based peridynamic equation of motion is:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}} \lambda(\boldsymbol{\xi})\,(\boldsymbol{\xi}\otimes\boldsymbol{\xi})\,(\mathbf{u}(\mathbf{x}+\boldsymbol{\xi},t)-\mathbf{u}(\mathbf{x},t))dV_{\boldsymbol{\xi}} + \mathbf{b}(\mathbf{x},t).$$

ρ: mass density, $\mathbf{u}$: displacement, $\boldsymbol{\xi}$: peridynamic bond,
λ: micromodulus, $\mathcal{H}$: peridynamic neighborhood, $\mathbf{b}$: body force.
Relationship between the micromodulus and elasticity tensor:

$$C_{ijkl} = \frac{1}{2}\int_{\mathcal{H}} \lambda(\boldsymbol{\xi})\xi_i\xi_j\xi_k\xi_l d\boldsymbol{\xi}. \tag{4}$$

Definition

An orthogonal transformation **Q** is a symmetry transformation of the micromodulus function $\lambda(\boldsymbol{\xi})$ if

$$\lambda(\mathbf{Q}\xi) = \lambda(\boldsymbol{\xi}),\ \forall\boldsymbol{\xi}\in\mathbb{R}^d. \tag{5}$$

Anisotropic Micromodulus

We propose a micromodulus of the form

$$\lambda(\boldsymbol{\xi}) = \frac{1}{m}\frac{\omega(\|\boldsymbol{\xi}\|)}{\|\boldsymbol{\xi}\|^2}\frac{(\boldsymbol{\xi}\otimes\boldsymbol{\xi})\boldsymbol{\Lambda}(\boldsymbol{\xi}\otimes\boldsymbol{\xi})}{\|\boldsymbol{\xi}\|^4} = \frac{1}{m}\frac{\omega(\|\boldsymbol{\xi}\|)}{\|\boldsymbol{\xi}\|^2}\frac{\xi_i\xi_j\xi_k\xi_l\Lambda_{ijkl}}{\|\boldsymbol{\xi}\|^4}$$

where $\boldsymbol{\Lambda}$ is a completely symmetric fourth-order tensor.

Using the relationship between $\lambda(\boldsymbol{\xi})$ and $\mathbb{C}$, we find

$$\begin{bmatrix}\Lambda_{1111}\\ \Lambda_{2222}\\ \Lambda_{1122}\end{bmatrix} = \begin{bmatrix}10 & -20 & 2\\ -\frac{10}{3} & \frac{76}{3} & -\frac{10}{3}\\ 2 & -20 & 10\end{bmatrix}\begin{bmatrix}C_{1111}\\ C_{2222}\\ C_{1122}\end{bmatrix}$$

$$\begin{bmatrix}\Lambda_{1112}\\ \Lambda_{2212}\end{bmatrix} = \begin{bmatrix}20 & -12\\ -12 & 20\end{bmatrix}\begin{bmatrix}C_{1112}\\ C_{2212}\end{bmatrix}$$

Material Stability in Peridynamics

The linear bond-based peridynamic material is stable if speeds are real for all plane waves [2]. Substituting an arbitrary plane wave

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{a} e^{i(k\mathbf{N}\cdot\mathbf{x} - \omega t)},$$

into the linear bond-based peridynamic equation of motion with null body force results in:

$$\rho\omega^2 \mathbf{a} = \mathbf{M}(\mathbf{N}, \kappa)\mathbf{a}, \qquad (6)$$

where

$$\mathbf{M}(\mathbf{N}, \kappa) := \int_{\mathcal{H}} \lambda(\boldsymbol{\xi})\boldsymbol{\xi} \otimes \boldsymbol{\xi} \left(1 - \cos\left(\kappa\mathbf{N} \cdot \boldsymbol{\xi}\right)\right) dV_{\boldsymbol{\xi}}. \qquad (7)$$

The eigenvalues of $\mathbf{M}(\mathbf{N}, \kappa)$ are $\rho\omega^2 = \rho c^2 \kappa^2$. To ensure propagation of waves at all wavelengths, it is necessary and sufficient for $\mathbf{M}(\mathbf{N}, \kappa)$ to be positive definite.

[2] S. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48, 175-209, 2000.

Sufficient Condition for Material Stability

Proposition

If $\lambda(\boldsymbol{\xi}) \geq 0$ is positive on a set of nonzero measure, then $\mathbf{M}(\mathbf{N}, \kappa)$ is positive definite.

Proof.

Let $K(\boldsymbol{\xi}) := \lambda(\boldsymbol{\xi})\,(1 - \cos(\kappa \mathbf{N} \cdot \boldsymbol{\xi}))$ so that $M_{ij} = \int_{\mathcal{H}} \xi_i \xi_j K(\boldsymbol{\xi}) d\boldsymbol{\xi}$.
Sylvester's criterion:

$$M_{11} = \int_{\mathcal{H}} \xi_1^2 K(\boldsymbol{\xi}) d\boldsymbol{\xi} > 0$$

and

$$\begin{aligned} 2(M_{11}M_{22} - M_{12}^2) = & \int_{\mathcal{H}} \xi_1^2 K(\boldsymbol{\xi}) d\boldsymbol{\xi} \int_{\mathcal{H}} \zeta_2^2 K(\boldsymbol{\zeta}) d\boldsymbol{\zeta} + \int_{\mathcal{H}} \xi_2^2 K(\boldsymbol{\xi}) d\boldsymbol{\xi} \int_{\mathcal{H}} \zeta_1^2 K(\boldsymbol{\zeta}) d\boldsymbol{\zeta} \\ & - 2 \int_{\mathcal{H}} \xi_1 \xi_2 K(\boldsymbol{\xi}) d\boldsymbol{\xi} \int_{\mathcal{H}} \zeta_1 \zeta_2 K(\boldsymbol{\zeta}) d\boldsymbol{\zeta} \\ = & \int_{\mathcal{H}} \int_{\mathcal{H}} (\xi_1 \zeta_2 - \xi_2 \zeta_2)^2 K(\boldsymbol{\xi}) K(\boldsymbol{\zeta}) d\boldsymbol{\xi} d\boldsymbol{\zeta} > 0 \end{aligned}$$

Sufficient Condition for Material Stability

We consider positivity of the oblique micromodulus

$$\lambda(\boldsymbol{\xi}) = \frac{1}{m} \frac{\Lambda_{11}\xi_1^4 + 4\Lambda_{16}\xi_1^3\xi_2 + 6\Lambda_{12}\xi_1^2\xi_2^2 + 4\Lambda_{26}\xi_1\xi_2^3 + \Lambda_{22}\xi_2^4}{\|\boldsymbol{\xi}\|^4} \frac{\omega(\|\boldsymbol{\xi}\|)}{\|\boldsymbol{\xi}\|^2}.$$

For this study we focused on the angular portion of the micromodulus and thus we need to determine the positivity of a quartic polynomial.

Theorem ([3])

The quartic function $f(z) = z^4 + 2az^2 + 2bz + c$ is nonnegative for all z if and only if $c \geq 0$ and

$$|b| \leq \frac{2}{3\sqrt{3}} \left(-a + \sqrt{a^2 + 3c}\right)^{\frac{1}{2}} \left(2a + \sqrt{a^2 + 3c}\right).$$

[3] V. Powers and B. Reznick. Notes towards a constructive proof of Hilbert's Theorem on ternary quartics. *Contemp. Math*, 272, 209-227, 1999.

Sufficient Condition for Material Stability

Theorem

The oblique micromodulus function is nonnegative if and only if one of the following conditions holds:

1. $\Lambda_{11} = \Lambda_{22} = \Lambda_{16} = \Lambda_{26} = 0, \Lambda_{12} > 0$.
2. $\Lambda_{11} = \Lambda_{16} = 0, \Lambda_{22} > 0, \Lambda_{12}\Lambda_{22} \geqslant \frac{2}{3}\Lambda_{26}^2$.
3. $\Lambda_{11} > 0, \Lambda_{22} \geqslant 0, c \geqslant 0$, *and*

   $|b| \leqslant \frac{2}{3\sqrt{3}} \left(-a + \sqrt{a^2 + 3c}\right)^{\frac{1}{2}} \left(2a + \sqrt{a^2 + 3c}\right)$ *where*

   $$a := -3\,\frac{{\Lambda_{16}}^2}{{\Lambda_{11}}^2} + 3\,\frac{\Lambda_{12}}{\Lambda_{11}}, \quad b := 4\,\frac{{\Lambda_{16}}^3}{{\Lambda_{11}}^3} - 6\,\frac{\Lambda_{12}\Lambda_{16}}{{\Lambda_{11}}^2} + 2\,\frac{\Lambda_{26}}{\Lambda_{11}}$$

   $$c := -3\,\frac{{\Lambda_{16}}^4}{{\Lambda_{11}}^4} + 6\,\frac{\Lambda_{12}{\Lambda_{16}}^2}{{\Lambda_{11}}^3} - 4\,\frac{\Lambda_{16}\Lambda_{26}}{{\Lambda_{11}}^2} + \frac{\Lambda_{22}}{\Lambda_{11}}$$

Micromodulus Positivity Requirements

Sandia National Laboratories

Corollary (Rectangular)

The rectangular micromodulus is nonnegative if and only if one of the following conditions holds:

1. $\Lambda_{11}, \Lambda_{22}, \Lambda_{12}$ *are all nonnegative.*
2. $\Lambda_{11} > 0, \Lambda_{12} < 0$*, and* $9\Lambda_{12}^2 \leqslant \Lambda_{11}\Lambda_{22}$*.*

Corollary (Square)

The square micromodulus is nonnegative if and only if one of the following conditions holds:

1. Λ_{11} *and* Λ_{12} *are nonnegative.*
2. $\Lambda_{12} < 0$ *and* $-3\Lambda_{12} \leqslant \Lambda_{11}$*.*

Corollary (Isotropic)

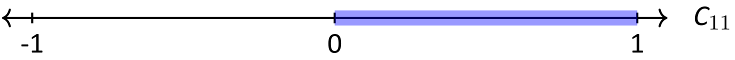
The isotropic micromodulus is nonnegative if and only if $\Lambda_{11} > 0$*.*

Comparison With Classical (Isotropic)

Corollary (Isotropic)

The isotropic micromodulus is nonnegative if and only if $C_{11} > 0$.

Stability in classical linear elasticity: $(C_{11} > 0)$



Region of stability on $B_1(0)$ for isotropic symmetry.

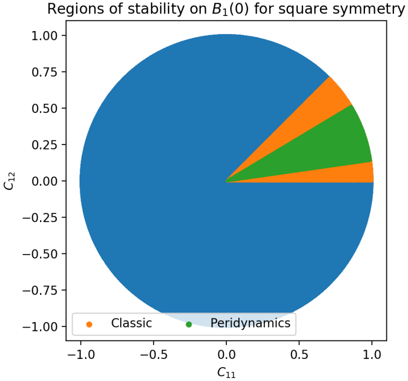
Comparison With Classical (Square)

Corollary (Square)

The square micromodulus is nonnegative if and only if:

$$\frac{1}{7}C_{11} < C_{12} < \frac{3}{5}C_{11}.$$

Stability in classical linear elasticity: $(C_{11} > C_{12} > 0)$



Comparison With Local (Rectangular)

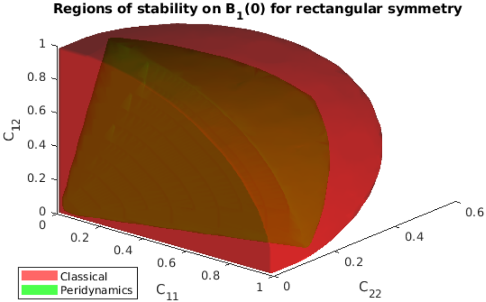
Corollary (Rectangular)

The rectangular micromodulus is nonnegative if and only if:

1. $\frac{5}{38}(C_{11}+C_{22}) \leqslant C_{12} \leqslant \min\left\{\frac{1}{2}C_{11}+\frac{1}{10}C_{22}, \frac{1}{10}C_{11}+\frac{1}{2}C_{22}\right\}$
2. $C_{12} < \min\left\{\frac{1}{2}C_{11}+\frac{1}{10}C_{22}, \frac{1}{10}C_{11}+\frac{1}{2}C_{22}, \frac{5}{38}(C_{11}+C_{22})\right\}$ *and*

   $(84C_{12} - 10(C_{11}+C_{22}))^2 \leqslant -5\left(C_{11}^2 + C_{22}^2\right) + 74C_{11}C_{22}.$

Stability in classical linear elasticity: $C_{11} > 0, C_{12} > 0, C_{11}C_{22} > C_{12}^2$



Future work

- Show positivity of the anisotropic kernel is more restrictive than elastic stability in classical linear elasticity for oblique symmetry.
- Explore the full material stability picture for the anisotropic kernel.
- Explore material stability dependence on the influence function.
- Explore material stability for a micromodulus which potentially changes signs angularly and radially.
- Involve external forces in the calculations.

Conclusions and Acknowledgements

- Explored material stability for a two-dimensional anisotropic peridynamic model.
- Proved that positivity of the rectangular micromodulus is more restrictive than material stability in classical linear elasticity.
- Numerically explored stability for possibly sign changing micromodulus.

Acknowledgments

- Laboratory Directed Research and Development program at the Oak Ridge National Laboratory.
- U.S. Defense Advanced Research Projects Agency (DARPA) (contract HR0011619523 and award 1868-A017-15)