Sandia National Laboratories

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Determination of Influential Parameters on Concrete Fracture using Peridynamics

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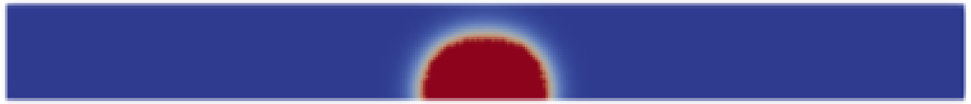
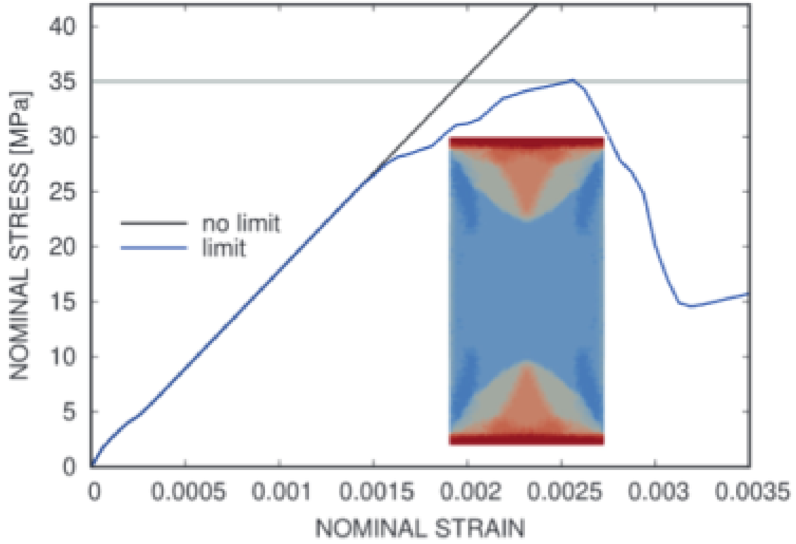
Why study concrete fracture using peridynamics?

- Concrete is a critical infrastructure material
- Fracture can cause:
  - Reduced mechanical properties
  - Increased surface area for chemical attack
  - Catastrophic failure
- Peridynamics is uniquely advantageous to model fracture
  - Handles spatial discontinuities
- Realistic 3D concrete microstructures used in this work
  - Shape effects

Water ingress from crack



Compression test on cement



R. E. Jones et al. *Construction and Building Materials* 286 (2021).

What is Peridynamics?

- Developed in 2000 by Stewart Silling at Sandia National Laboratory
- Continuum mechanics meets molecular dynamics
- No spatial derivatives
  - Suitable for fracture modeling
- Meshless method
  - Regular grid of nodes
- Non local
  - User defined radius of non-locality - horizon
  - Typically 2-3x node spacing

Equation of motion:

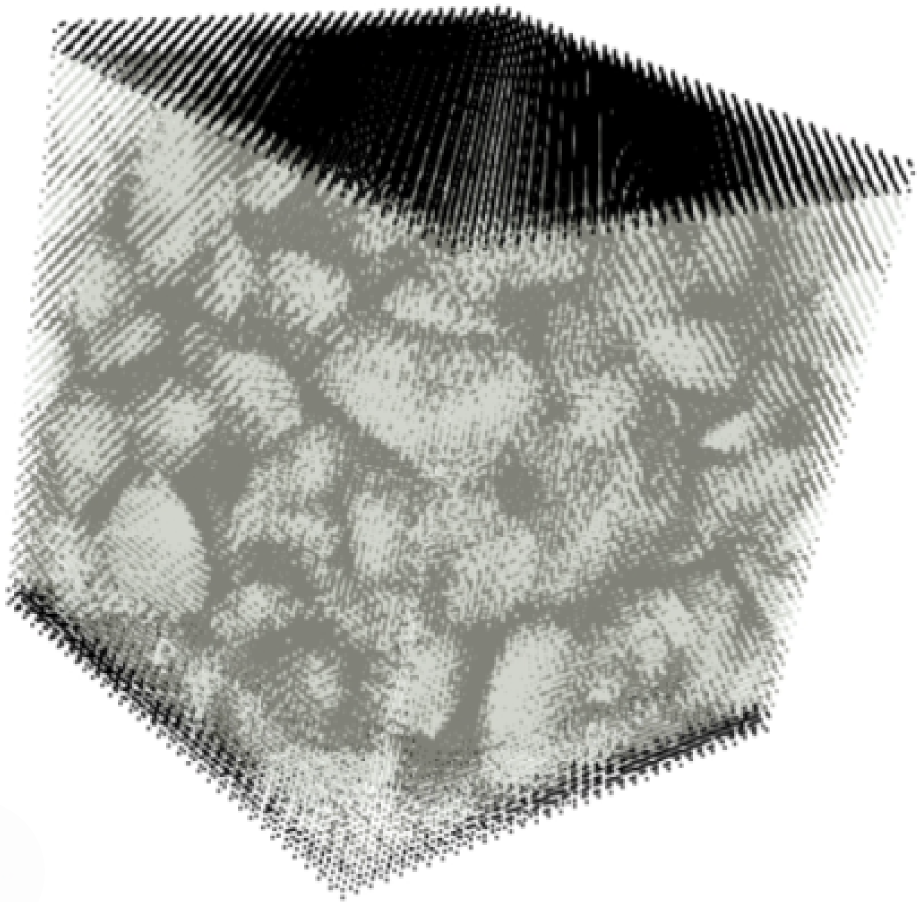
$$\rho \ddot{\mathbf{u}} = \mathbf{L}_{\mathbf{u}} + \mathbf{b} \quad \text{on} \quad \mathscr{R}, \qquad t \geq 0$$

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}\left(\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t), \mathbf{x}' - \mathbf{x}\right) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

S. A. Silling. *Journal of the Mechanics and Physics of Solids* 48 (2000) 175-209.

Concrete Microstructure Generation

- Mortar + coarse aggregates
- Real aggregate shapes from NIST database
- Particles placed randomly into a cube
    - Cored boundary conditions
    - 40% volume fraction of coarse aggregates
    - 75mm cube edge length
- Microstructure converted to a grid of nodes
    - FCC lattice pattern
    - Node spacing 1.5 - 2.1mm
    - Steel plates on top and bottom



E. J. Garboczi. *Cement and Concrete Research* 32 (2002).

Computational Parameters

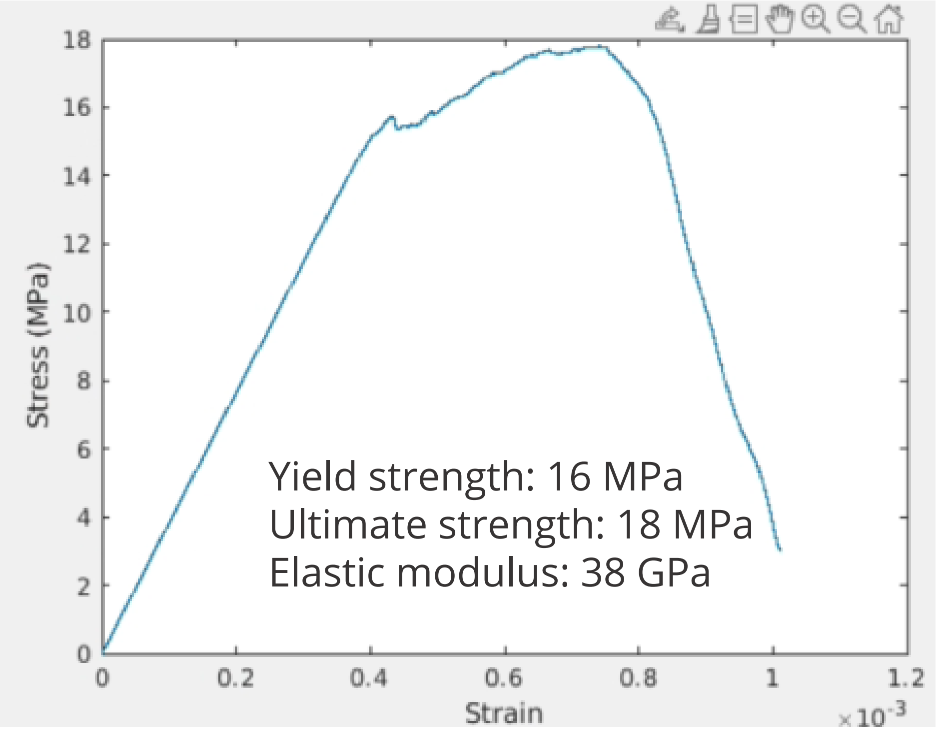
- Microstructure converted to a grid of nodes
  - FCC lattice
  - Lattice spacing 1.5 – 2.1mm
- Horizon – 5mm
- Applied uniaxial displacement
  - Constant rate 0.75 mm/s
  - Applied by 'plates' on top and bottom of the microstructure

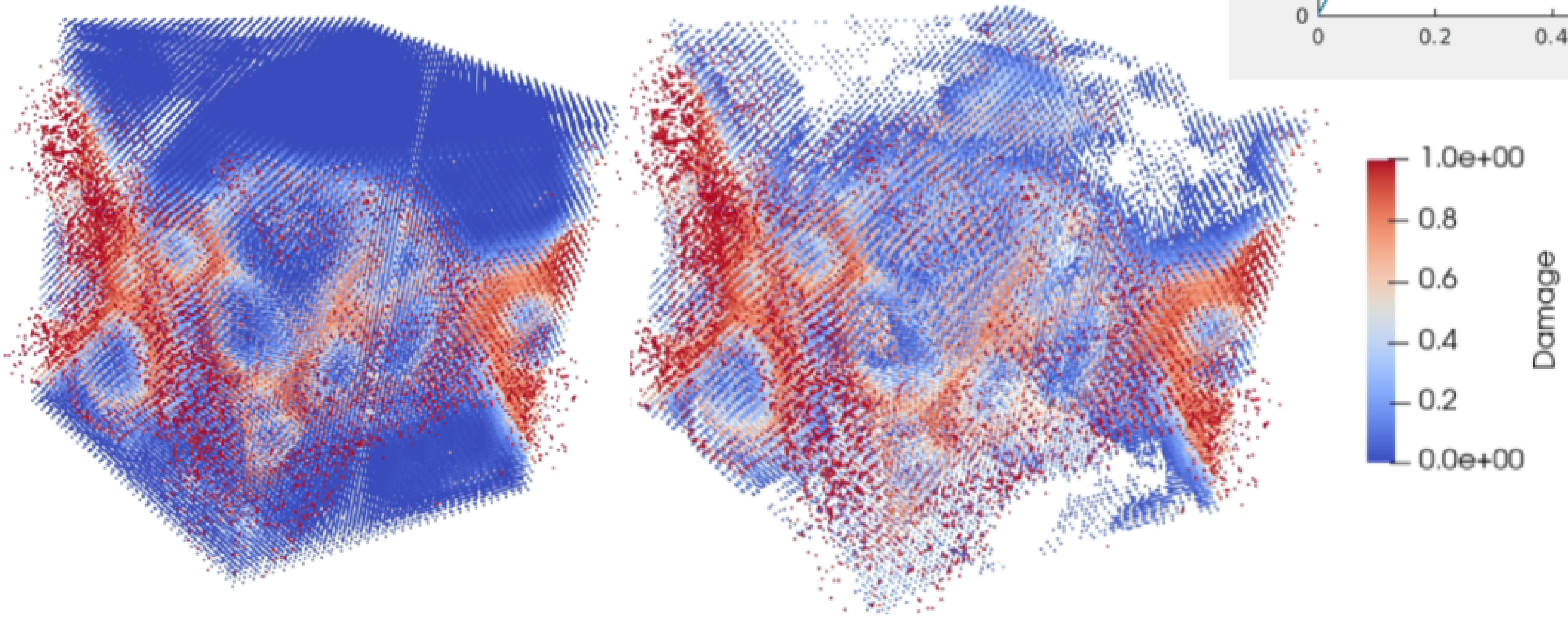
Concrete		
Volume fraction (coarse)	ϕ	0.4
Mortar		
Young's modulus [GPa]	E	26.7
Poisson's ratio	ν	0.23
Fracture toughness [MPa-m$^{1/2}$]	K_{Ic}	0.30
Aggregate		
Young's modulus [GPa]	E	55
Poisson's ratio	ν	0.3
Fracture toughness [MPa-m$^{1/2}$]	K_{Ic}	1.92
Interface		
Modulus [GPa]		0.92 E_{mortar}
Fracture Toughness [MPa-m$^{1/2}$]		0.82 $K_{Ic_{mortar}}$

X. Gu, et al. *Construction and Building Materials* 46 (2013) 156–166.
M. Dehestani, et al. *Theoretical and Applied Fracture Mechanics* 107 (2020).
C. Kurtulus, et al. *Soil Mechanics and Foundation Engineering* 52 (6) (2016) 348–354.
X. Zhou, et al. *Journal of Central South University of Technology* 17 (1) (2010) 150–155.
Li and Guo, *Construction and Building Materials* 161 (2018) 665–675.

Results - Compression

- Damage patterns form an 'X' shape seen in experimental work
- Elastic modulus, 38 GPa, matches published values
- Yield strength is lower than expected



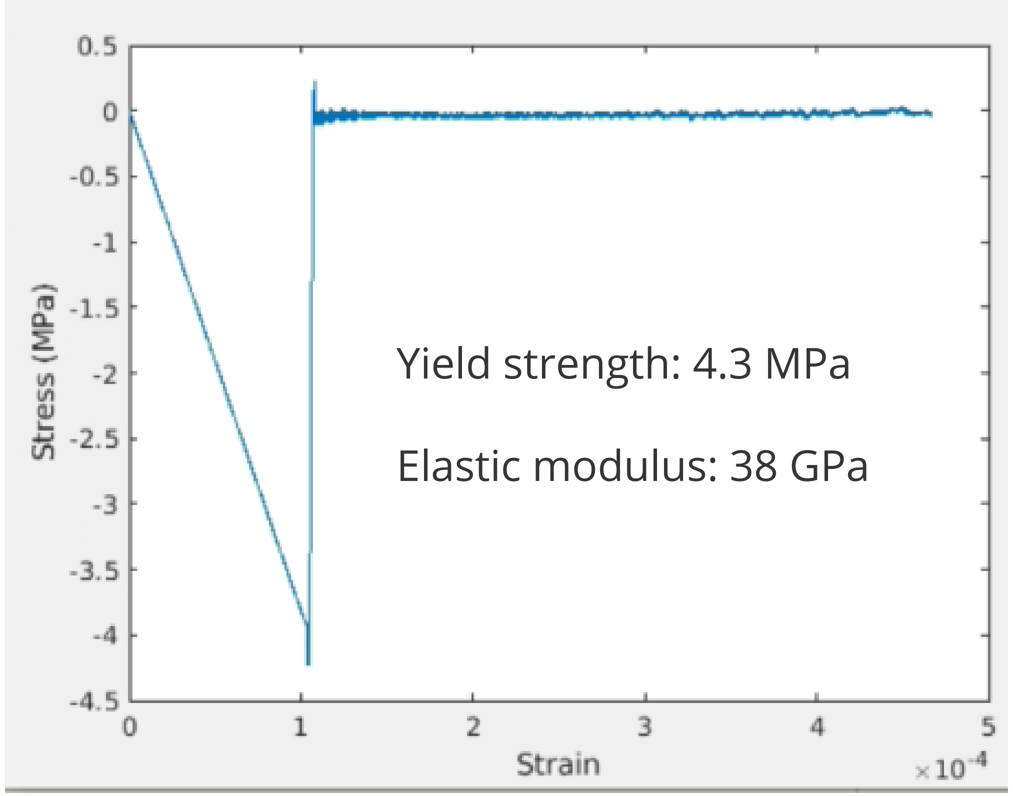


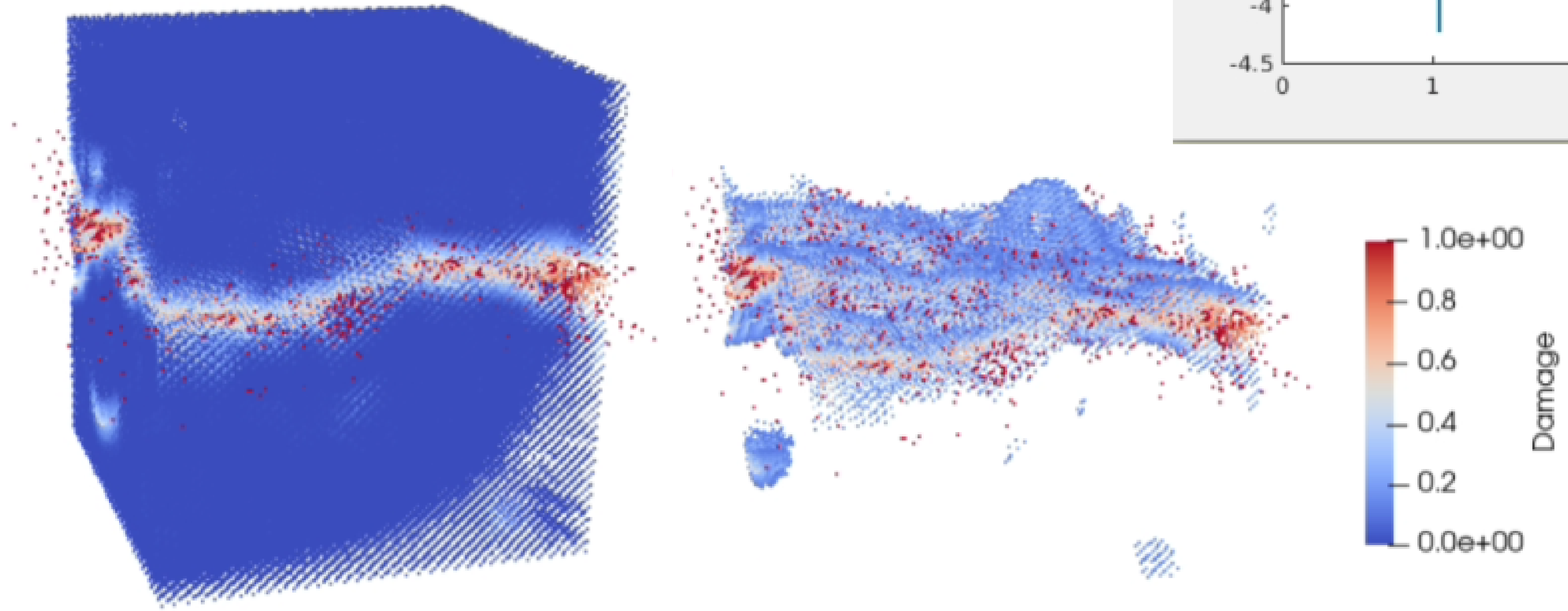
N. A. Farhan et al. *Construction and Building Materials* 196 (2019) 26-42.

V. Toufign et al. *ACI Materials Journal* 114 (2017).

Results - Tension

- Tensile strength and elastic modulus matches range of published values for concrete
- Fracture network forms a failure surface consistent with tensile experiments

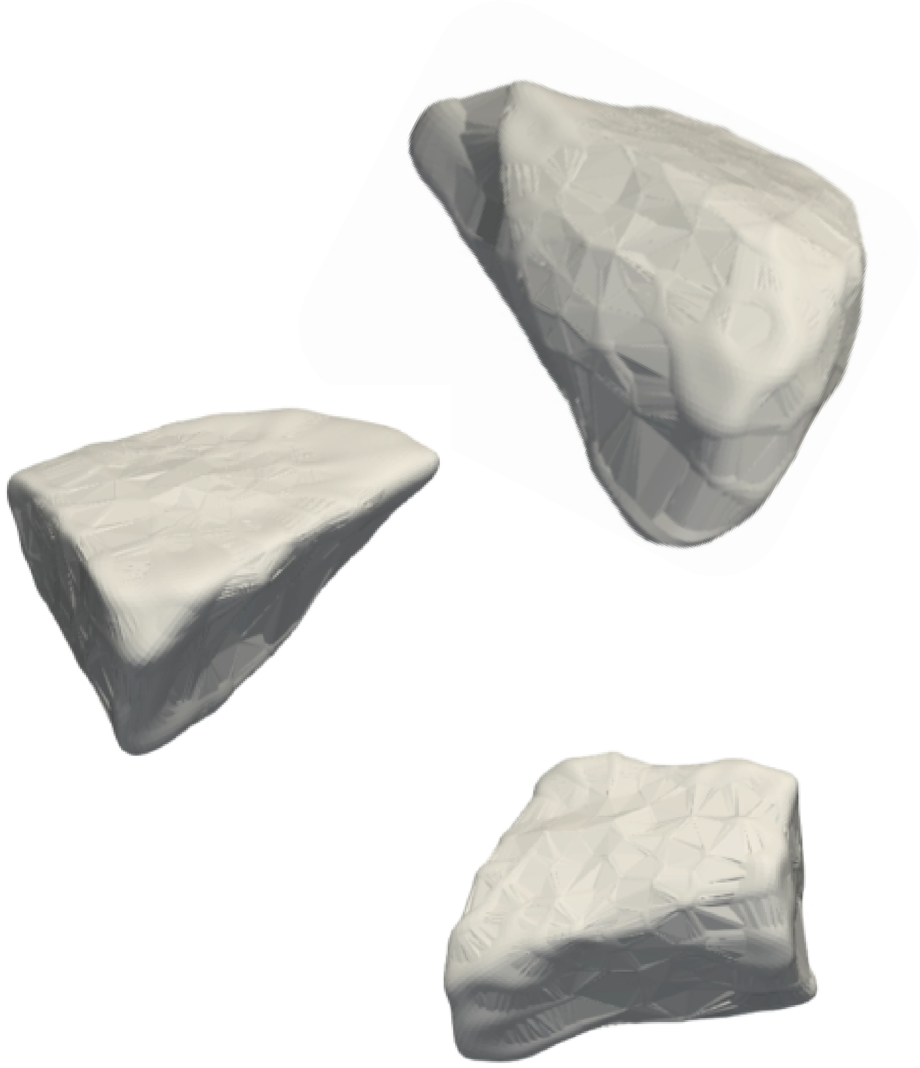




N. A. Farhan et al. *Construction and Building Materials* 196 (2019) 26-42.

Data Analysis

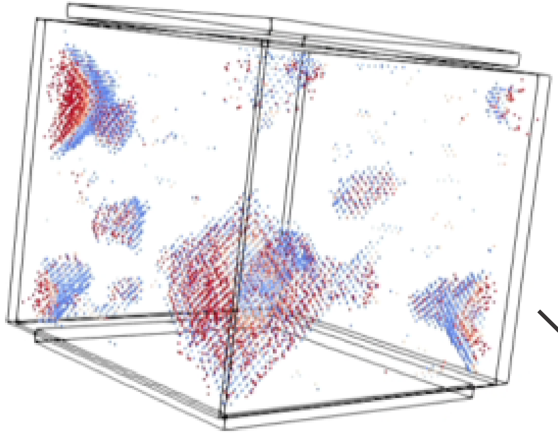
- Define “*good*” and “*bad*” damage resilience
  - Yield strength
  - Total number of damaged nodes
  - Ultimate stress
- *What is unique about the best and worst performers?*
  - Assess aggregate properties
    - Variation with size ranges
    - Shape & aspect ratios
  - Assess microstructure properties
    - Aggregate size gradation
    - Number of aggregate-boundary intersections
- Determine statistical significance:
  - T-Tests
  - Correlation tests



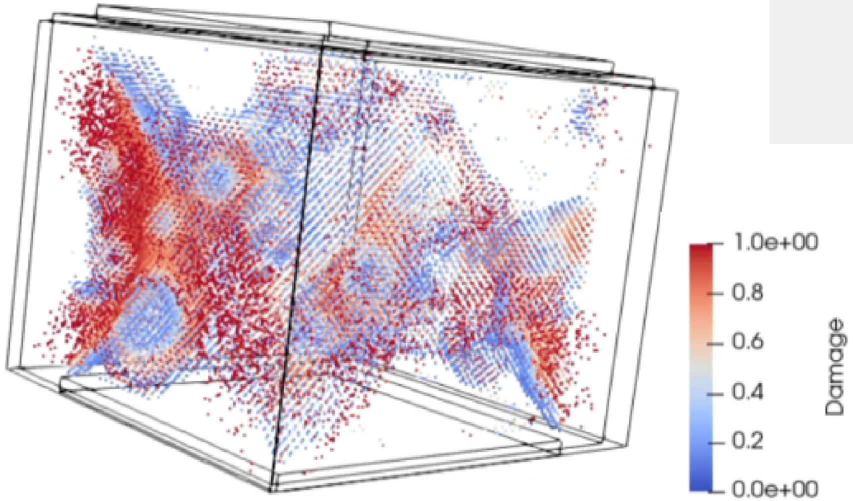
Data Analysis

Damage clusters

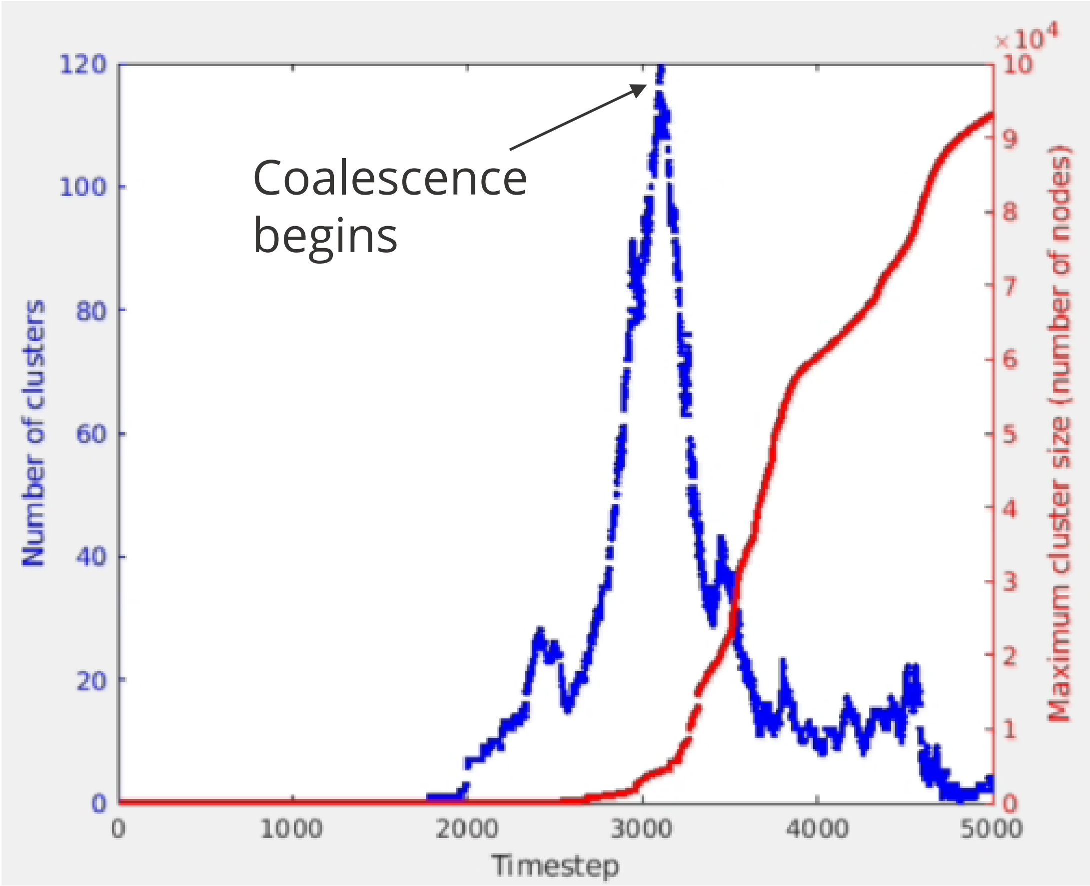
- Assess the formation of damage clusters
- Track the coalescence of damage clusters



Many small, defined clusters



Clusters coalesced into one main, large cluster



Insights

- Rounder aggregates correlate to improved fracture resistance
  - Ratio of maximum and minimum radii
  - Wadell roundness:

$$\frac{Surface\ area\ of\ volume\ equivalent\ sphere}{Surface\ area\ of\ particle}$$

- Aggregates with a width of 9.5mm – 12.5mm show the strongest correlation to yield strength
  - Next strongest correlation was the parameters of the entire aggregate set
  - Correlations identified by statistical tests comparing the best and worst performing microstructures

- Microstructures with lower total aggregate surface area have higher fracture resistance
  - Less ITZ phase

H. A. Wadell. *The Journal of Geology*, 40 (1932), 443-451

Conclusions

- Peridynamics is used to model 3D fracture of concrete under uniaxial loading
  - Tension and compression
  - Meshless method overcomes challenges of meshing composite geometry
  - Lack of spatial derivatives ideal for modeling fracture
- Simulated compressive yield strength is low for concrete
  - Calibration of model is ongoing
- Tensile behavior matches published data well
- Data is analyzed for impactful parameters
  - Aggregates
  - Microstructure

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