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Multiphysics Peridynamic Models for Crack Growth in Brittle Materials

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Outline

- Peridynamic theory of solid mechanics
- Capturing the formation of cracks in the direct-write additive manufacturing process
- A multiphysics approach for modeling damage in concrete structures subjected to aqueous environments

Peridynamic Theory of Solid Mechanics

What is peridynamics?

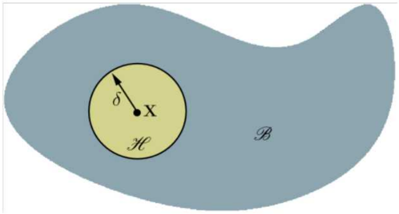
- Peridynamics is a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles

How does it work?

- Peridynamics is a nonlocal extension of continuum mechanics
- Remains valid in presence of discontinuities, including cracks
- Balance of linear momentum is based on an integral equation:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \underbrace{\int_{\mathscr{B}} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}'-\mathbf{x}\right\rangle - \underline{\mathbf{T}}'[\mathbf{x}',t]\left\langle \mathbf{x}-\mathbf{x}'\right\rangle \right\} \, \mathrm{d}V_{\mathbf{x}'}}_{\text{Divergence of stress replaced with integral of nonlocal forces.}} + \mathbf{b}(\mathbf{x},t)$$

The material point X interacts directly with all points within its horizon



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

S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.

F. Bobaru, J.T. Foster, P.H. Geubelle, and S.A. Silling, Eds., *Handbook of Peridynamic Modeling*, CRC Press, 2016.

Peridynamic Theory of Solid Mechanics

Constitutive laws in peridynamics

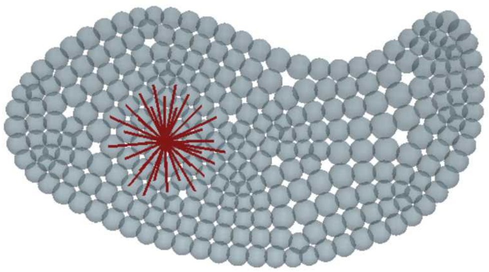
- Peridynamic bonds connect any two material points that interact directly
- Peridynamic forces are determined by force states acting on bonds

$$\underbrace{\underline{\mathbf{T}}[\mathbf{x}, t]}_{\text{Force State}} \quad \underbrace{\langle \mathbf{x}_i' - \mathbf{x} \rangle}_{\text{Bond}}$$

- Force states are determined by constitutive laws and are functions of the deformations of all points within a neighborhood, and possibly other variables
- Material failure is modeled through the weakening / breaking of peridynamic bonds

Meshfree discretization of a peridynamic body

- A body may be discretized using a finite number of nodal volumes



$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x}, t) = \sum_{i=0}^{N} \left\{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}_i' - \mathbf{x} \rangle - \underline{\mathbf{T}}'[\mathbf{x}_i', t] \langle \mathbf{x} - \mathbf{x}_i' \rangle \right\} \Delta V_{\mathbf{x}_i'} + \mathbf{b}(\mathbf{x}, t)$$

Peridynamic Constitutive Models

Peridynamic force states map bonds to pairwise force densities

- Peridynamic constitutive laws can be grouped into two categories
  - *Bond-based*: bond forces depend only on a single pair of material points
  - *State-based*: bond forces depend on deformations of all neighboring material points

Microelastic Material

- Bond-based constitutive model
- Pairwise forces are a function of bond stretch

$$s = \frac{y - x}{x}$$

- Magnitude of pairwise force density given by

$$\underline{t} = \frac{18k}{\pi\delta^4} s$$

Linear Peridynamic Solid

- State-based constitutive model
- Deformation decomposed into deviatoric and dilatational components

$$\theta = \frac{3}{m} \int_{\mathcal{H}} (\underline{\omega}\, \underline{x}) \cdot \underline{e}\, dV \qquad \underline{e}^d = \underline{e} - \frac{\theta\, \underline{x}}{3}$$

- Magnitude of pairwise force density given by

$$\underline{t} = \frac{3k\theta}{m} \underline{\omega}\, \underline{\mathrm{x}} + \frac{15\mu}{m} \underline{\omega}\, \underline{e}^{\mathrm{d}}$$

$\underline{x}$	bond vector
x	initial bond length
y	deformed bond length
s	bond stretch
$\underline{e}$	bond extension
$\underline{e}^d$	deviatoric bond extension
$\underline{\omega}$	influence function
V	volume
$\mathcal{H}$	neighborhod
m	weighted volume
θ	dilatation
δ	horizon
k	bulk modulus
μ	shear modulus
$\underline{t}$	pairwise force density

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

S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.

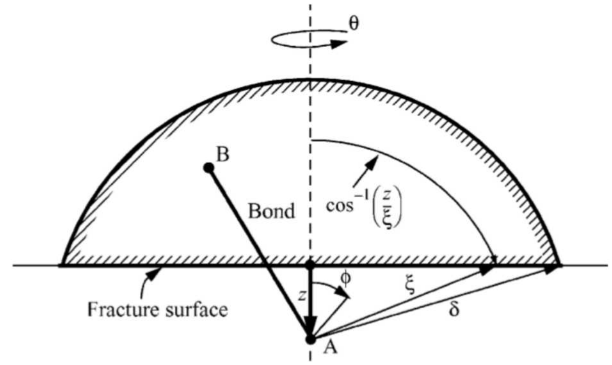
Bond Failure Laws

Material failure is captured through the breaking of peridynamic bonds

- Critical stretch model for brittle failure
  - Bond fails irreversibly when critical stretch is exceeded
  - Critical stretch value determined from the material's energy release rate

$$s_{\max} = \frac{y_{\max} - x}{x}$$

$$d = \begin{cases} 0 & \text{if} \quad s_{\max} < s_o \\ 1 & \text{if} \quad s_{\max} \geq s_0 \end{cases}$$



$$G_0 = \int_0^{\delta}\int_0^{2\pi}\int_z^{\delta}\int_0^{\cos^{-1} z/\xi} (c s_0^2 \xi/2)\xi^2 \sin\phi \, d\phi \, d\xi \, d\theta \, dz$$

$$s_0 = \sqrt{\frac{10 G_0}{\pi c \delta^5}} = \sqrt{\frac{5 G_0}{9 k \delta}}$$

[Images from Silling and Askari, 2005]

- Alternative models
  - Energy-based approach [Foster]
  - Ductile failure models [Silling]

Silling, S.A. and Askari, E. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures* 83:1526-1535, 2005.

Peridynamic Horizon Provides a Length Scale

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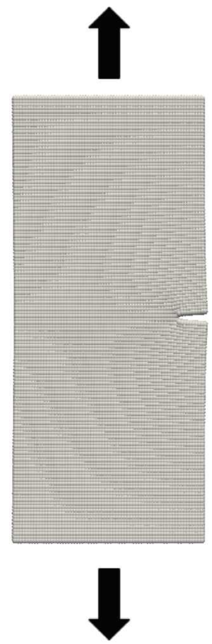
Nonlocality (length scale) relieves mesh dependence

- The peridynamic horizon introduces a length scale that is independent of the mesh size
- Decoupling from the mesh size enables consistent modeling of material response in the vicinity of discontinuities
- Example: mesh independent plastic zone in the vicinity of a crack

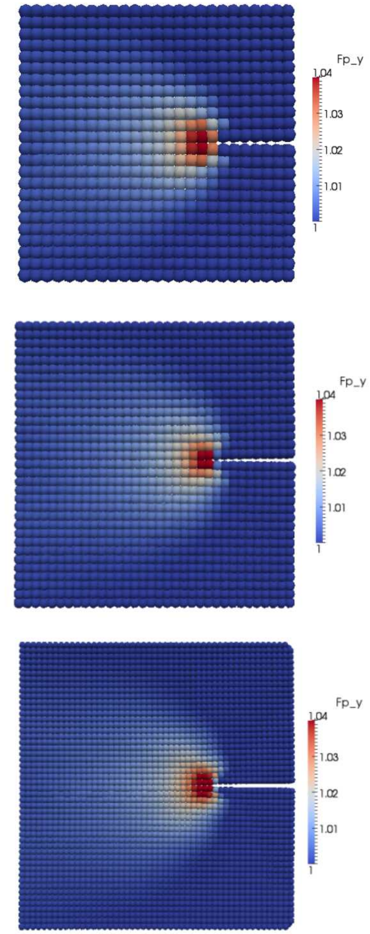


Pre-cracked specimen loaded in tension

Coarse mesh

Medium mesh

Fine mesh



Component of plastic deformation gradient in loading direction

Connection to Local and H.O.G. Models

- Local models contain no length scale

$$\ddot{u}(x) = a u''(x)$$

- Higher-order gradients introduce a length scale in a weak sense

$$\ddot{u}(x) = a u''(x) + b u''''(x)$$

Dimensional analysis shows that sqrt(b/a) has units of length

- Peridynamics is a strongly nonlocal model

Peridynamic model (nonlocal)

$$\rho \ddot{u}(x,t) = \int_{-\delta}^{\delta} \frac{c}{|\epsilon|} \left[u(x+\epsilon, t) - u(x,t) \right] d\epsilon$$

Taylor Series

Higher-order gradient model (weakly nonlocal)

$$\rho \ddot{u}(x,t) = \mathrm{K}_a \left[\frac{\partial^2 u}{\partial x^2} + \frac{\delta^2}{24} \frac{\partial^4 u}{\partial x^4} + \frac{\delta^4}{1080} \frac{\partial^6 u}{\partial x^6} + \dots \right]$$

$\lim \ \delta \to 0$

Local model

$$\rho \ddot{u}(x,t) = \mathrm{K}_a \frac{\partial^2 u}{\partial x^2}$$

S.A. Silling and R.B. Lehoucq, Convergence of peridynamics to classical elasticity theory, *Journal of Elasticity*, 93(1), 2008.

P. Seleson, M.L. Parks, M. Gunzburger, and R.B. Lehoucq. Peridynamics as an upscaling of molecular dynamics. *Multiscale Modeling and Simulation*, 8(1), 2009.

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Direct-Write Additive Manufacturing Process

1. Ceramic powder is mixed with polymeric binding agent to create a thixotropic slurry
2. Layered strands deposited onto substrate to form component geometry
   - Data recorded during deposition process (position, temperature, pressure)
3. Polymer binder is removed via burn-off process
   - Burn-off may lead to crack formation
4. Sintering phase to coalesce particles

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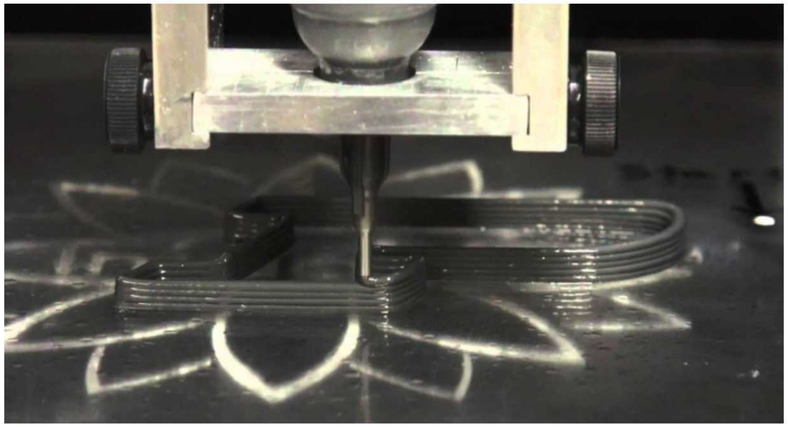
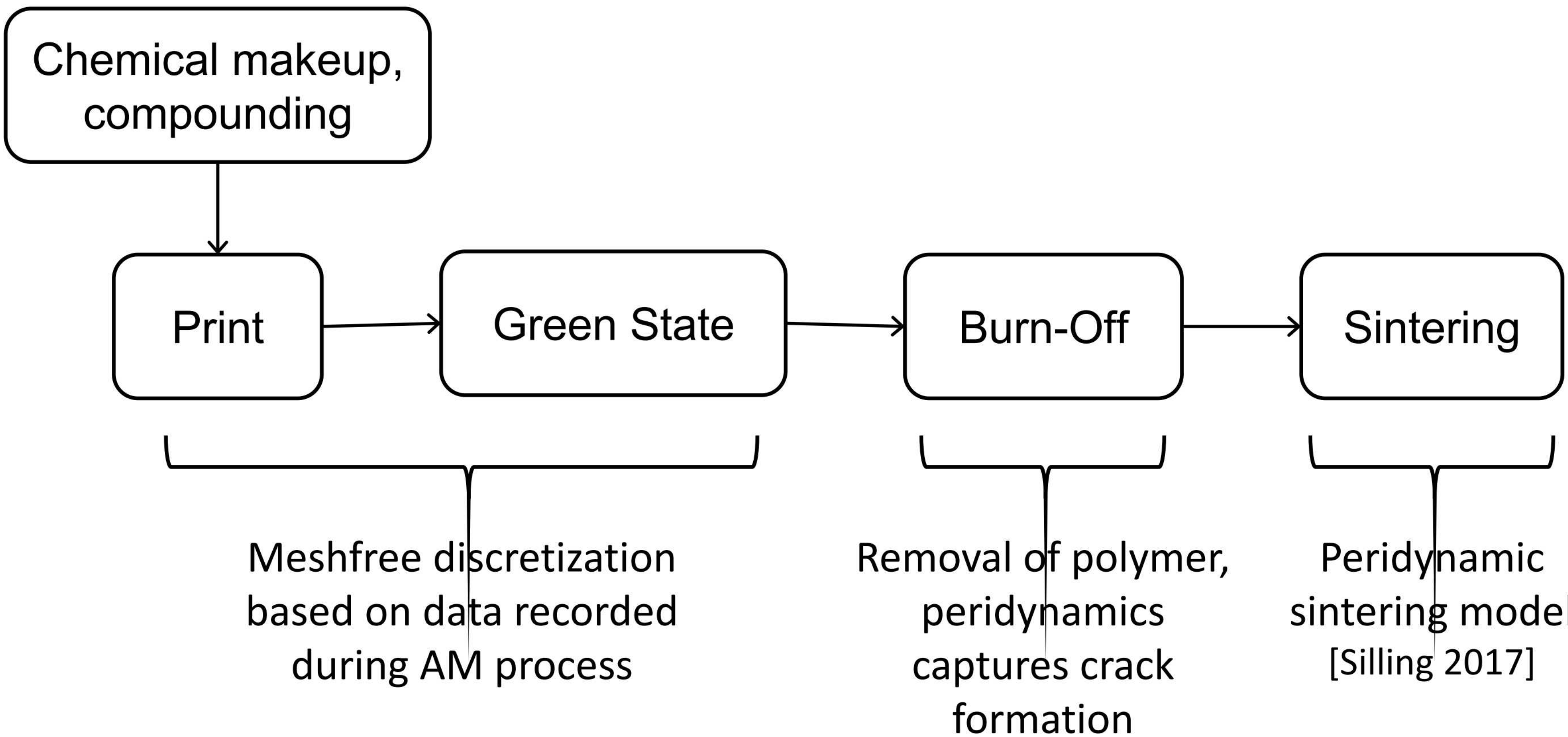


Peridynamic Modeling of Direct-Write AM Process

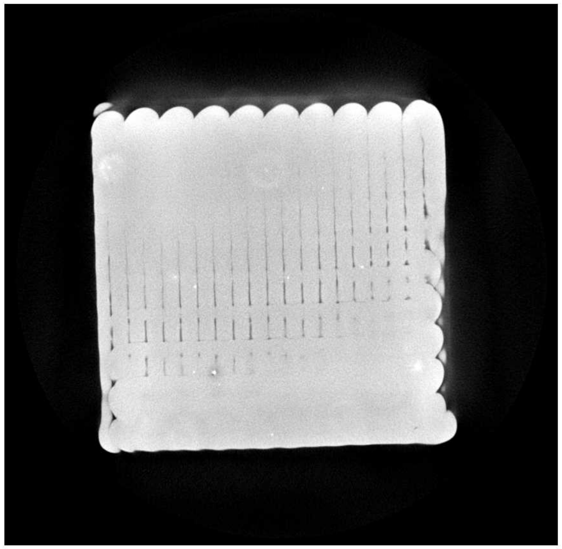
Goals:

- End-to-end model of direct-write AM process
- Future work: Apply optimization techniques for inversion and control

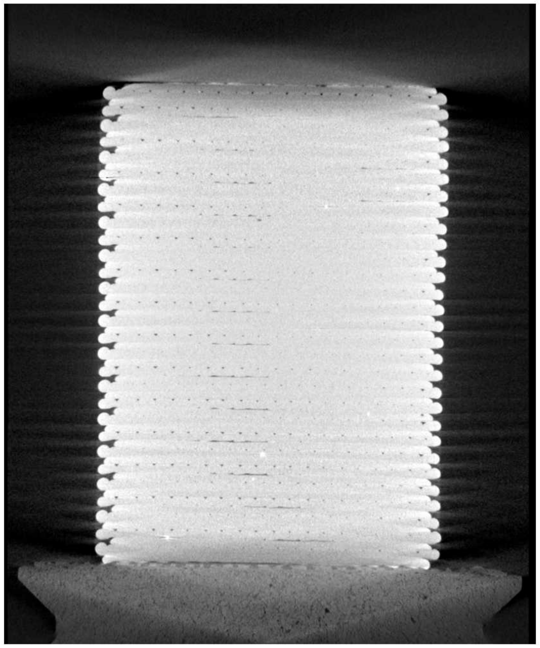


Geometry of Green State

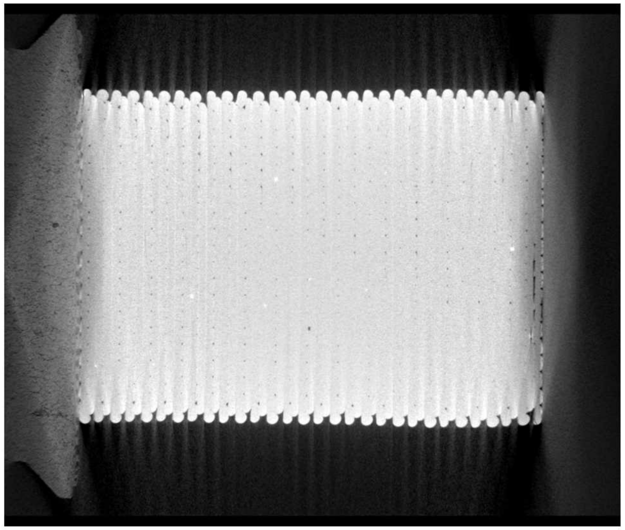
- Slurry (ceramic powder + binder) extruded through nozzle
- Strands layered to form specimen geometry
- Data recorded over course of direct-write process
  - Position, pressure, temperature



XY Plane



XZ Plane



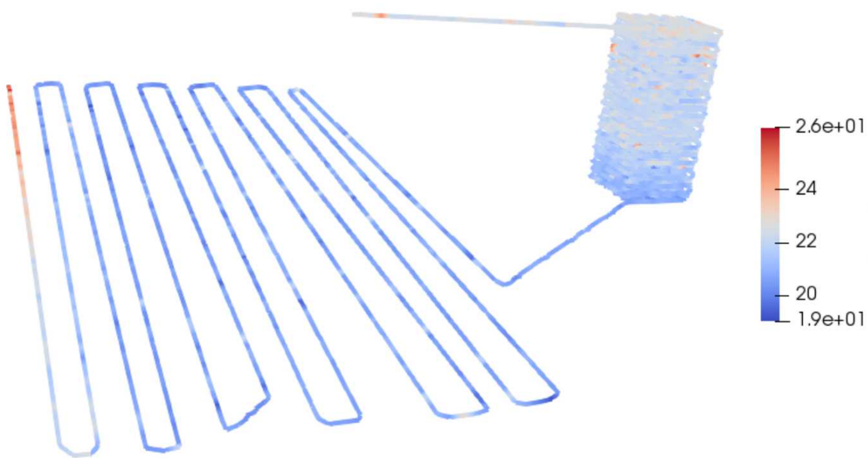
YZ Plane

Data Recorded During Direct-Write Process

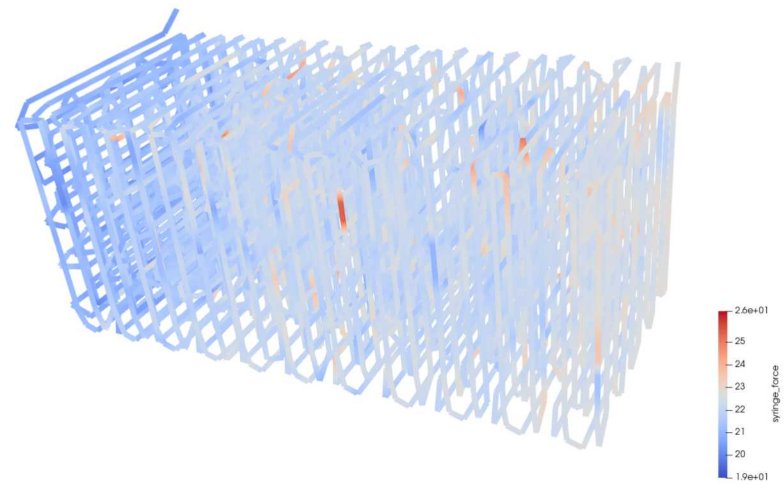
- Data file output by direct-write device

```
Elapsed Time (ms), X Position, Y Position, Z Position,, Extrusion Temp (C), Platen Temp (C), Syringe Force (Lbs)
"35890","22.0737","28.5888","0",,176.025,135.986,20.4386,
"35921","22.0737","29.06","0",,175.537,135.986,20.7682,
"35953","22.0737","29.5288","0",,175.537,135.498,20.9798,
...
```

- Data can be utilized for model construction



Syringe force & position



Isolation of component geometry

Construction of Meshfree Model

- Meshfree models provide a path for converting experimental data to model geometry

Simple cylindrical geometry provides a building block for modeling individual strands

- Many possibilities: strands can be modified to better capture observed geometry

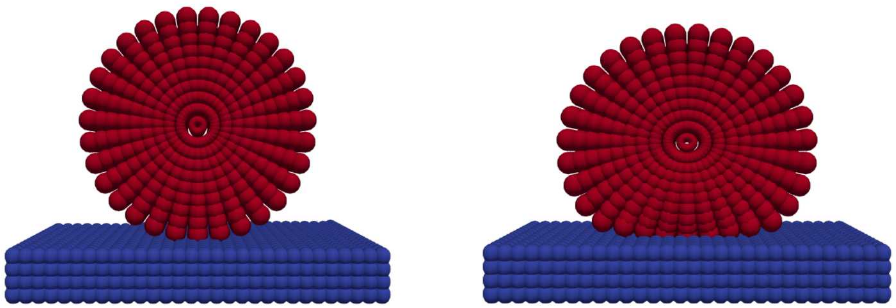
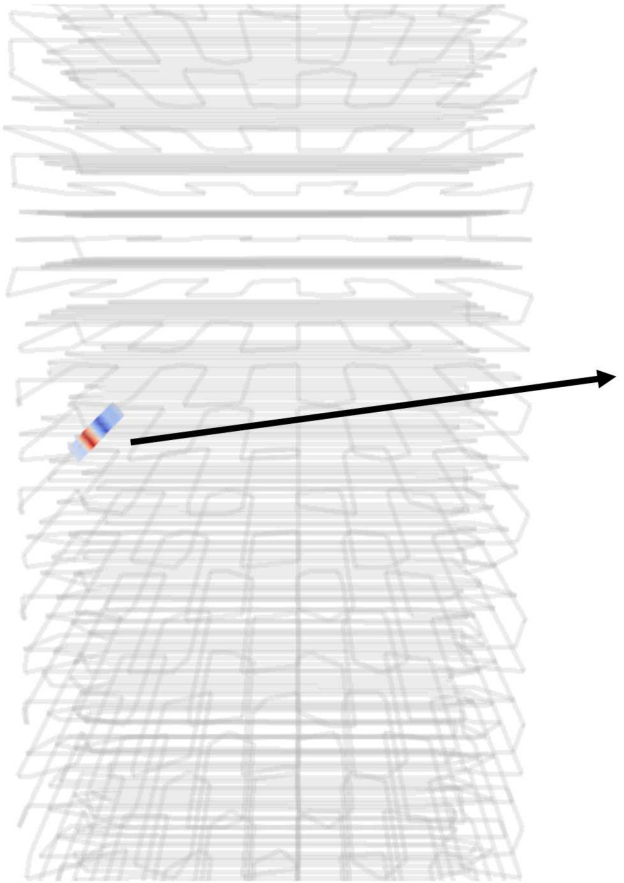


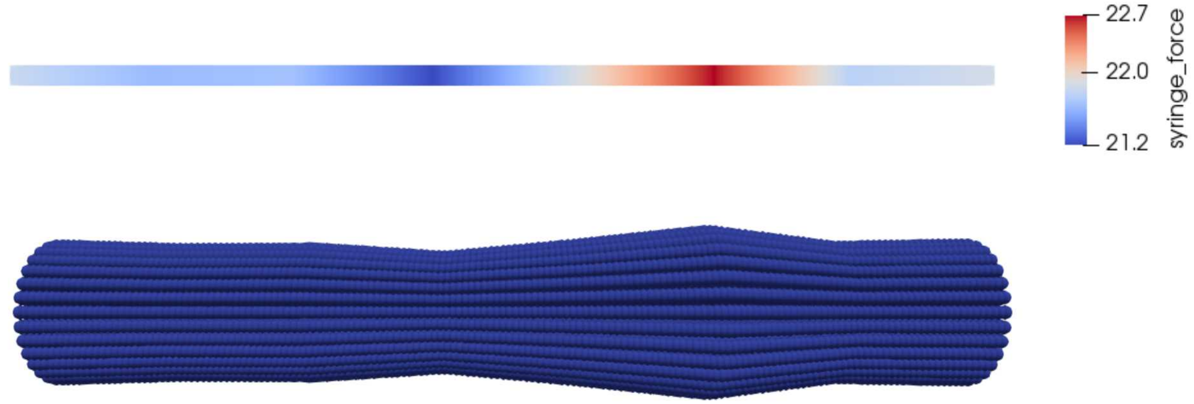
Illustration: application of body force to alter strand geometry

Construction of Meshfree Model

- Inconsistencies in strand geometry are observed experimentally
- Data recorded during direct-write process provides insight



Strand radius can be determined from recorded syringe force



Construction of Meshfree Model

- Pre-processing script constructs model of multiple strands
- Strand geometry and laydown pattern informed by data recorded during direct-write process

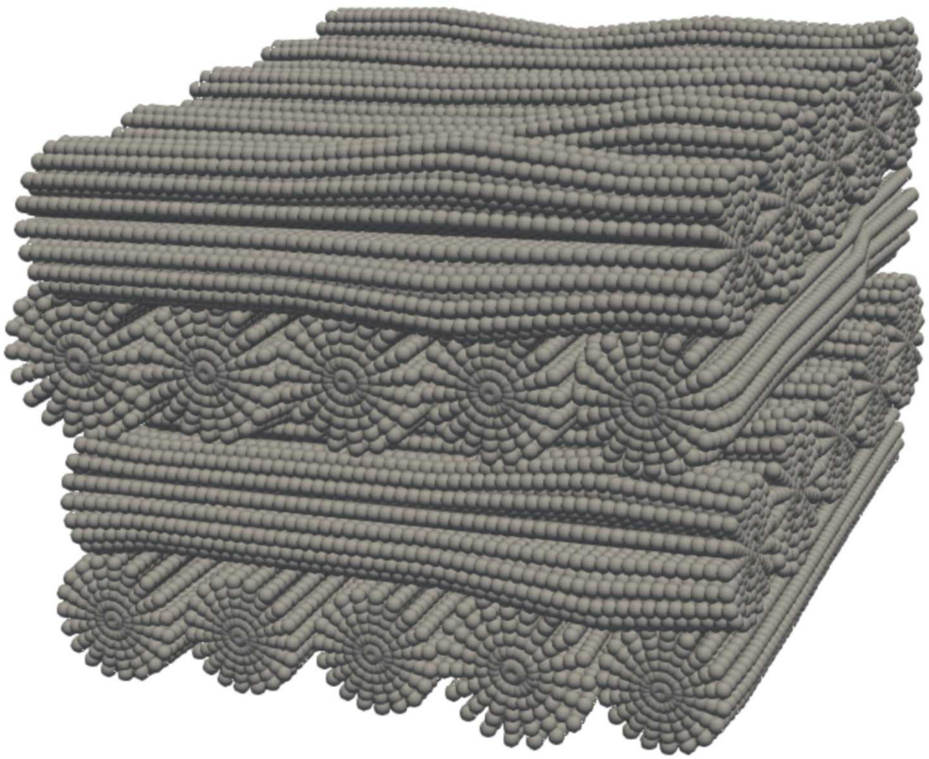


Illustration: subset of specimen geometry showing multiple strands

Proof-of-Concept Effort: Model of "Potato Chipping"

Incorporating thermal strains

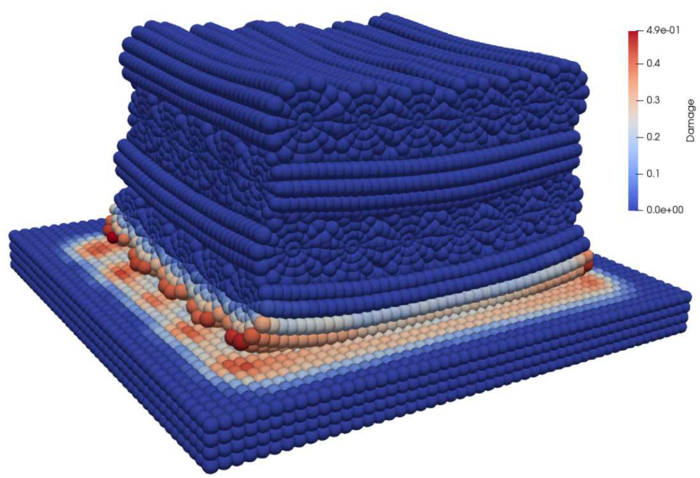
- Subtract thermal strain from bond extension
- Modify LPS constitutive model

$$\underline{e}^* = \underline{e} - \underline{e}^{\text{thermal}} = \underline{e} - \alpha\, \Delta T\, \underline{x}$$

$$\theta^* = \int_{\mathcal{H}} \frac{3}{m} \left(\underline{\omega}\, \underline{x}\right) \cdot \underline{e}^*\, dV$$

$$\underline{e}^{*d} = \underline{e}^* - \frac{\theta^*\, \underline{x}}{3}$$

$$\underline{t}^* = \frac{3k\theta^*}{m} \underline{\omega}\, \underline{x} + \frac{15\mu}{m} \underline{\omega}\, \underline{e}^{*d}$$

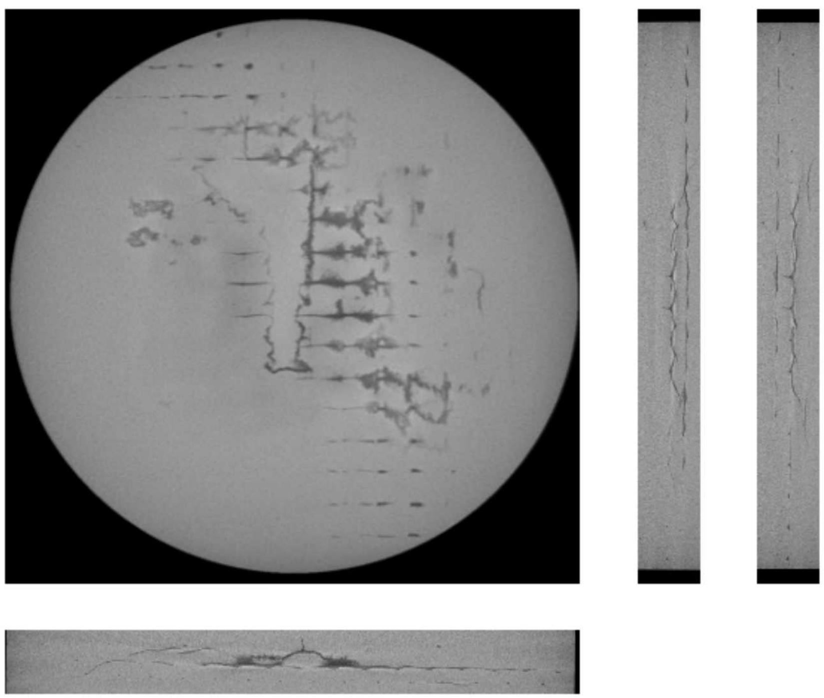


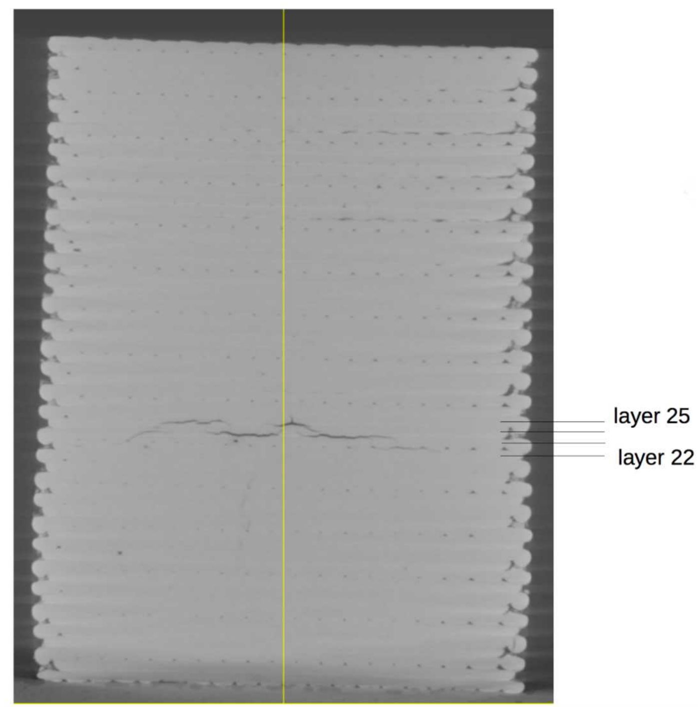
"Potato-chip" deformation results from thermal shrinkage and interaction with substrate

David Littlewood. Modeling Thermal Strains with Peridynamics. SAND Report 2013-2876P. Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2013.

Cracks Observed Following Burn-Off and Sintering

- Cracks observed in direct-write components are believed to be formed from the expansion of trapped binder during the burn-off phase
- Cracks are preserved during sintering
- Cracks are clearly tied to microstructure (strand geometry)





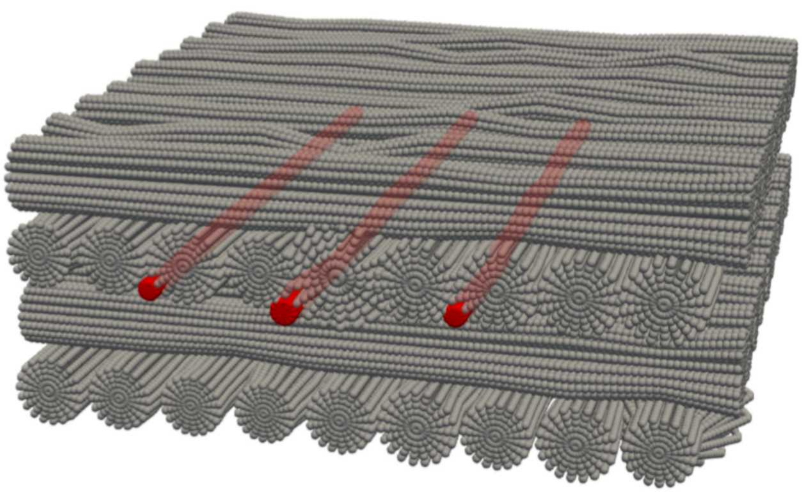
Modeling Effect of Trapped Polymer During Burn-Off

- Incorporate pressure due to expansion of trapped polymer

$$\theta = \int_{\mathcal{H}} \frac{3}{m} \left(\underline{\omega} \, \underline{x} \right) \cdot \underline{e} \, dV + \frac{p^{\mathrm{b}}}{-k}$$

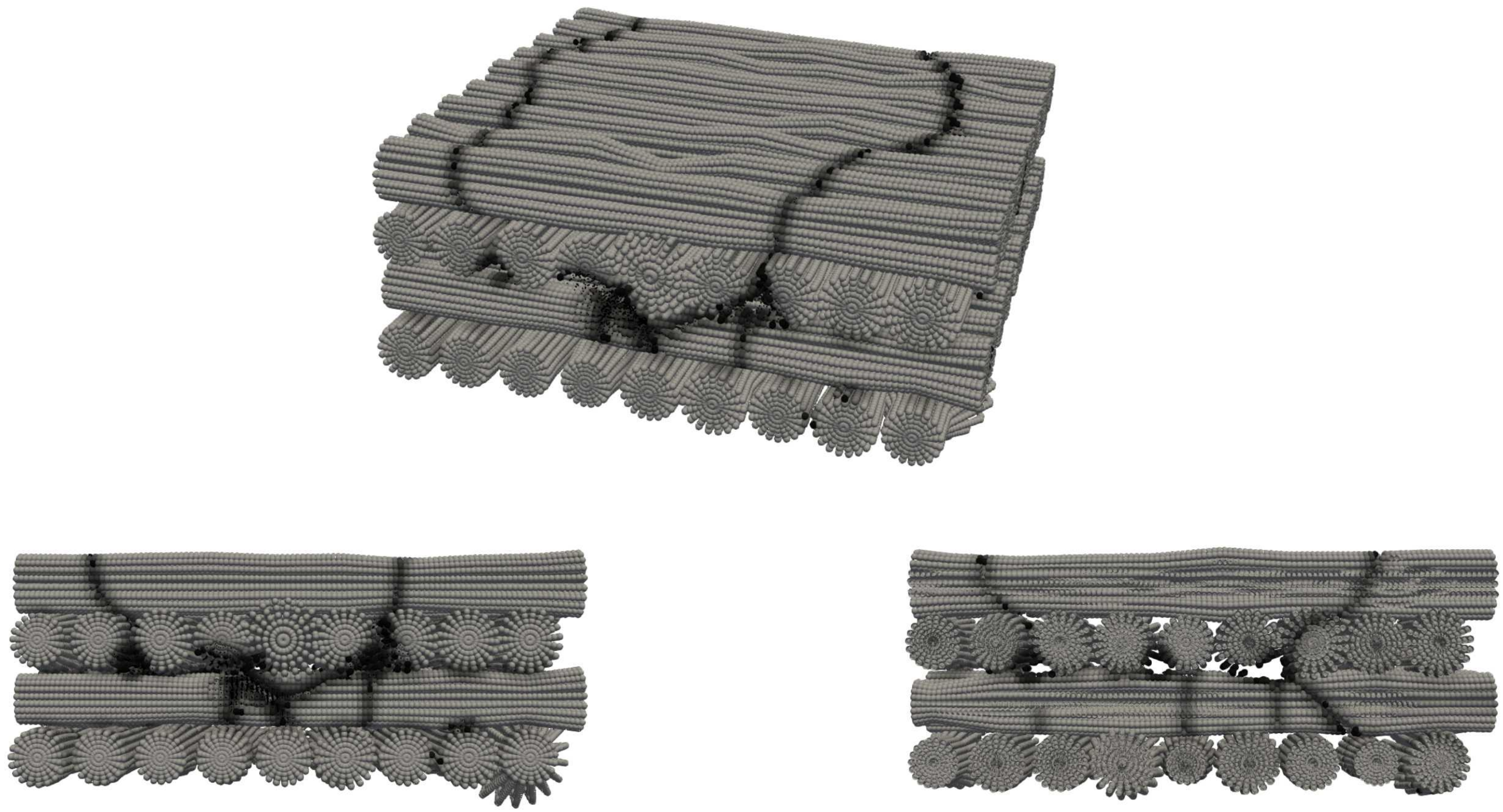
Additional "Burn-off" pressure

- Preliminary modification to strand geometry includes trapped polymer between strands



Capturing Crack Formation During Burn-Off

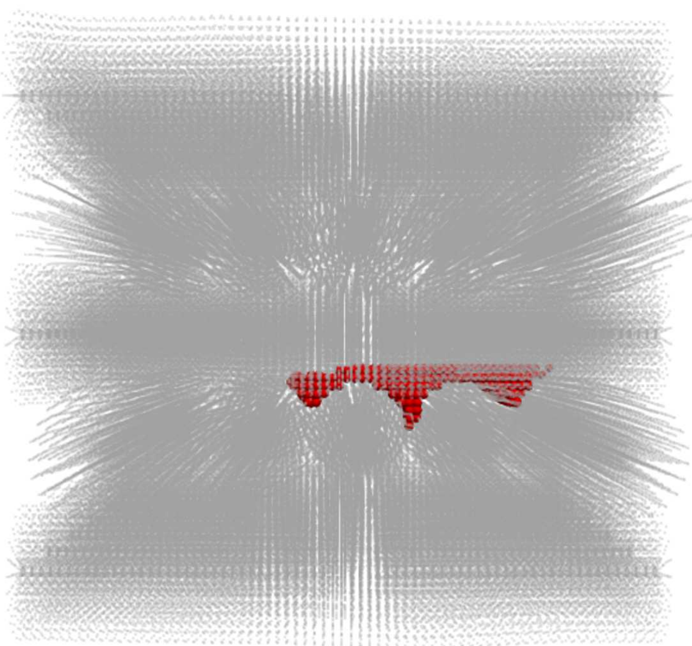
Initial results show good qualitative agreement with observed cracking

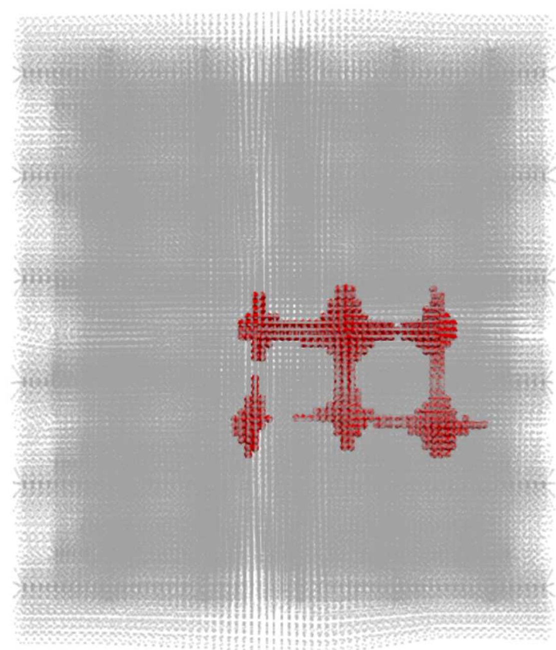


Improved Representation of Trapped Polymer

Ongoing work: Tools for inserting trapped polymer into strand model

- Nearest-neighbor search to identify voids within strand model
- Uniform grid clipped to match void geometry in specified subregion
- Strands and polymer combined into multi-material discretization





Red nodes represent trapped polymer within strand model

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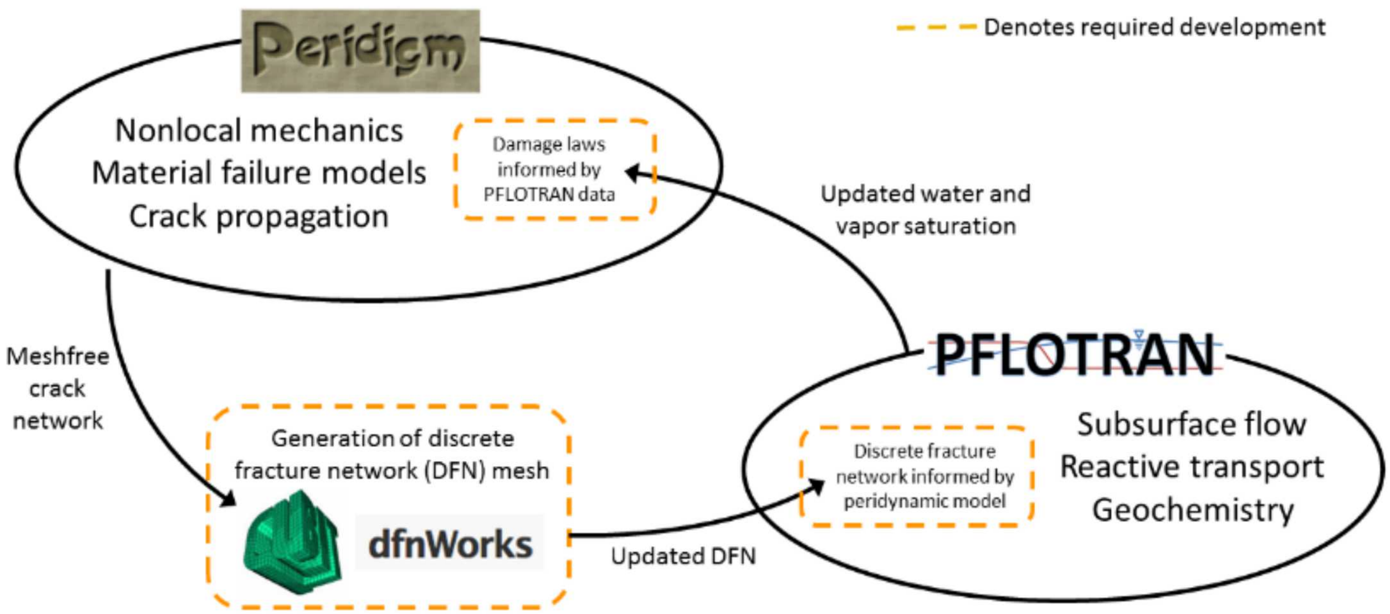
Peridynamic Modeling of Failure in Civil Structures

Integrated multiphysics modeling of environmentally assisted fracture

- *Goal*: Damage model for concrete structures in aqueous environments
- *Challenge*: Linking mechanics model and flow/transport model
- *Strategy*: Couple peridynamic mechanics model (Peridigm) with flow/transport model from geomechanics community (PFLOTRAN)



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Coupling Peridynamics and Flow/Transport Models

Two-way coupling strategy

- Peridynamic mechanics model determines material damage (bond failure)
  - Permeability is determined as a function of peridynamic damage, passed to flow model
  - Candidate relationships between damage and permeability

$$\frac{k_d}{k_o} = e^{(\alpha d)^\beta}$$ [Picandet, et al.]

$$\frac{k_d}{k_o} = e^{(1-\alpha d)}$$ [Zhou, et al.]

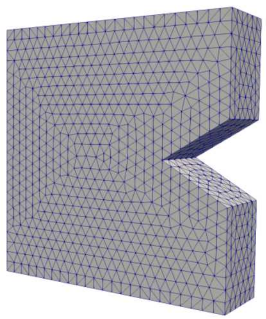
- Flow and transport model determines fluid saturation and/or pressure
  - Elastic properties and peridynamic damage law are a function of fluid saturation

V. Picandet, A. Khelidj, and G. Bastian, Effect of axial compressive damage on gas permeability of ordinary and high-performance concrete, *Cement and Concrete Research*, 31(9), 2001.

C. Zhou, K. Li, and Han J., Characterizing the effect of compressive damage on transport properties of cracked concretes, *Materials and Structures*, 45(3), 2012.

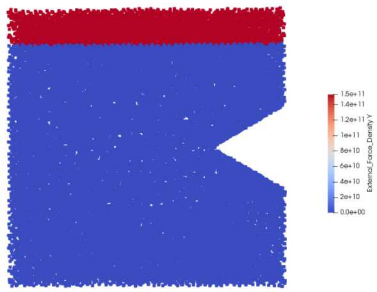
Proof-of-Concept Coupling Demonstration

- Problem setup

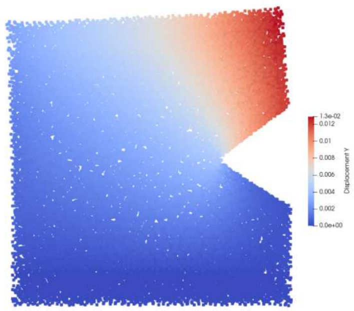


FEM mesh
(PFLOTRAN)

Meshfree
(Peridgm)

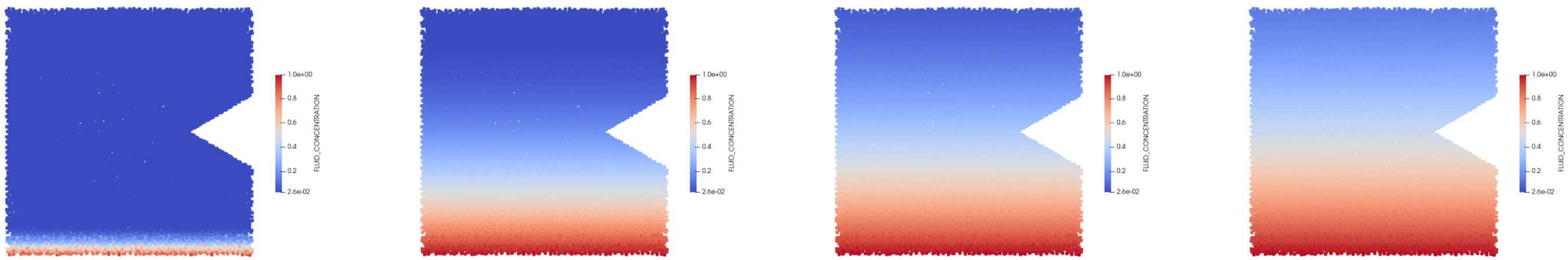


Applied
loading



Nominal
Displacement
(magnified 20x)

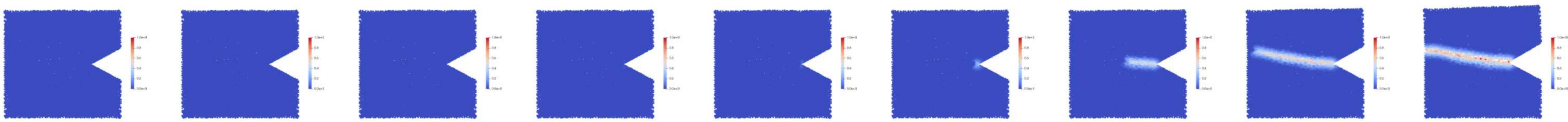
- Fluid saturation coupled to mechanical response



Water diffuses into body over time → alters mechanics response → damage influences diffusion

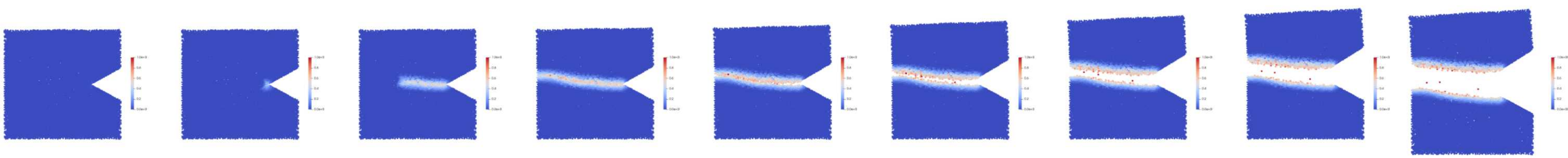
Proof-of-Concept Coupling Demonstration

- Damage progression in unmodified model



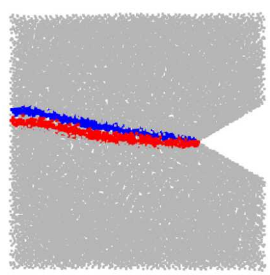
Step 900 Step 1000 Step 1100 Step 1200 Step 1300 Step 1400 Step 1500 Step 1600 Step 1700

- Damage progression in modified model
  - Critical stretch is reduced as a function of fluid saturation



Step 900 Step 1000 Step 1100 Step 1200 Step 1300 Step 1400 Step 1500 Step 1600 Step 1700

- Damage initiates under smaller load and follows different crack path



Blue = Unmodified Model
Red = Modified model

Colored nodes have damage > 40%

Resources

Peridigm peridynamics code

https://github.com/peridigm/peridigm

PFLORTRAN reactive flow and transport code

https://www.pflotran.org