SAND2022-8769C

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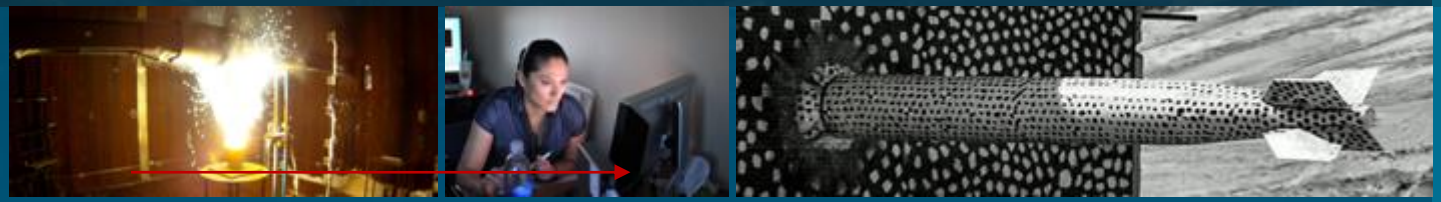
Peridynamic modeling of multilayer graphene



Stewart Silling

July 11, 2022
SIAM AN22
Pittsburgh, PA

SAND2022-xxxxx

U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

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Outline

- Strategy for coarse graining of molecular dynamics (MD) into peridynamics.
- New peridynamic state-based material model.
- Mix-and-match state-based and bond-based terms for different physical effects in the same model.
- Examples.

Motivation

- There has been a lot of MD work on graphene.
- MD is not practical for many engineering applications.
- Find a material model within a continuum theory.

Acknowledgments

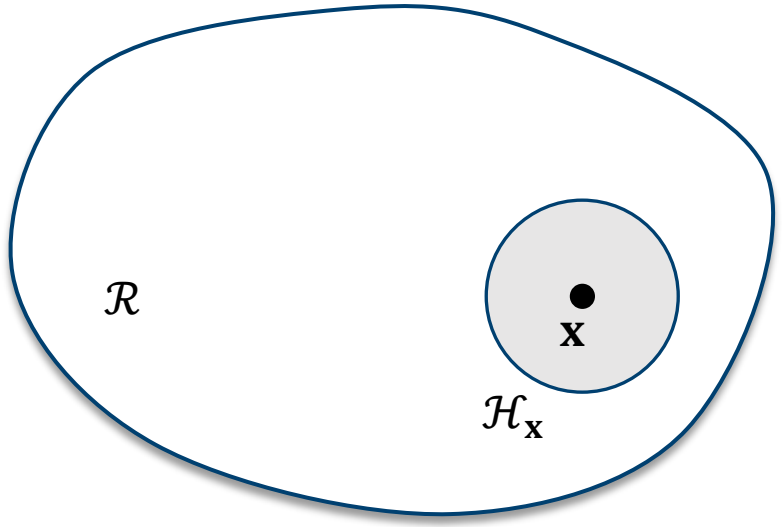
Muge Fermen-Coker (ARL), Yue Yu, Huaiqian You (Lehigh Univ), Marta D'Elia (Sandia)

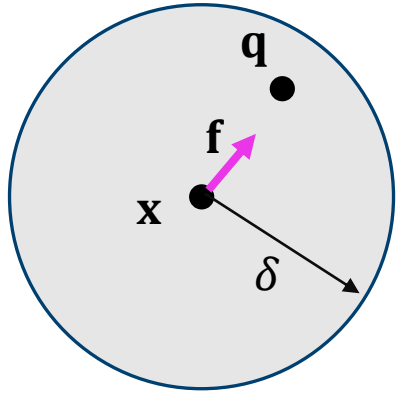
Peridynamics background

- Peridynamic momentum balance in 3D:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}_\mathbf{x}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\, d\mathbf{q} + \mathbf{b}(\mathbf{x},t) \qquad \forall \mathbf{x} \in \mathcal{R},\ t \geq 0.$$

- $\mathbf{f}$ is the *pairwise bond force density* of the *bond* from $\mathbf{q}$ to $\mathbf{x}$.
- $\mathcal{H}_\mathbf{x}$ is the *family* of $\mathbf{x}$, which is a ball centered at $\mathbf{x}$ with radius δ (the *horizon*).





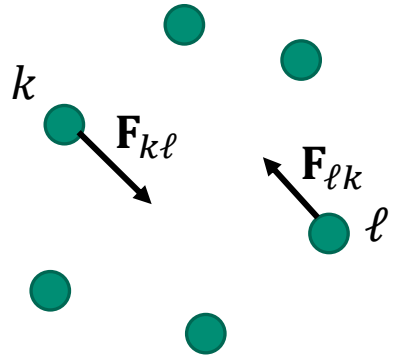
Coarse graining of MD into peridynamics

- Consider a set of discrete particles that exert forces $\mathbf{F}_{k\ell}(t)$ on each other,

$$\mathbf{F}_{\ell k}(t) = -\mathbf{F}_{k\ell}(t).$$

- Particles are subjected to external forces $\mathbf{B}_k(t)$.
- The particles obey Newton's second law,

$$M_k \ddot{\mathbf{u}}_k(t) = \sum_{\ell} \mathbf{F}_{k\ell}(t) + \mathbf{B}_k(t).$$

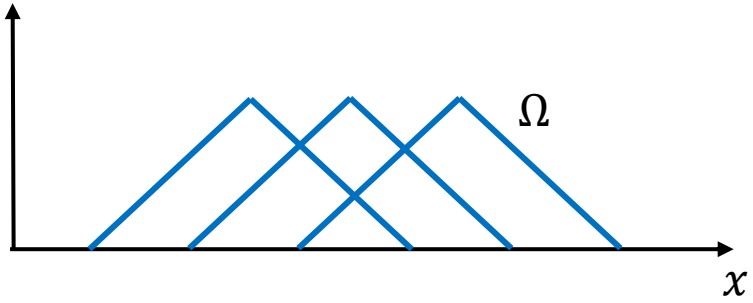


- Define smoothing functions $\Omega(\mathbf{x}, \cdot)$ normalized such that

$$\int \Omega(\mathbf{x}, \mathbf{p})\, \mathrm{d}\mathbf{x} = 1 \qquad \forall \mathbf{p}.$$

Center of smoothing function

Atom position



- This derivation: SS, Chapter 1 in *Peridynamic Modeling, Numerical Techniques, & Applications*, E. Oterkus, ed., Elsevier (2021).
- Statistical physics derivation: R. B. Lehoucq & M. P. Sears, *Physical Review E* (2011).

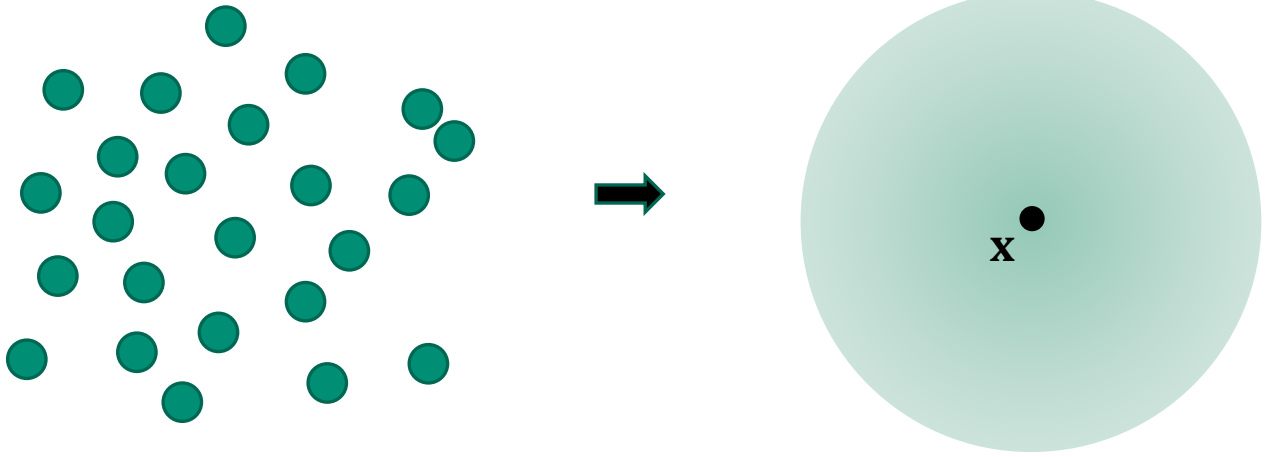
Continuous density, external force, and displacement

- Define the smoothed mass density and body force density fields by

$$\rho(\mathbf{x}) = \sum_k \Omega(\mathbf{x}, \mathbf{x}_k) M_k, \qquad \mathbf{b}(\mathbf{x}, t) = \sum_k \Omega(\mathbf{x}, \mathbf{x}_k) \mathbf{B}_k(t).$$

- Define the smoothed displacement field by

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x})} \sum_k \Omega(\mathbf{x}, \mathbf{x}_k) M_k \mathbf{u}_k(t).$$



Atoms

Each $\mathbf{u}(\mathbf{x})$ represents a weighted average of atomic displacements

Smoothed displacements follow a nonlocal evolution law

- Combine all of the above, find

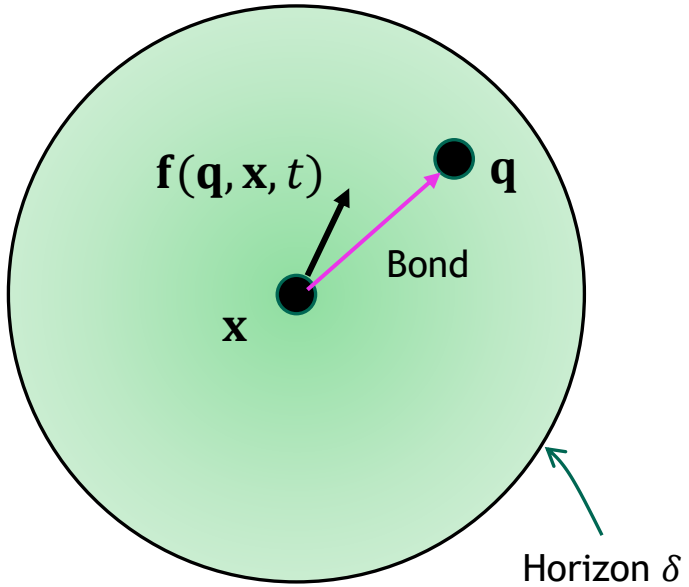
$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int \mathbf{f}(\mathbf{q},\mathbf{x},t)\,\mathrm{d}\mathbf{q} + \mathbf{b}(\mathbf{x},t) \qquad (1)$$

where

$$\mathbf{f}(\mathbf{q},\mathbf{x},t) = \sum_k \sum_\ell \Omega(\mathbf{x},\mathbf{x}_k)\Omega(\mathbf{q},\mathbf{x}_\ell)\mathbf{F}_{k\ell}(t).$$

- Observe

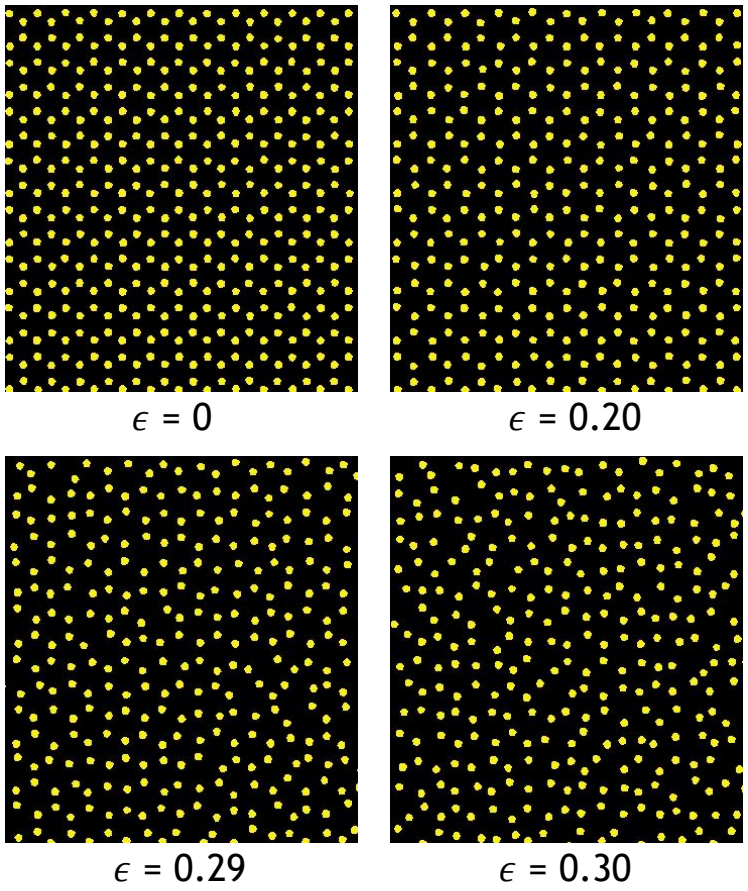
$$\mathbf{f}(\mathbf{q},\mathbf{x},t) = -\mathbf{f}(\mathbf{x},\mathbf{q},t) \qquad \forall \mathbf{x},\mathbf{q},t.$$

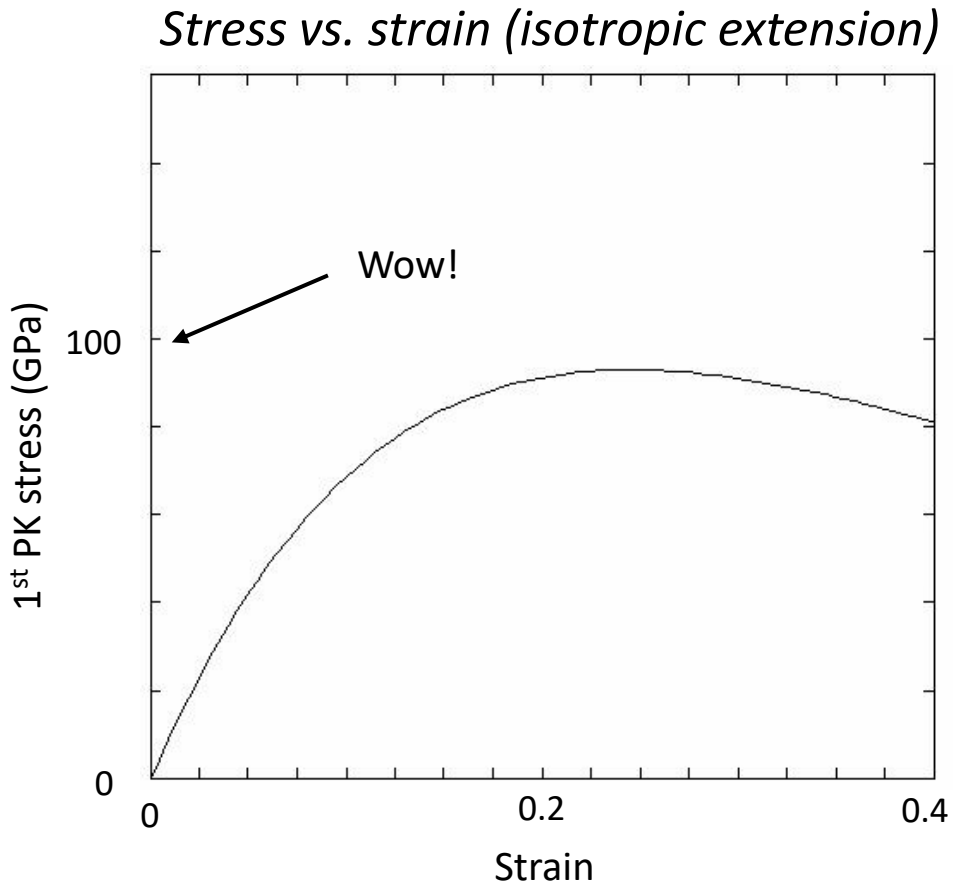


- We will use these **f** values from MD to calibrate a peridynamic material model.

MD model of single-sheet graphene

- Tersoff potential*.
- In isotropic extension, the stress-strain curve reaches a maximum at a strain of about 0.24.



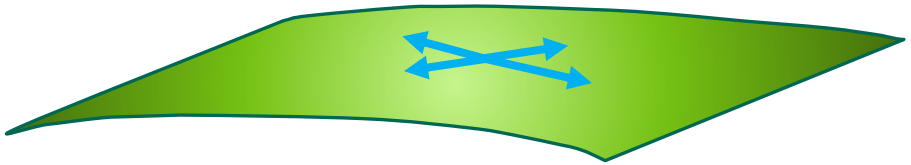


* J. Tersoff, *Physical Review Letters*(1988).

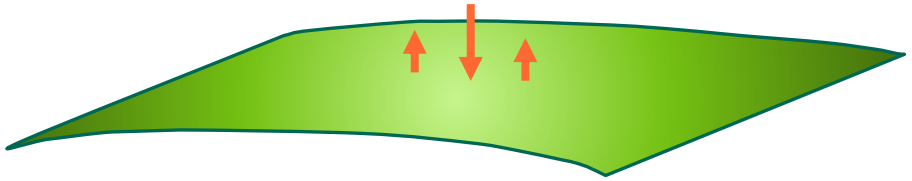
Peridynamic continuum material model

- Separate terms for
  - Stretching of the lattice
  - Bending
  - Adhesion
- Calibration with coarse grained MD bond forces.

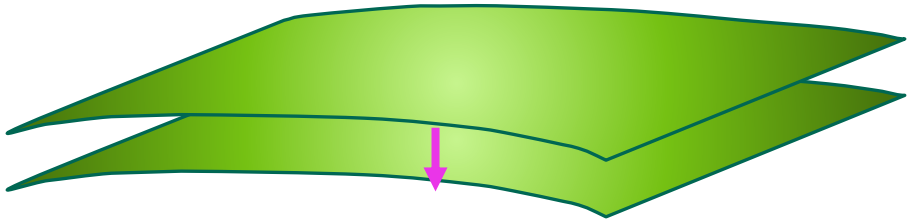
$$\mathbf{f} = \mathbf{f}_{\text{membrane}} + \mathbf{f}_{\text{bend}} + \mathbf{f}_{\text{adhesion}}$$



$\mathbf{f}_{\text{membrane}}$



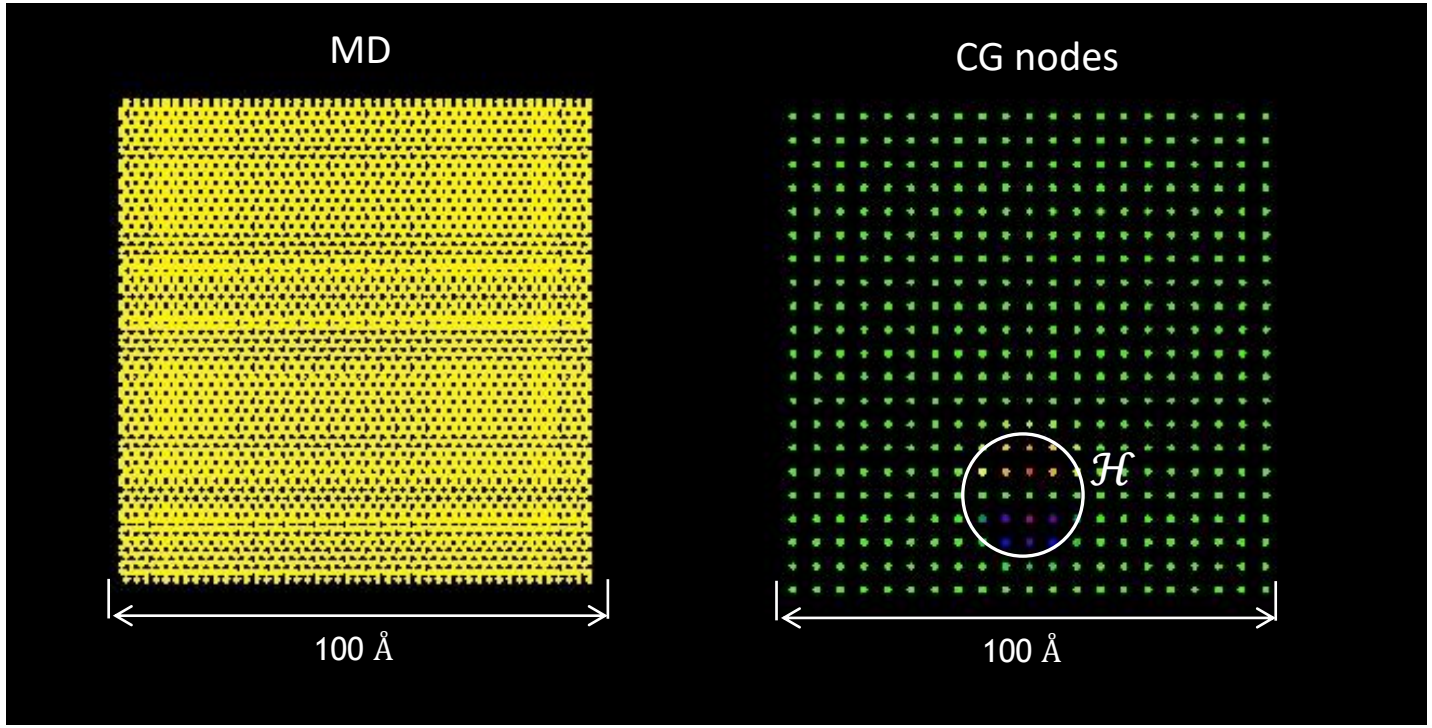
$\mathbf{f}_{\text{bend}}$



$\mathbf{f}_{\text{adhesion}}$

MD model of graphene: Coarse graining

- Perform MD modeling of a perfect graphene sheet under isotropic extension and uniaxial strain.
- Compute the smoothed (peridynamic) forces and displacements.
- Fit the forces to the bond strains.
- CG nodes have a spacing of about 5 Angstroms (≈ 4 atomic spacings).



Membrane forces: Ordinary state-based model*

- Bond force density in bond $\boldsymbol{\xi}$:

$$t = A\mathrm{R}(r)\mathrm{S}(s^+)\left[\left(1-\frac{\beta}{2}\right)s+\beta\bar{s}\right]$$

where $r = |\boldsymbol{\xi}|/\delta$.

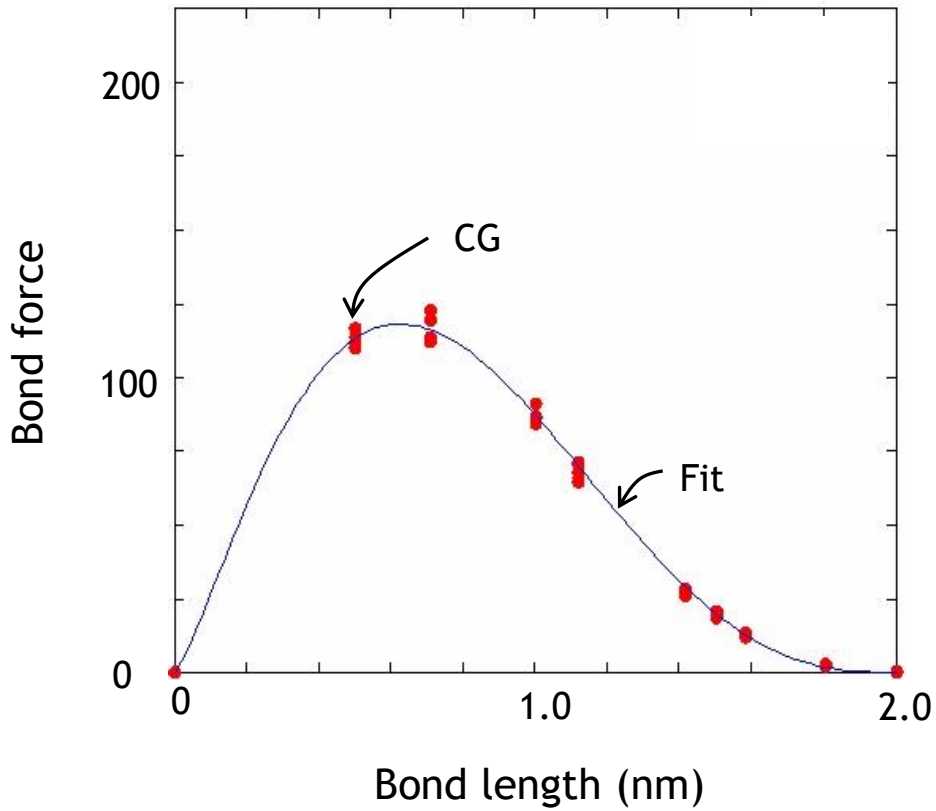
- s^+ is the *maximum* bond strain in the family.
- $\bar{s}$ is the *mean* bond strain in the family.
- The dependence on bond length is

$$\mathrm{R}(r) = r^{\mu_1}(1-r)^{\mu_2}.$$

- The softening term is

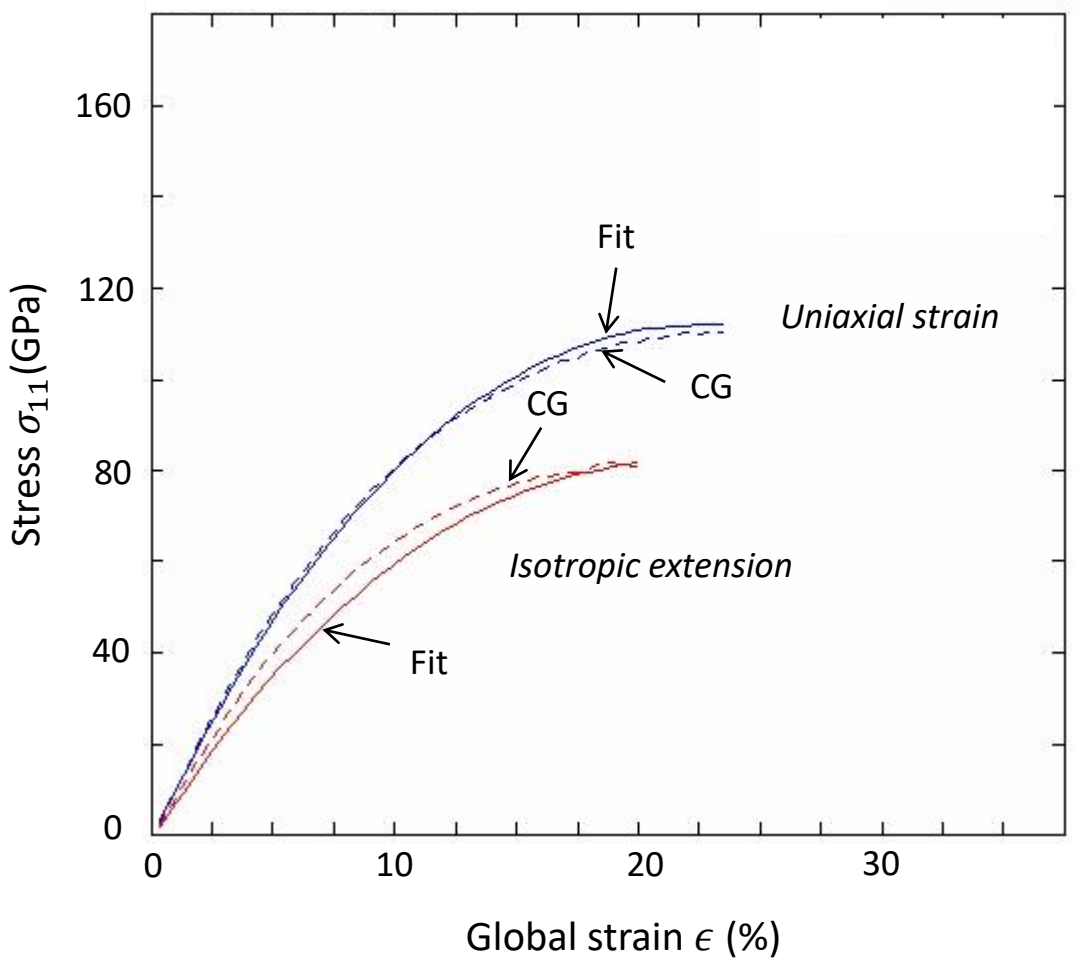
$$\mathrm{S}(p) = \begin{cases} n/s_0 & \text{if } p \le 0, \\ \dfrac{1}{p}\left(1-\left|1-\dfrac{p}{s_0}\right|^n\right) & \text{if } 0 < p < 2s_0, \\ 0 & \text{if } 2s_0 < p. \end{cases}$$

- A, β, μ_1, μ_2, s_0, and n are constants.



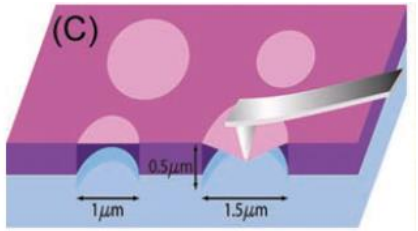
*SS et al. "Peridynamic Model for Single-Layer Graphene Obtained from Coarse-Grained Bond Forces." *Journal of Peridynamics and Nonlocal Modeling* (2022)

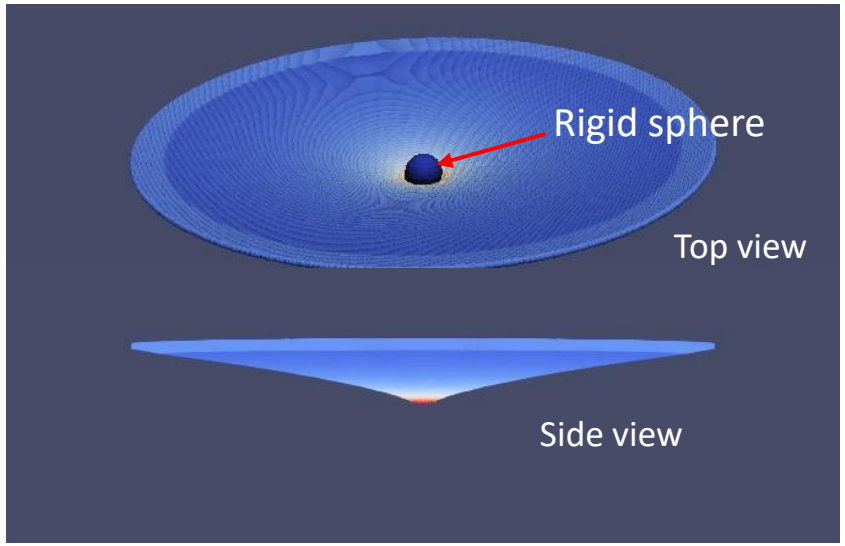
Fit of the softening and bond strain terms



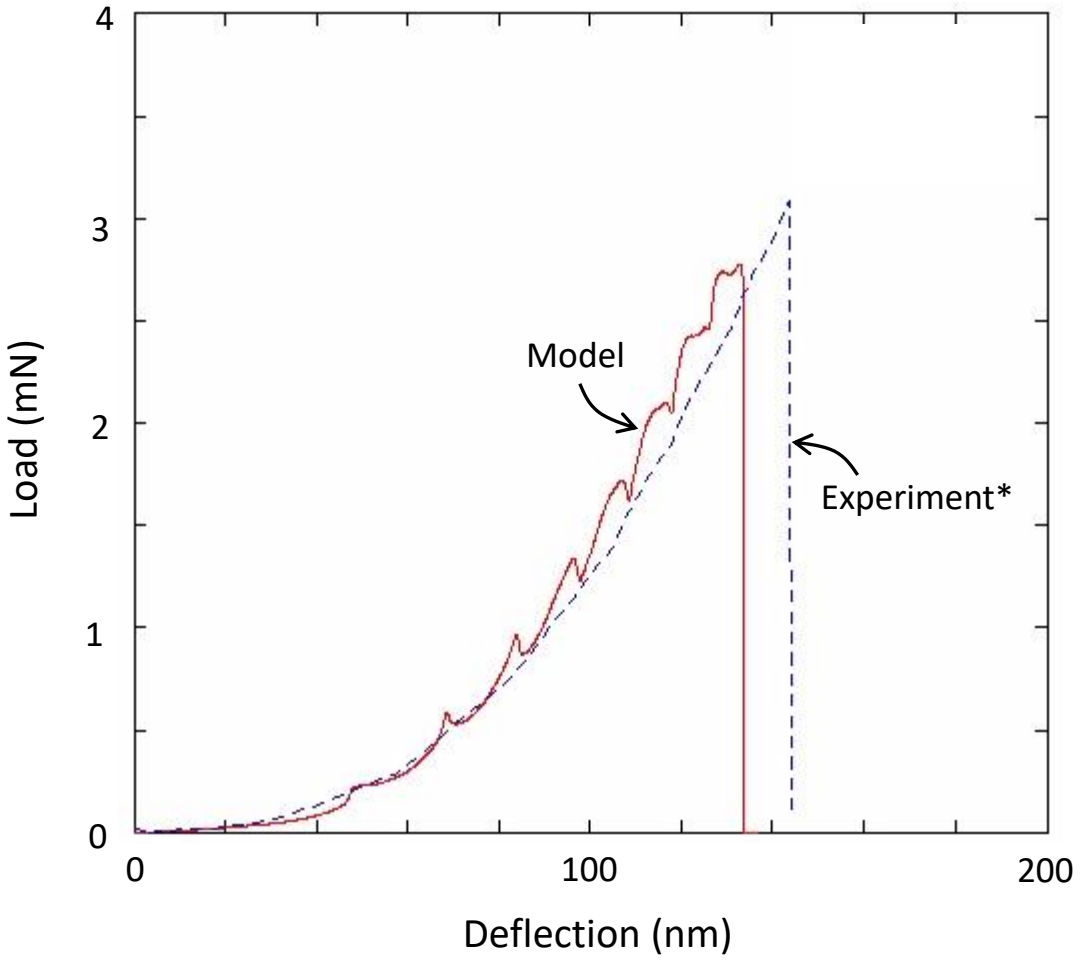
Comparison with experimental data for single-sheet graphene

- Atomic force microscope probe deflects a graphene sheet fixed at edges*.





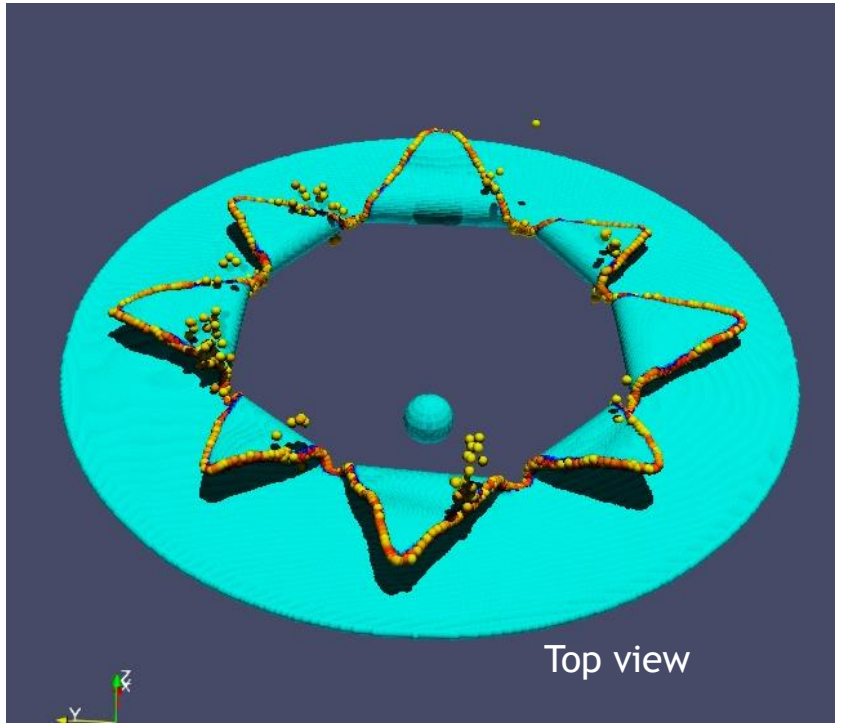
Colors show strain

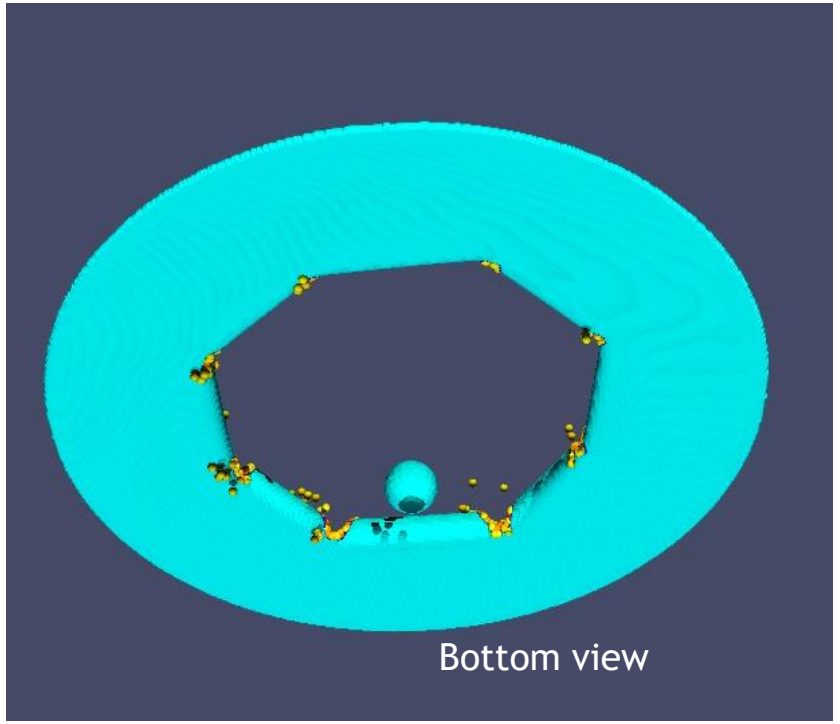


* C. Lee et al., *Science* (2008).

Post-failure graphene sheet

- Radial cracks result in petals.



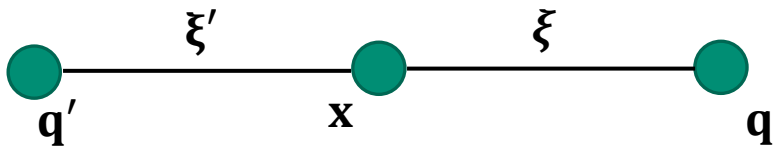


Colors show damage

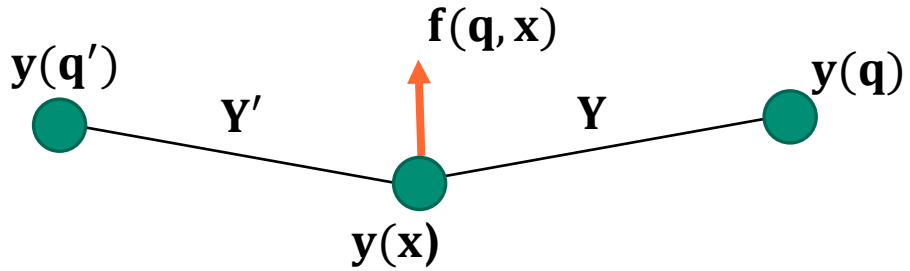
- C. Lee et al., *Science* (2008).

Now add bending to the peridynamic model

- Everything up to now was restricted to in-plane deformation.
- Now include bending – with single or multiple sheets.
- We can do this without adding rotational degrees of freedom.
- Use a non-ordinary state-based model that exerts out-of-plane forces that resist bending.*



Initial



Deformed

- J. O'Grady & J. Foster, *Intl J Solids & Structures* (2014).
- J. O'Grady & J. Foster, *Computational Mechanics* (2016).

NOSB peridynamic model for bending forces

- The bond forces in $\mathbf{f}_{\text{bend}}$ are out-of-plane and tend to resist bending:

$$\mathbf{f}_{\text{bend}}(\mathbf{x}+\boldsymbol{\xi},\mathbf{x}) = \mathbf{t}_{\text{bend}}(\mathbf{x}+\boldsymbol{\xi},\mathbf{x}) - \mathbf{t}_{\text{bend}}(\mathbf{x},\mathbf{x}+\boldsymbol{\xi}),$$

$$\mathbf{t}_{\text{bend}}(\mathbf{x}+\boldsymbol{\xi},\mathbf{x}) = \lambda r^2 \mathsf{R}(r) \frac{\mathbf{Y}\times(\mathbf{M}'\times\mathbf{M})}{|\mathbf{Y}|^2}$$

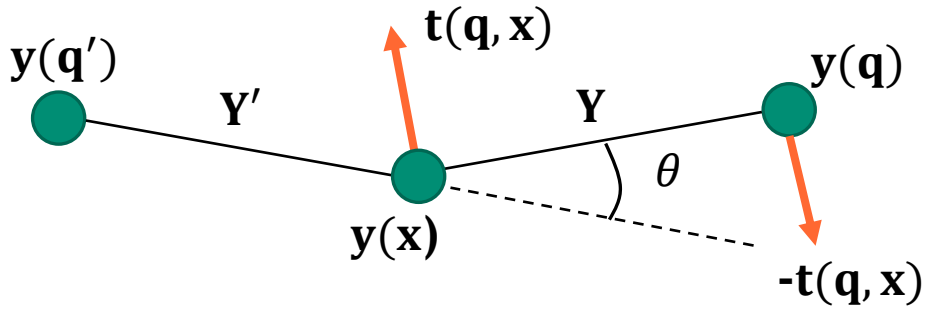
where λ is a constant, $r = |\boldsymbol{\xi}|/\delta$,

$$\mathbf{Y} = \mathbf{y}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{y}(\mathbf{x}), \qquad \mathbf{M} = \frac{\mathbf{Y}}{|\mathbf{Y}|}$$

and the prime denotes the "twin" bond $\boldsymbol{\xi}' = -\boldsymbol{\xi}$:

$$\mathbf{Y}' = \mathbf{y}(\mathbf{x}-\boldsymbol{\xi}) - \mathbf{y}(\mathbf{x}), \qquad \mathbf{M}' = \frac{\mathbf{Y}'}{|\mathbf{Y}'|}.$$

Numerator is basically the angle change

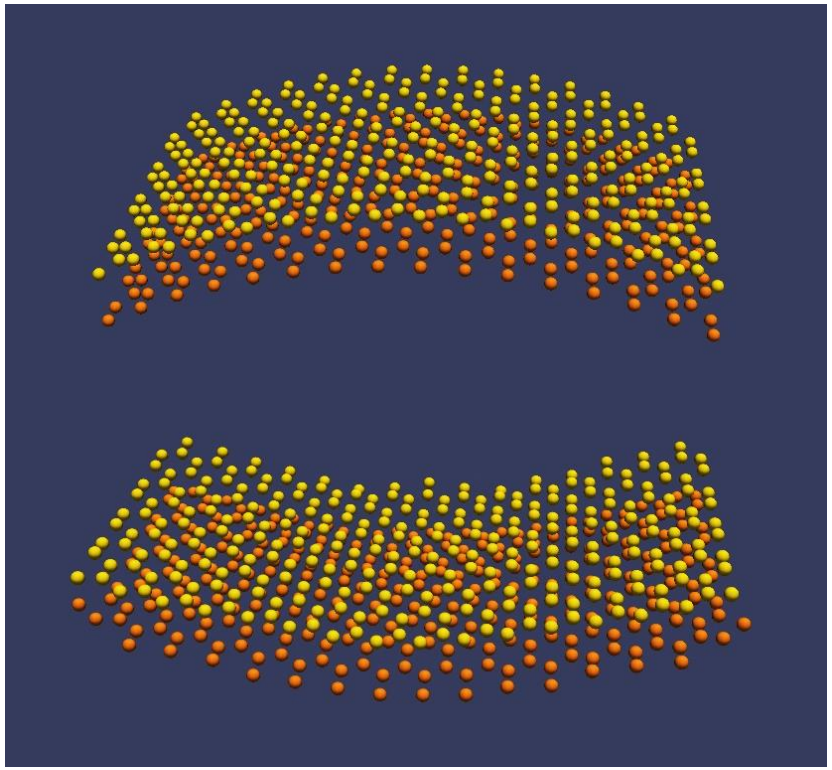


- J. O'Grady & J. Foster, *Intl J Solids & Structures* (2014).
- J. O'Grady & J. Foster, *Computational Mechanics* (2016).

Calibrating the NOSB bending model

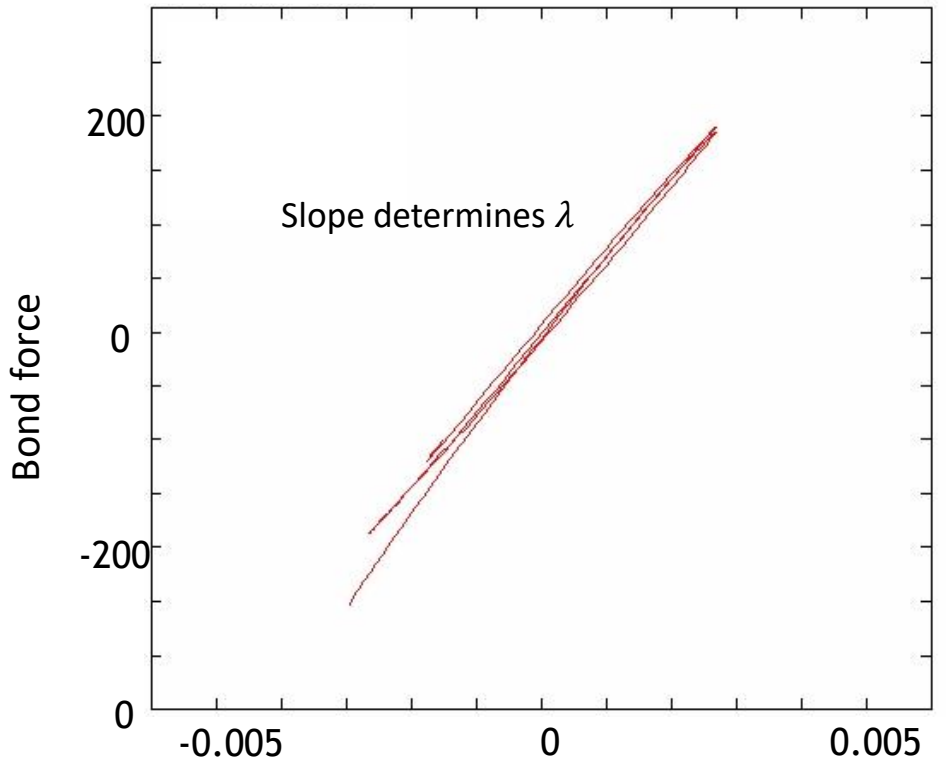
- It's hard to think up MD simulations where the membrane stresses don't mask the bending response in a curved sheet.
- Use free bending vibrations to avoid imposing boundary conditions.

Free bending mode vibrations in MD



Coarse graining

CG bending forces from MD



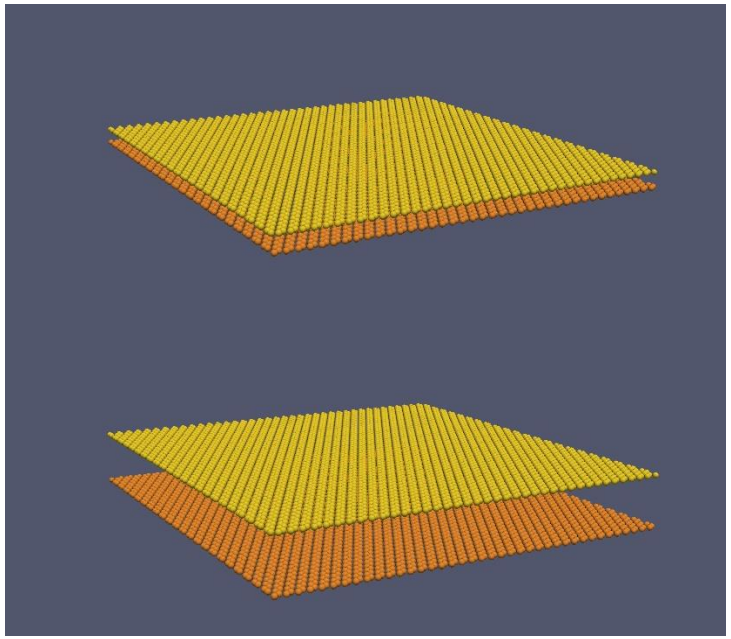
Adhesion between sheets

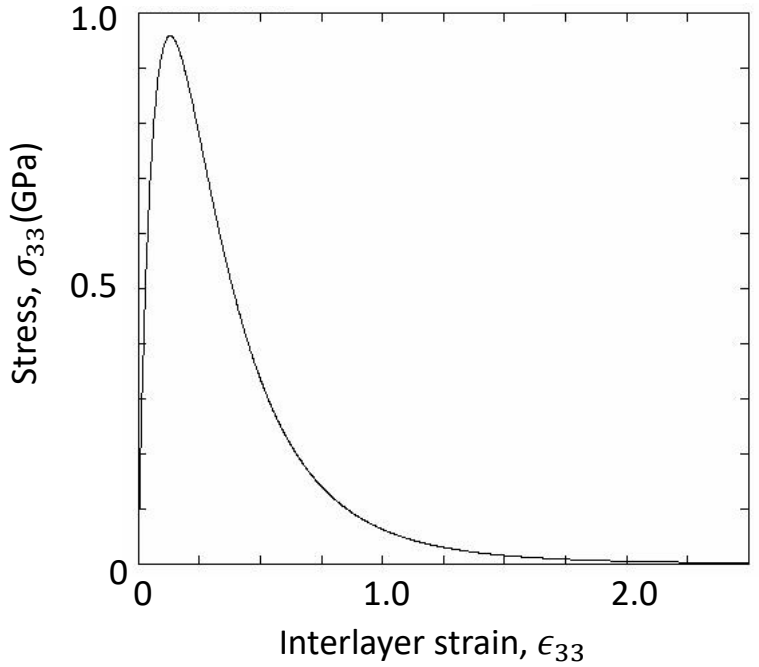
- Sheets adhere to each other by van der Waals forces.
  - These are much more compliant than the covalent bonds in the hex lattice.

$$E_{\text{membrane}} \approx 1000\text{GPa}, \qquad E_{\text{adhesion}} \approx 3\text{GPa}$$

  - Interlayer forces in MD are modeled with a Lennard-Jones potential.*

MD simulation of two sheets separating

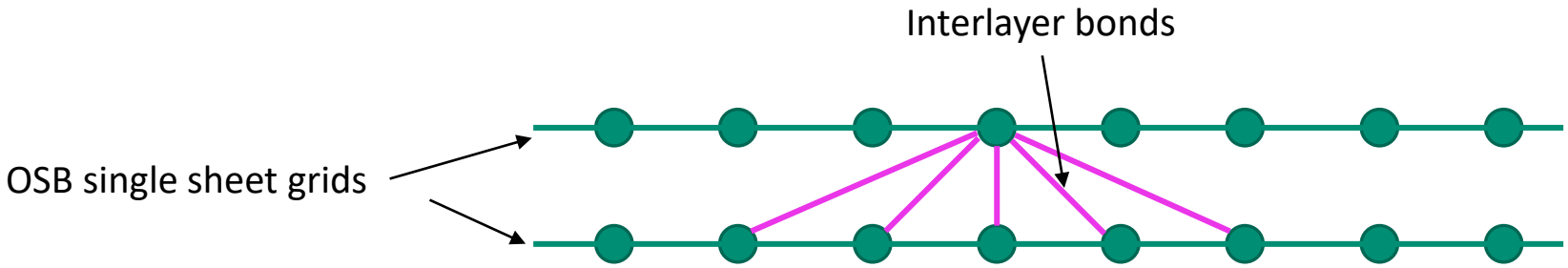


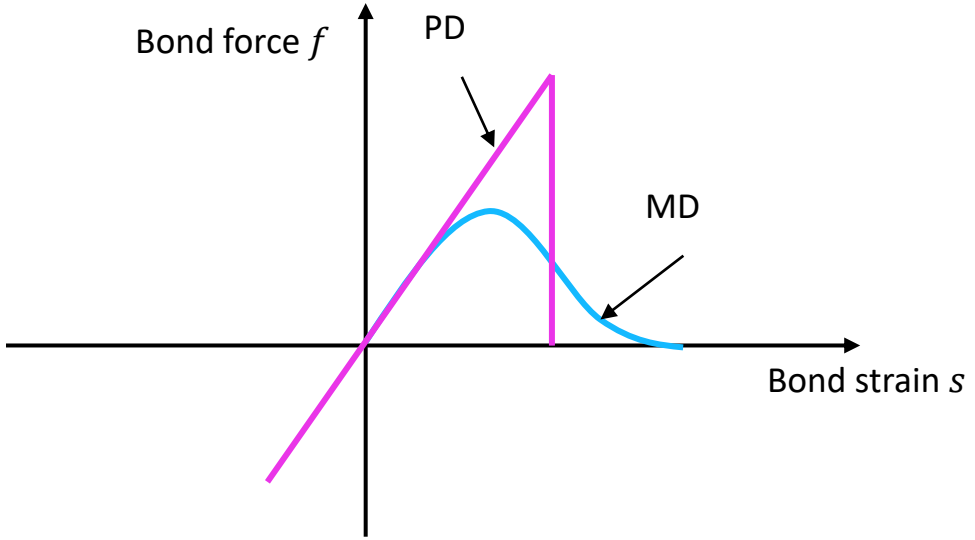


*S. J. Stuart et al., *J. Chem. Phys* (2000)

Bond-based model for adhesive forces

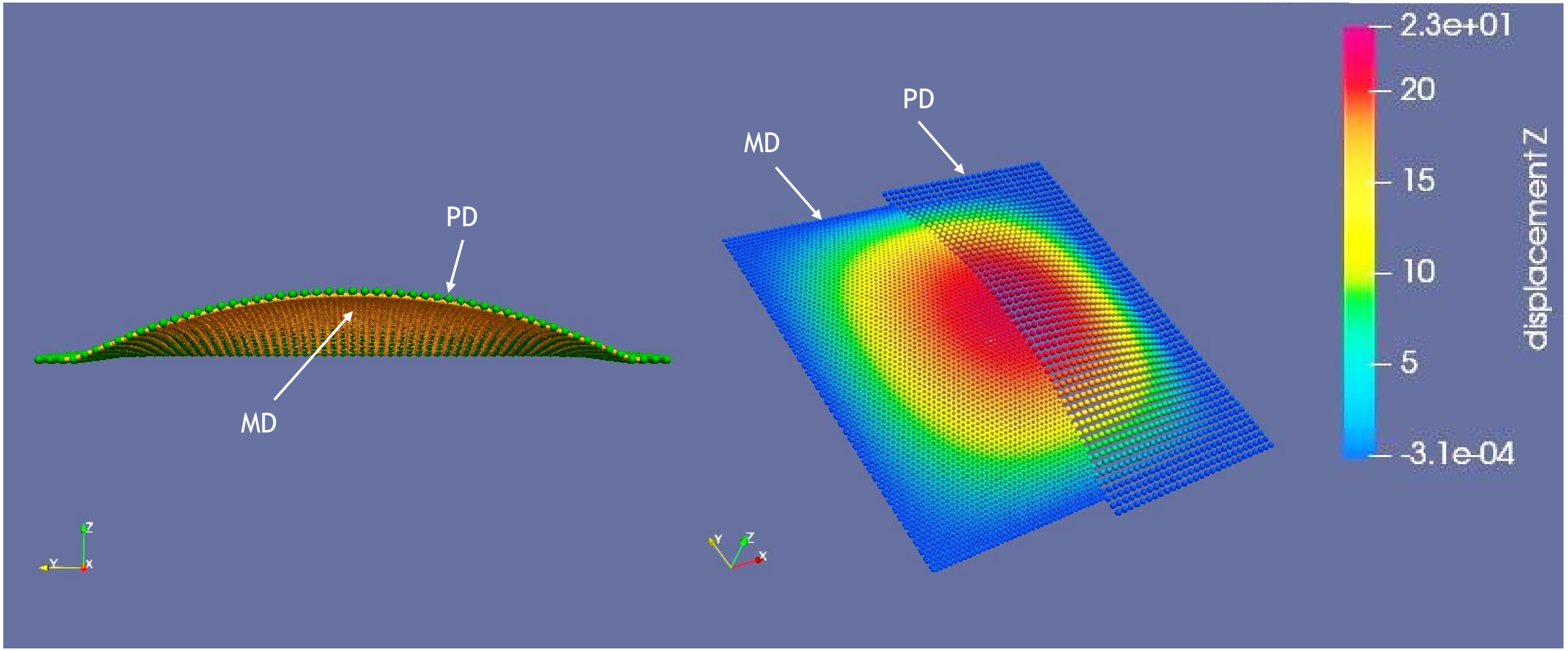
- $\mathbf{f}_{\text{adhesion}}$ is found from linear bond-based interactions.
- Calibrated to match MD results for elastic modulus and fracture energy (area under curve).





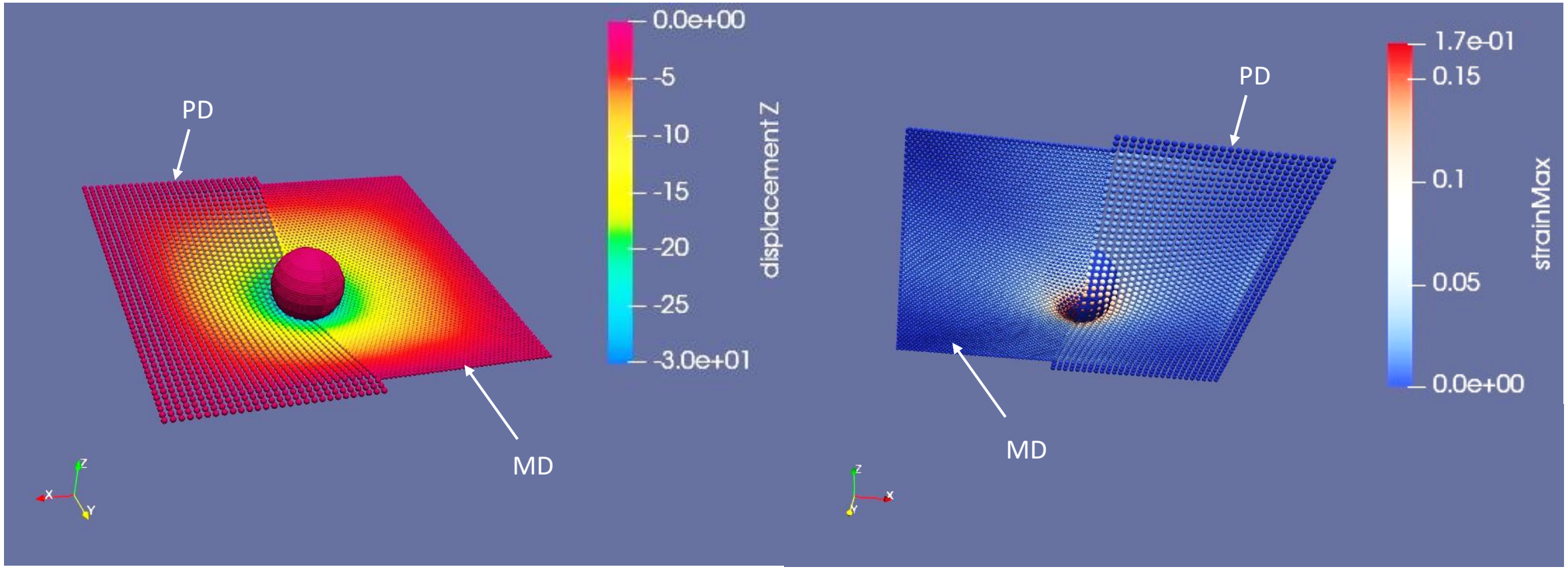
Verification: 2-layer film under transverse loading

- Compare the new peridynamic model with MD.



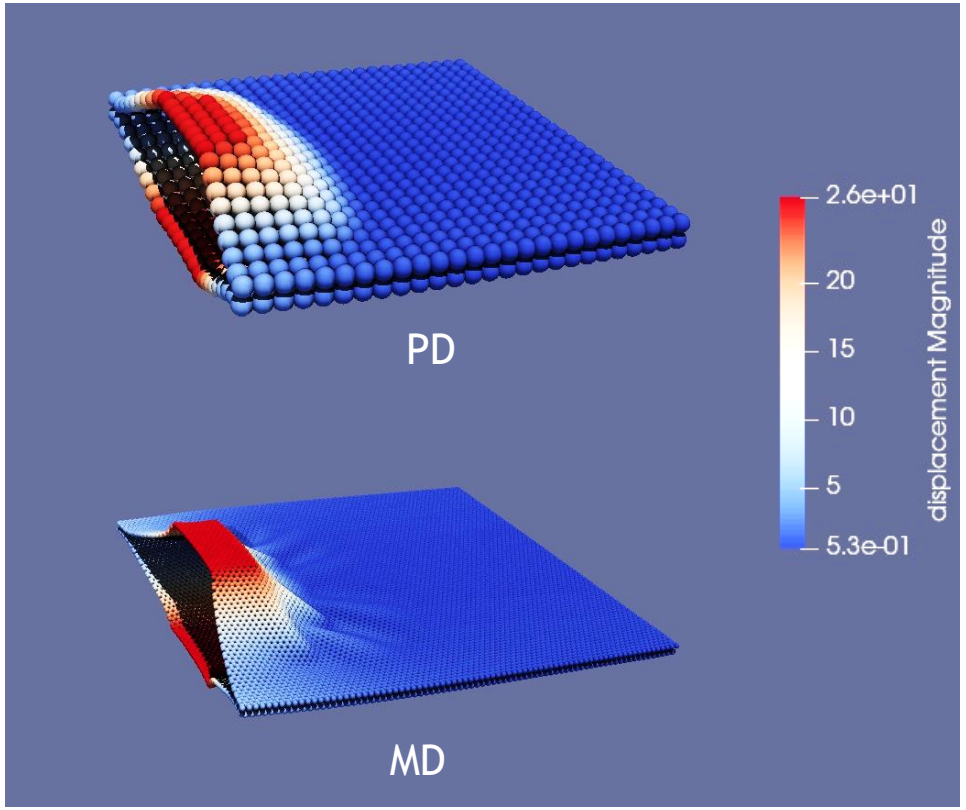
Verification: Impact of a sphere on a 2-layer film

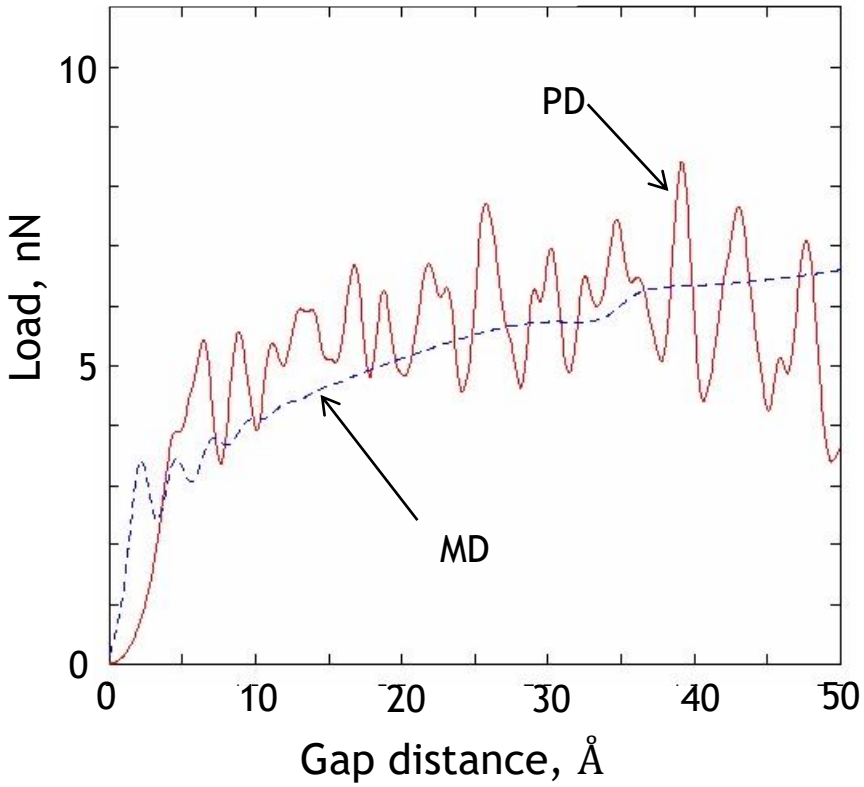
- Compare the new peridynamic model with MD.



Verification: Decohesion of two layers

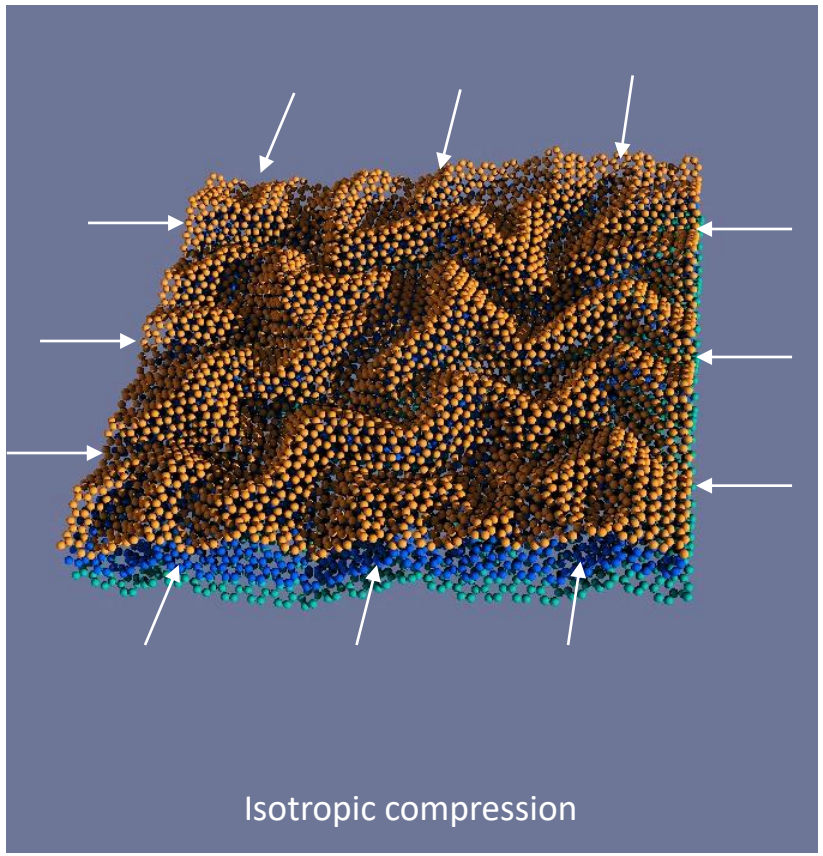
- Two rectangular subregions separate, creating a tent-like feature behind the advancing crack.



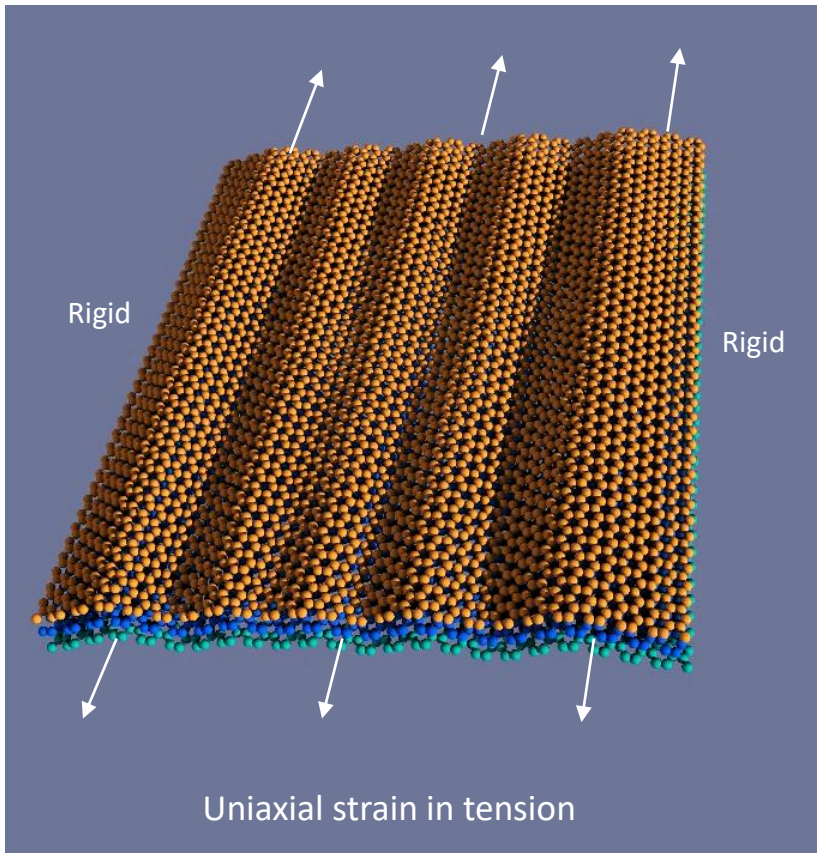


Wrinkling

- Buckling happens easily under compression due to low bending rigidity.
- Negative Poisson ratio makes the membrane try to puff out under tension.



Isotropic compression



Uniaxial strain in tension

Discussion

- The new material model adds bending and adhesive forces to the in-plane forces.
- Big reduction in computational resources over MD due to fewer nodes and larger time step size.
- Bond breakage criterion can be calibrated to get the right fracture energy.
- Machine learning was not used here but has been applied to develop nonlocal kernels for graphene in simpler cases*.

* H. You et al. "A data-driven peridynamic continuum model for upscaling molecular dynamics." *Computer Methods in Applied Mechanics and Engineering* (2022).