A bond-based peridynamics model for polymeric material fracture under finite deformation

Caglar Tamur, Shaofan Li

Department of Civil and Environmental Engineering, University of California, Berkeley

caglar.tamur@berkeley.edu, shaofan@berkeley.edu

Introduction

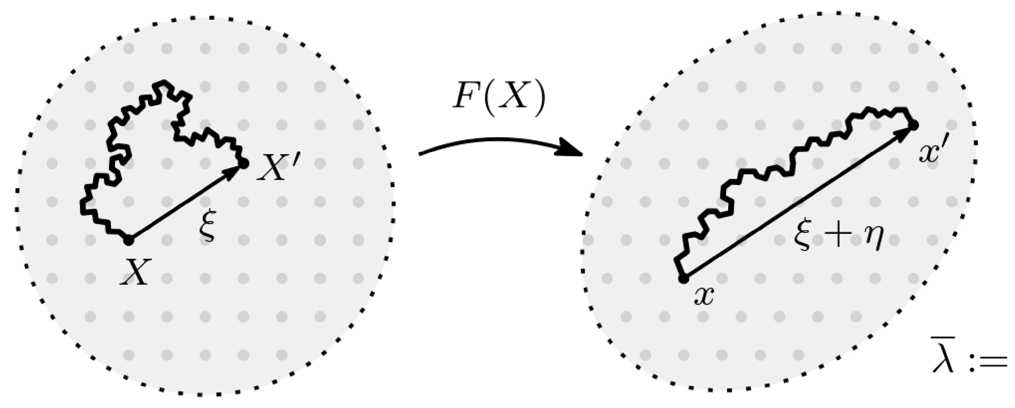
- Peridynamics (PD) is a nonlocal theory of mechanics that is developed as an alternative to continuum mechanics. It is highly effective in modeling discontinuous material behavior, such as crack propagation.
- Attempts of PD modeling of polymers are limited to correspondence models. A microstructurally informed nonlocal theory for general polymeric materials is highly sought after.
- By introducing a novel mesoscale potential function, we developed a nonlocal continuum framework to simulate large deformation response, crack propagation and fracture of elastomeric materials.

Constitutive relations for polymer networks

Non-Gaussian chain statistics theory: the Kuhn-Grün [1] idealization of the free energy of a single polymer chain, inverse Langevin type potential:

$$\phi_{KG}(r) = k\theta n\left[\frac{r}{nl}\beta + \ln\left(\frac{\beta}{\sinh\beta}\right)\right] \qquad \beta = \mathcal{L}^{-1}\left(\frac{r}{nl}\right) \qquad \mathcal{L}(\beta) = \coth\beta - \frac{1}{\beta}$$

Peridynamics kinematics description of a chain with rigid links:



$$\bar{\lambda} := \frac{|\xi+\eta|}{|\xi|}$$

Figure 1. Peridynamic representation of a rubber chain with rigid Kuhn segments in the initial and deformed configurations.

Utilizing Arruda-Boyce 8-chain model [2], peridynamics bond stretch is related to the molecular level chain stretch:

$$\bar{\lambda} = \sqrt{\frac{tr\bar{C}}{3}} = \sqrt{\frac{\lambda^{4/3} + 2\lambda^{-2/3}}{3}}$$

Introducing a novel bond-based peridynamics potential

$$\phi(\bar{\lambda}, \lambda_b) = \underbrace{k\theta\bar{n}\left[\frac{\bar{\lambda}}{\lambda_b\sqrt{\bar{n}}}\beta + \ln\left(\frac{\beta}{\sinh\beta}\right)\right]|\boldsymbol{\xi}|}_{\text{Chain untangling}} + \underbrace{\bar{n}\frac{1}{2}D(\ln\lambda_b)^2}_{\text{Kuhn segment stretching [3]}}|\boldsymbol{\xi}|$$

- $k\theta$: Rubber modulus, can be linked to continuum elastic constants
- $\bar{n}$: Number of links per chain
- D : Bond constant, can be computed via MD or DFT simulations
- $\bar{\lambda}$: PD bond stretch
- λ_b : Kuhn segment stretch (C-C backbones)

Bond force density corresponding to the potential:

$$\boldsymbol{t}(\bar{\lambda}, \lambda_b) = \frac{\partial\phi}{\partial\boldsymbol{\eta}} = k\theta\sqrt{\bar{n}}\frac{\beta}{\lambda_b}\frac{\boldsymbol{\zeta}}{|\boldsymbol{\zeta}|}$$

The model describes a two-way deformation mechanism:

1. Polymer chains untangle, no atomistic bond stretch. ($\bar{\lambda} > 1,\ \lambda_b = 1$)
2. After $\bar{\lambda}$ reaches a threshold, the C-C bonds start stretching. ($\bar{\lambda} > 1,\ \lambda_b > 1$)

Material constants can be fine tuned according to the microstructure. A critical bond stretch λ_{crit} shall be chosen to account for PD bond breaking. Bond force density is utilized in the nonlocal balance of linear momentum. In numerical applications, PD equation of motion is solved using the adaptive dynamic relaxation scheme to obtain the quasi-static solution.

Numerical examples

1. Thin plate under simple shear

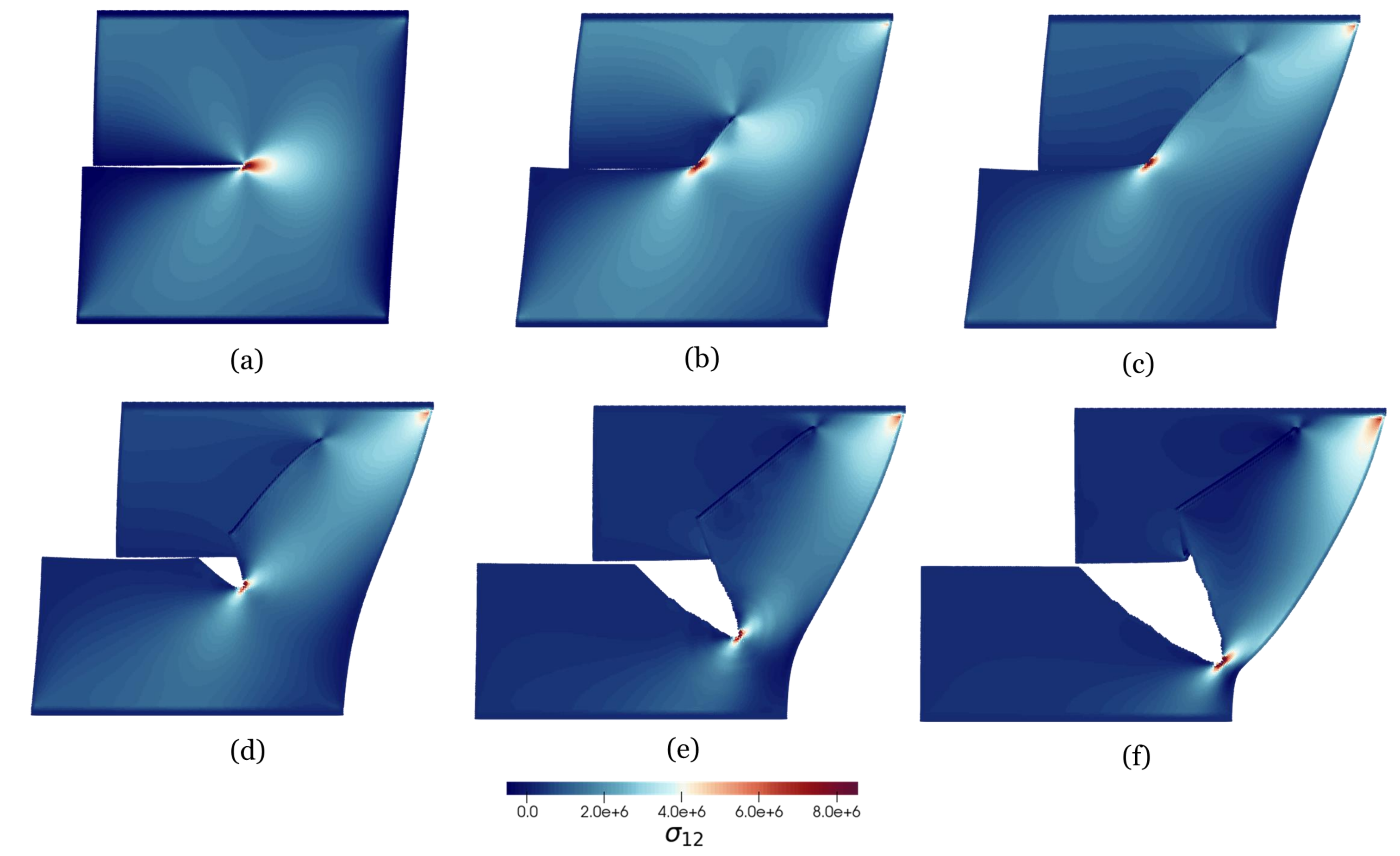


Figure 2. Shear stress (σ_{12}) distribution during different stages of deformation.

- Formation of a compressive crack at the crack tip (Fig 2.b), followed by the initiation of a tensile crack (Fig 2.d) are observed.
- The failure phenomenon requires the bifurcation solution of the large deformation problem, which is *captured for the first time* in a peridynamics simulation.

2. Fracture in a 3D cylindrical bar in tension

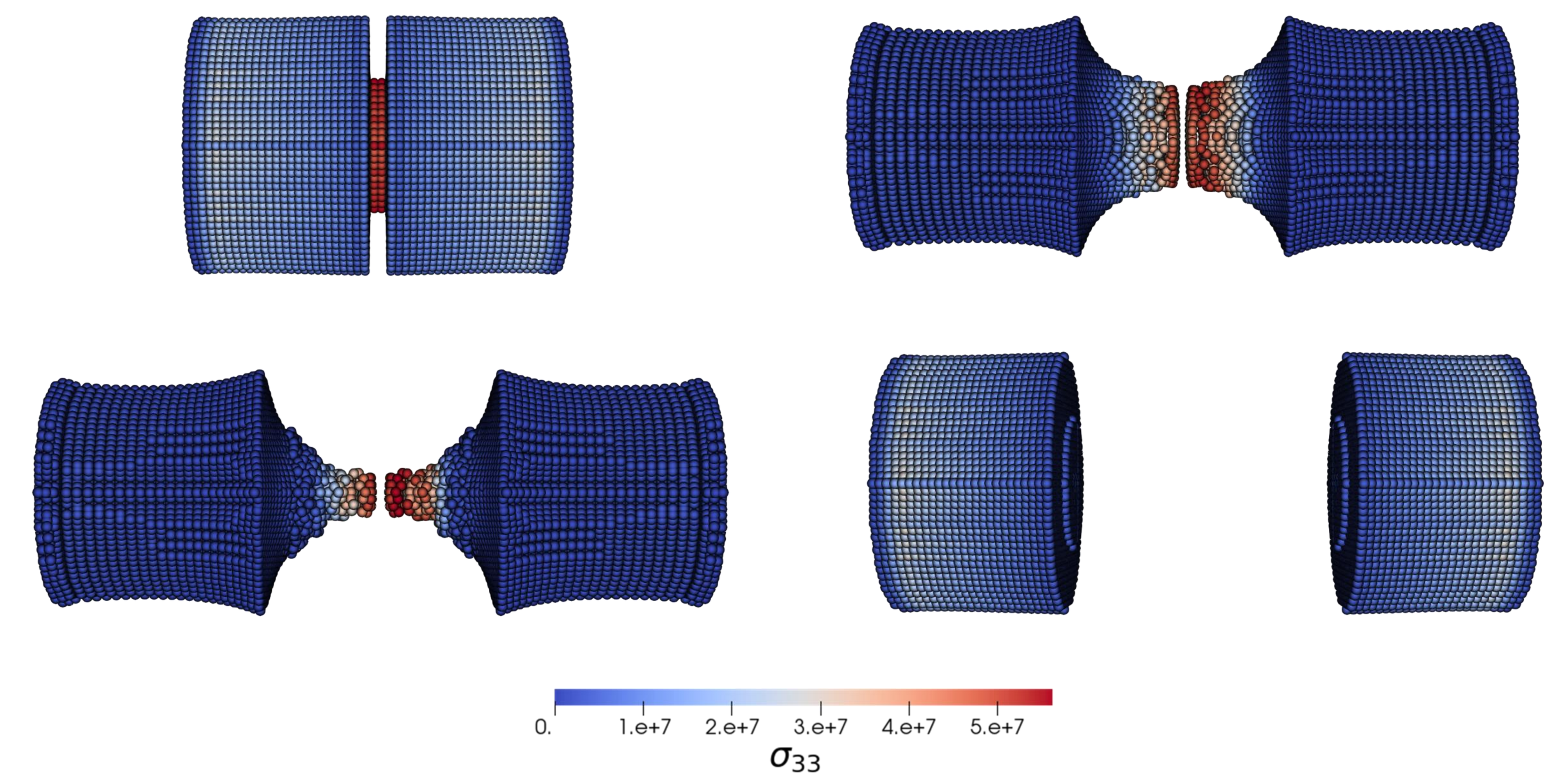


Figure 3. Tensile stress (σ_{33}) distribution during different stages of deformation.

- Effect of notch size on the fracture energy is investigated.

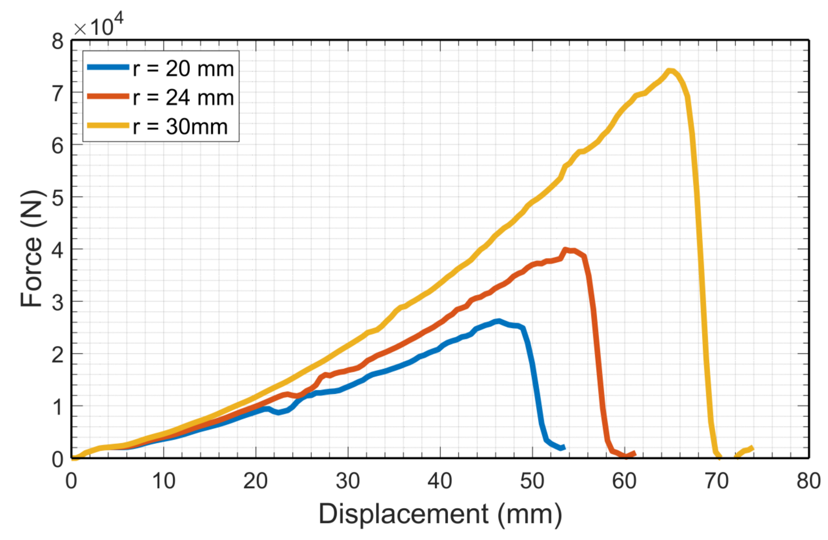


Figure 4. Force-displacement relations for different mid-section radii.

Conclusions and Future

- A microstructurally informed nonlocal potential is introduced.
- It is demonstrated through a series of numerical examples that the proposed model can capture the fracture, damage process and large deformation in elastomeric materials with simplicity and accuracy. See [**4**] for more details.
- Incompressibility needs to be addressed.
- Application under consideration: Elastomer-matrix composites.

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