The use of AI in Materials Fracture and Damage

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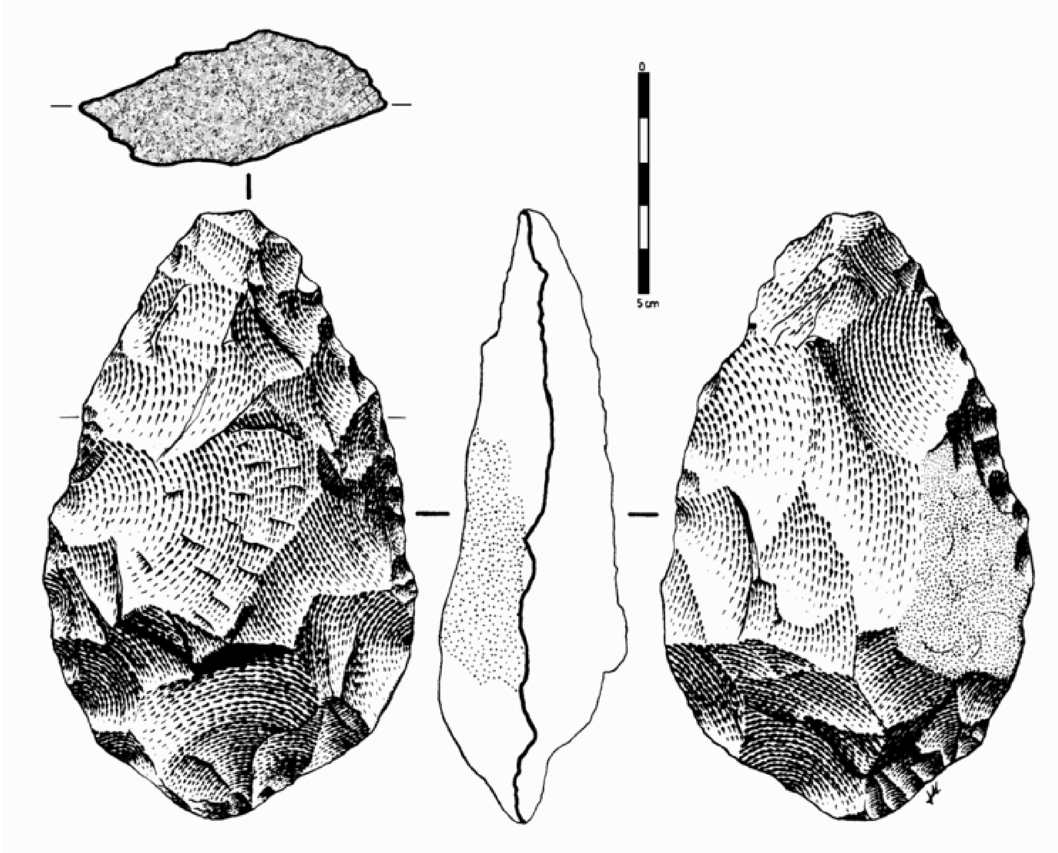
Brittle fracture is almost always to be avoided, unless...

Pre-historic fracture

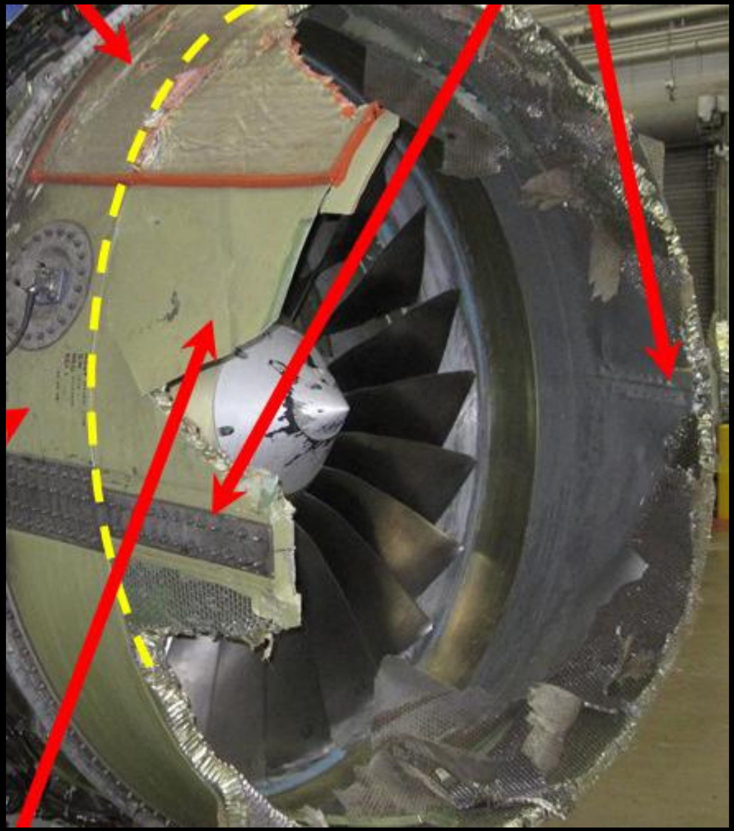
- Stone-age tools: most durable prehistoric remains;
- Flint, quartzite, fine-grained or amorphous materials, silicates (obsidian=volcanic glass).
- Conchoidal (shell-like) fractures can be produced only by mechanical impact (dynamic fracture), rather than, e.g. frost cracking; a method to differentiate prehistoric stone tools from natural stones.



Importance of predicting fracture and damage

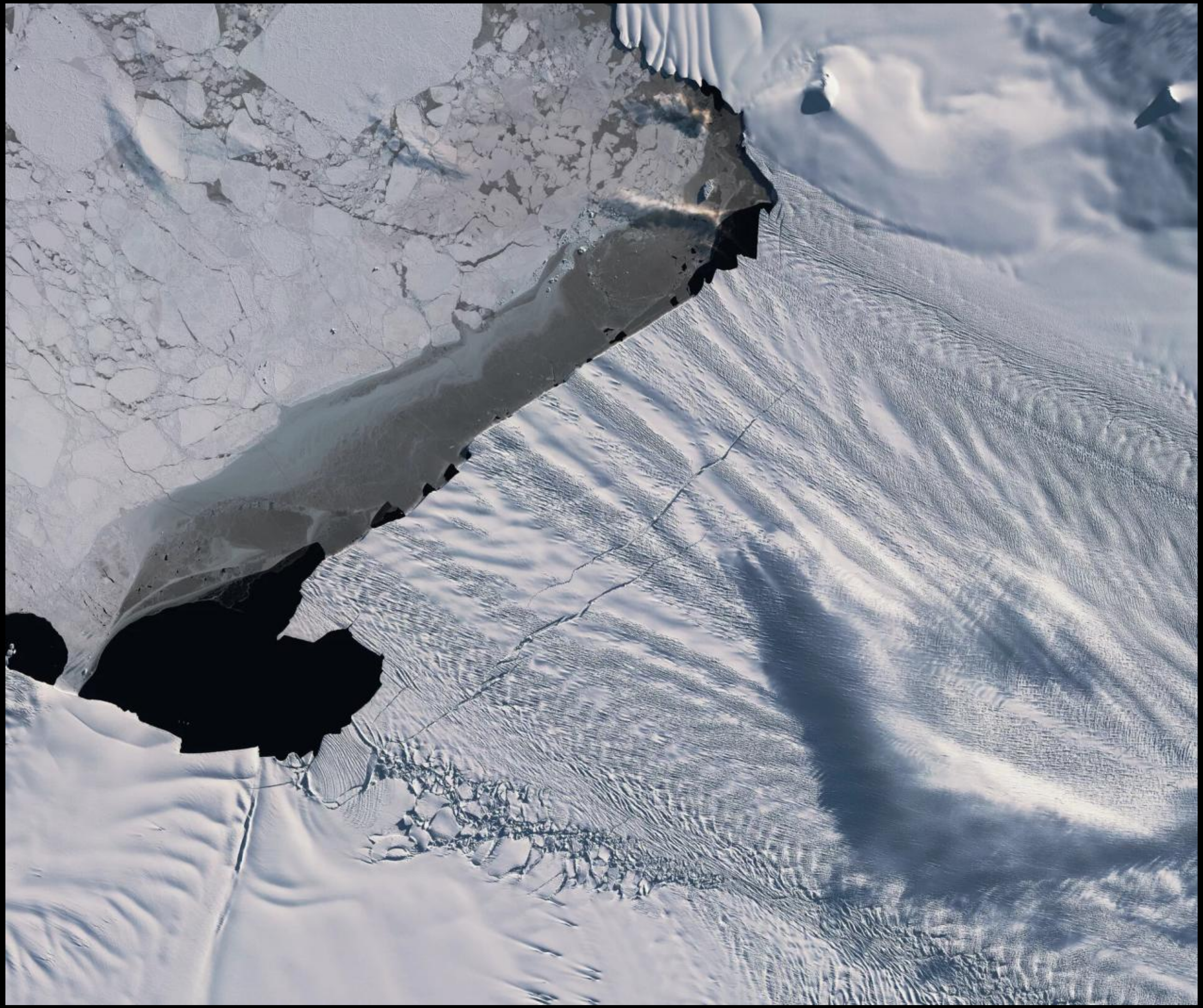
Fracture, damage

- Sometimes catastrophic ….



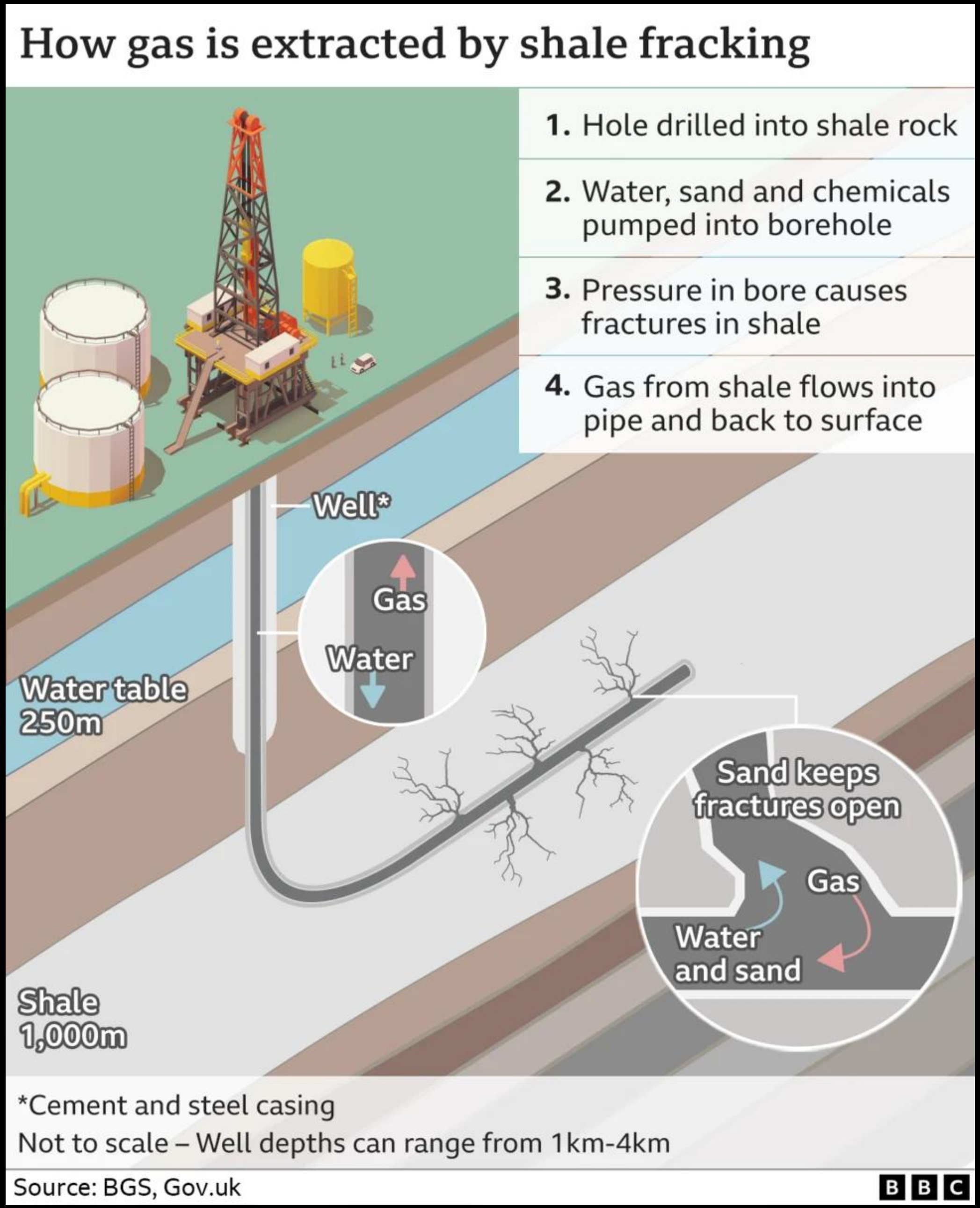
Ice sheet fracture

- its fracture influences melting



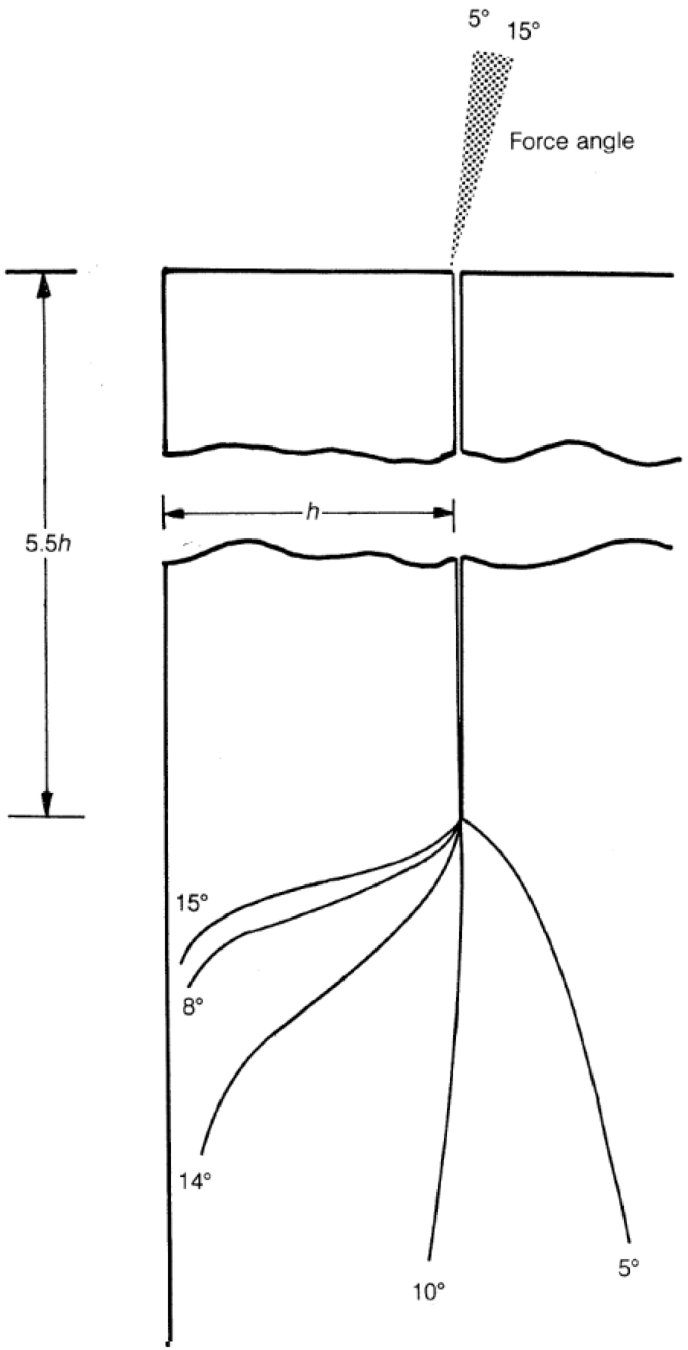
Hydraulic fracturing (fracking):

- Rock fracture induced by pressure pulse
- Can we control the fracture process?



Sensitivity in Brittle Fracture

- Crack path dependence on force impact angle
- Can AI predict what happens for an angle of, e.g., 8°?



Potential Solutions using AI

- Sufficient amount of experimental data (not feasible)
- Sufficient amount of synthetic data (produced by a physics-based model) to train an accurate AI system (possible)
- Are there physics-based models that can accurately simulate dynamic brittle fracture?

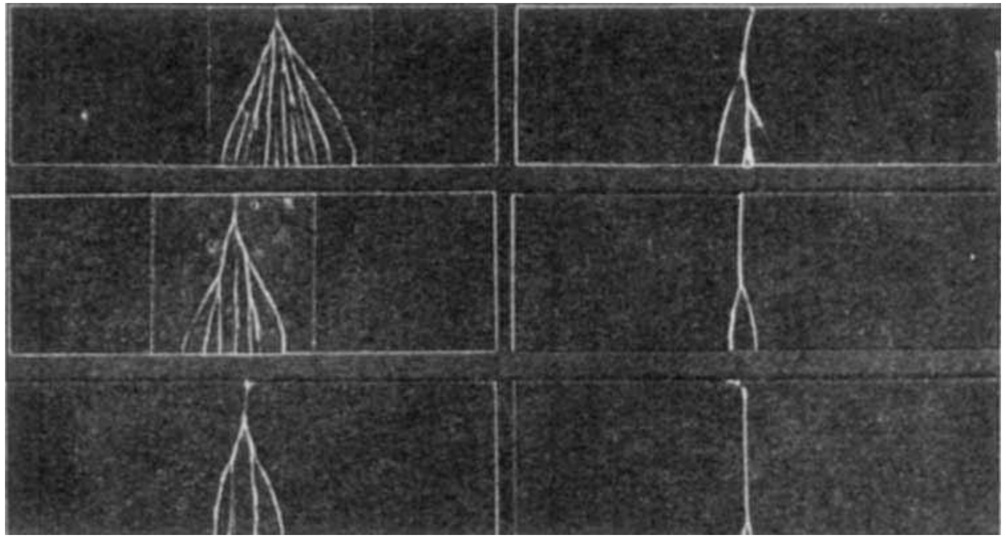
Physics-based models for fracture

- DFT/atomistic models
- Macro-scale (continuum) models:
  - based on classical continuum mechanics: work well for ductile failure, but difficulties predicting dynamic brittle fracture.
  - Peridynamic models: nonlocal extension of classical continuum mechanics

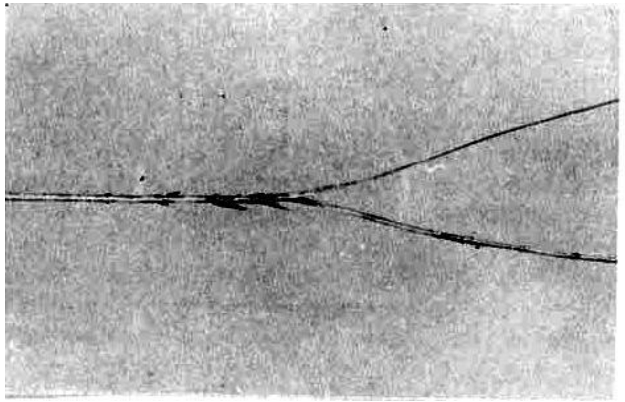
Dynamic brittle fracture and crack branching

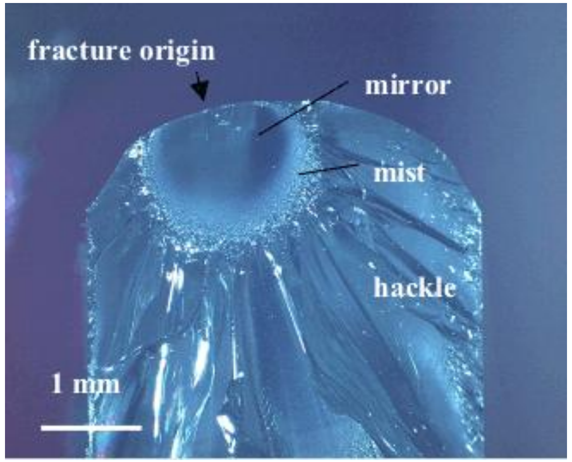
Dynamic fracture/Crack branching

Bowden et al, Nature 1967.



Crack branching in edge-notch homalite (**Ramulu and Kobayashi, IJFM 1985**).

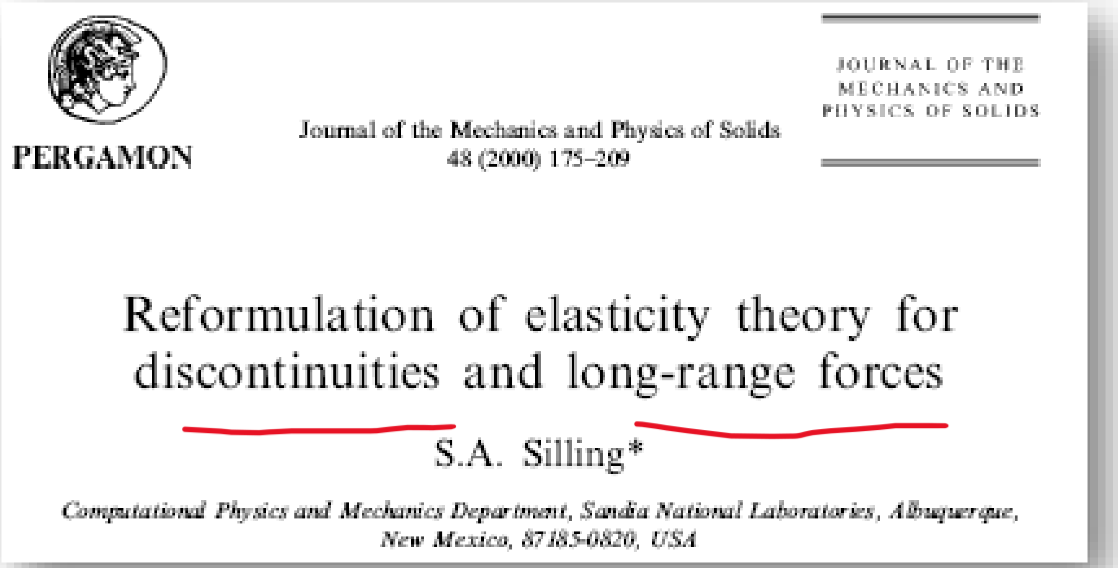




- Roughening of crack surface before branching (mirror-mist-hackle).
- Based on experiments: when a crack reaches a critical state, “it splits into two or more branches, each propagating **with about the same speed as the parent crack, but with a much reduced process zone”** (Ravi-Chandar, 2004).
- **Classical fracture mechanics** predicts crack speed to drop by half after branching. This does not happen!

What is Peridynamics?

Dr. Stewart Silling (Sandia National Labs)



PERGAMON

Journal of the Mechanics and Physics of Solids
48 (2000) 175–209

JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS

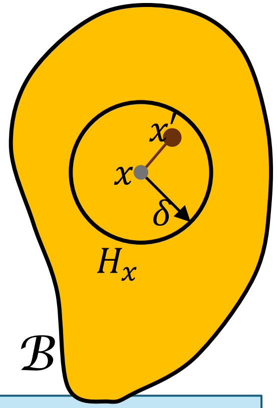
Reformulation of elasticity theory for discontinuities and long-range forces

S.A. Silling*

Computational Physics and Mechanics Department, Sandia National Laboratories, Albuquerque, New Mexico, 87185-0820, USA

Classical continuum mechanics

$$\rho\ddot{\mathrm{u}}(\mathrm{x},t) = div(\sigma(\mathrm{x},t)) + \mathrm{b}(\mathrm{x},t)$$



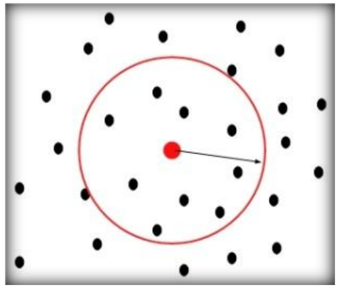
Peridynamics

$$\rho\ddot{\mathrm{u}}(\mathrm{x},t) = \int_{H_x} \mathrm{f}(\mathrm{u}(\mathrm{x}',t) - \mathrm{u}(\mathrm{x},t), \mathrm{x}' - \mathrm{x})dV\mathrm{x}' + \mathrm{b}$$

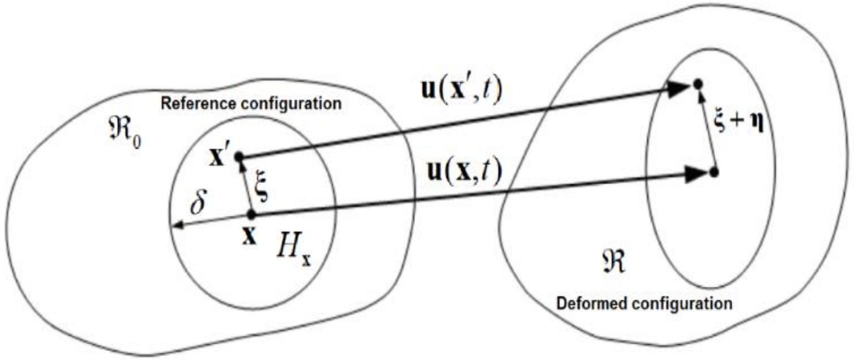
- Integro-differential equation
- No spatial derivatives (integral operators);
- Damage (from which fracture evolves): a general nonlinear mapping (not a scalar or even a tensor)

Introduction to PD

- Material point *x* interacts with other points (via PD *bonds*) within a distance called "*horizon*".



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

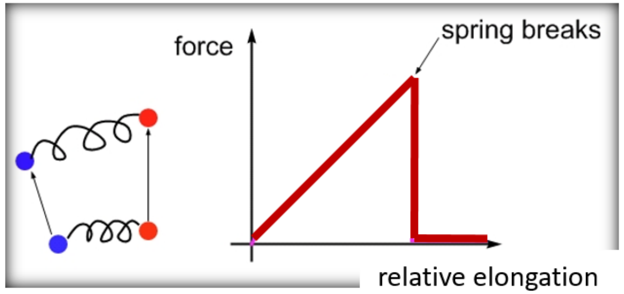


- **<u>Prototype Microelastic Brittle (PMB) material model</u>**

$$f(\boldsymbol{\eta},\boldsymbol{\xi}) = \begin{cases} \dfrac{\boldsymbol{\xi}+\boldsymbol{\eta}}{\|\boldsymbol{\xi}+\boldsymbol{\eta}\|} c(\xi)s & \xi \le \delta \\ \mathbf{0} & \xi > \delta \end{cases}$$

Relative bond elongation:

$$s(\boldsymbol{\eta},\boldsymbol{\xi}) = \frac{\|\boldsymbol{\eta}+\boldsymbol{\xi}\| - \|\boldsymbol{\xi}\|}{\|\boldsymbol{\xi}\|}$$



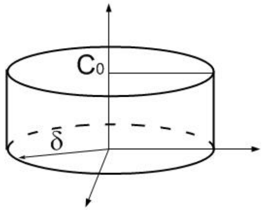
Z. Chen, D. Bakenhus, F. Bobaru. "A constructive peridynamic kernel for elasticity, *CMAME*, **311**, 356-373 (2016).

- Silling, S. A., *JMPS*, 2000.
- Ha, Y. D., & Bobaru, F., *IJF*, 2010.
- Silling, S. A., & Askari, E., *Computers & structures*, 2005.

Calibration of bond properties

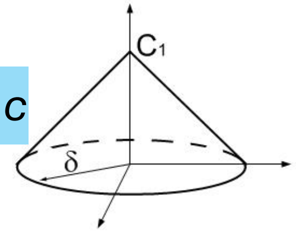
- **Micro-modulus function (c):**
  - match **elastic strain energy** for **a homogeneous deformation** to classical elasticity value

constant c



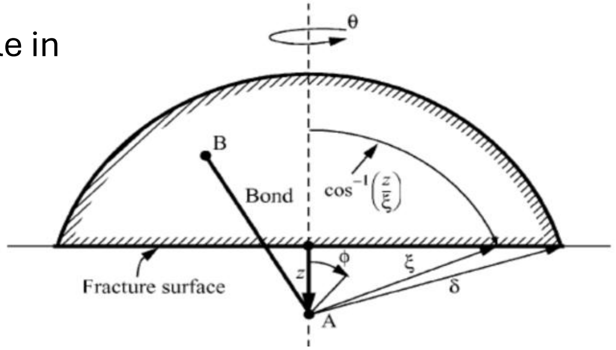
$$c(\xi) = c_0 = \frac{6E}{\pi\delta^3(1-\nu)}$$

conical c



$$c(\xi) = \frac{24E}{\pi\delta^3(1-\nu)}\left(1 - \frac{\|\xi\|}{\delta}\right)$$

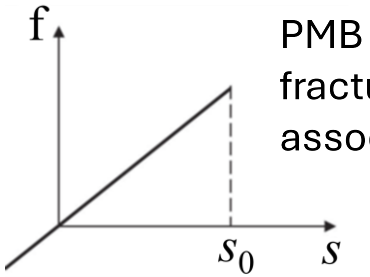
- **Critical relative elongation (s_0):** match **fracture energy** with the energy required to break sample in two



$$G_c = \begin{cases} \int_0^{\delta}\int_0^{2\pi}\int_z^{\delta}\int_0^{\cos^{-1}\left(\frac{z}{\xi}\right)}\left[\frac{c(\xi)s_0^2\xi}{2}\right]\xi^2\sin\phi\, d\phi\, d\xi\, d\theta\, dz, & \text{3D} \\ 2\int_0^{\delta}\int_z^{\delta}\int_0^{\cos^{-1}\left(\frac{z}{\xi}\right)}\left[\frac{c(\xi)s_0^2\xi}{2}\right]\xi\, d\theta\, d\xi\, dz, & \text{2D} \end{cases}$$

constant c

$$s_c = \begin{cases} \sqrt{\frac{5G_c}{6E\delta}}, & 3D \\ \sqrt{\frac{4\pi G_c}{9E\delta}}, & \text{2D plane stress} \\ \sqrt{\frac{5\pi G_c}{12E\delta}}, & \textit{2D plane strain} \end{cases}$$

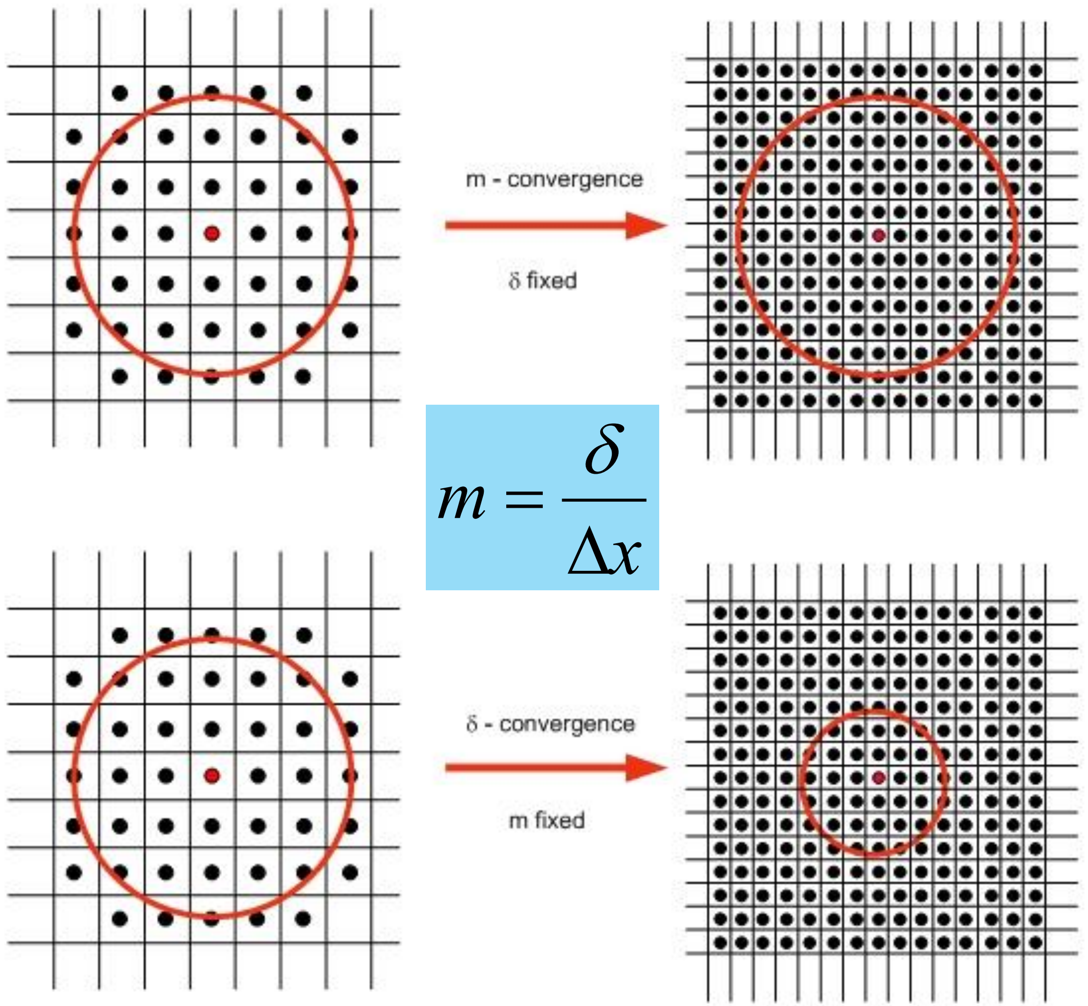


PMB model uses a single fracture parameter, associated with G_c

- Ha, Y. D., & Bobaru, F., *IJF*, 2010.
- Silling, S. A., & Askari, E., *Computers & structures*, 2005.

Convergence in Peridynamics

- Graphical description for ***m*-convergence** and **δ-convergence**:



$$m = \frac{\delta}{\Delta x}$$

Convergence to exact nonlocal solution

Chen, Peng, Jafarzadeh, Bobaru. “Analytical solutions of peridynamic equations. Part II: Elastic wave propagation”- *International Journal of Engineering Science*, (2023)

m: horizon factor
δ: horizon size
Δx: discretization size

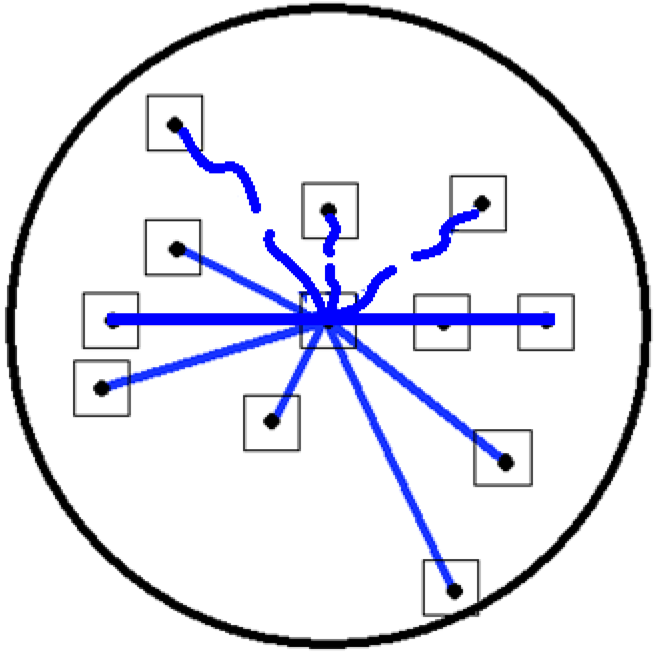
Convergence to exact classical solution (if one exists)

- Ha & Bobaru, *International Journal of Fracture* (2010)

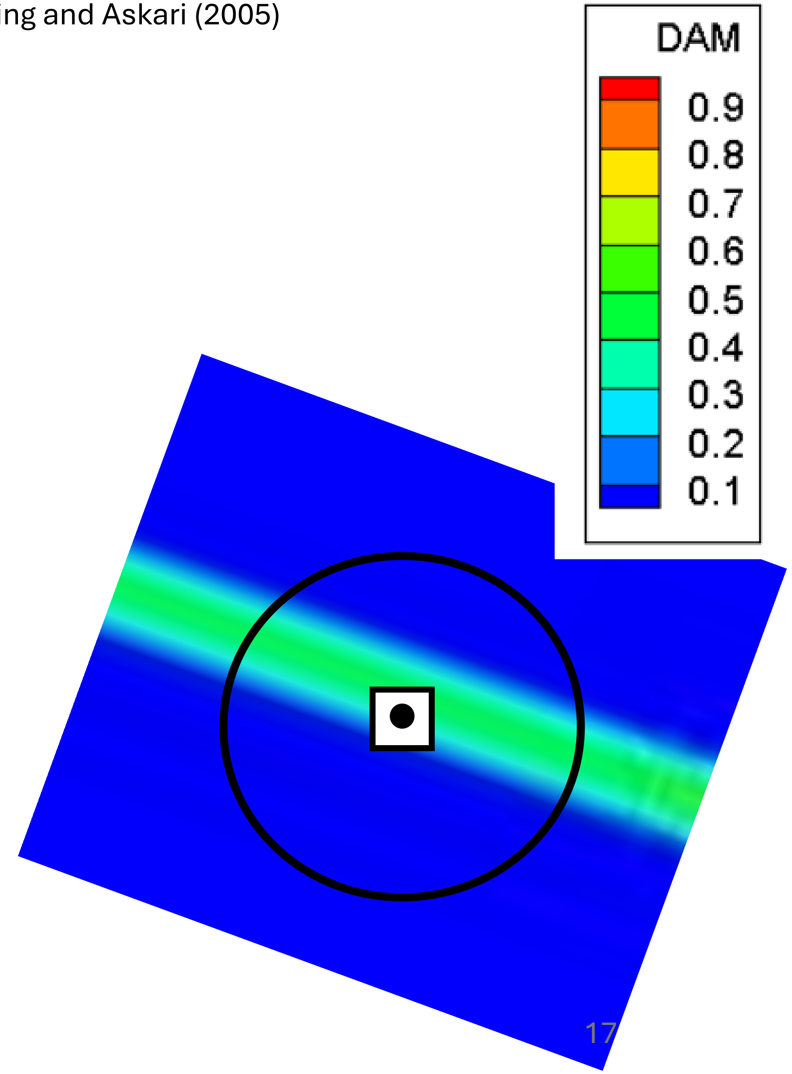
How do cracks form in PD?

Nodal Damage Index

$$d = \frac{n_{\text{broken}}}{n}$$



S.A. Silling (2000)
Silling and Askari (2005)



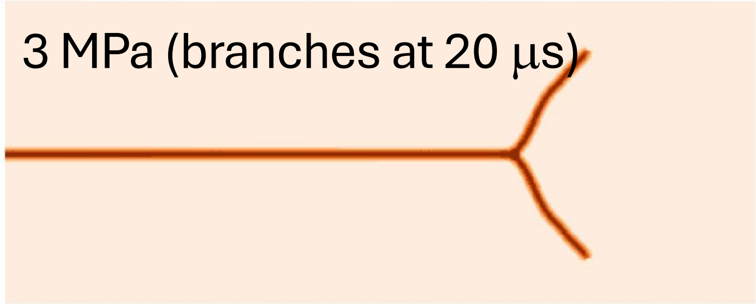
- d is between 0 and 1.
- A value d= 0.4-0.5 localized along a line (in 2D) or surface (in 3D) indicates that a crack has formed.
- Cracks/damage are autonomous
- PD Damage ≠ Nodal damage Index

in PD, damage has directionality (a nonlinear mapping, more general than scalar or tensor quantities used in Continuum Damage Mechanics).

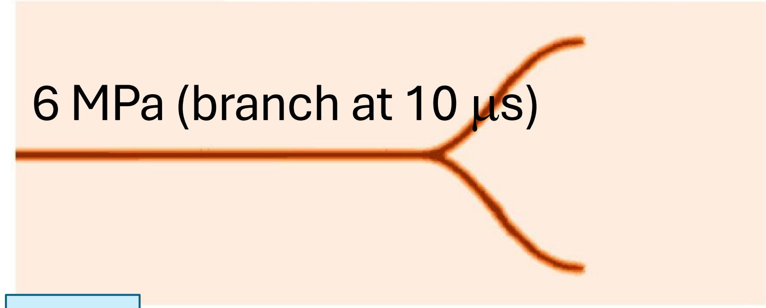
Peridynamic model results for crack branching

0.5 MPa

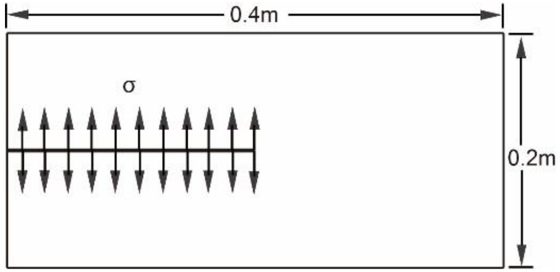
3 MPa (branches at 20 μs)



6 MPa (branch at 10 μs)



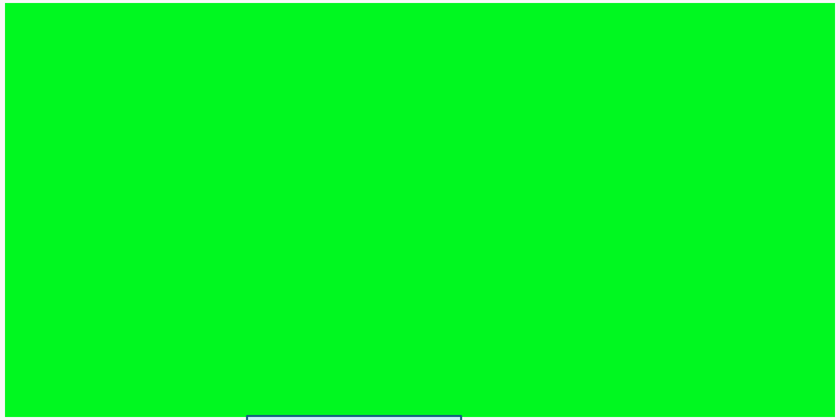
glass



Vertical velocity

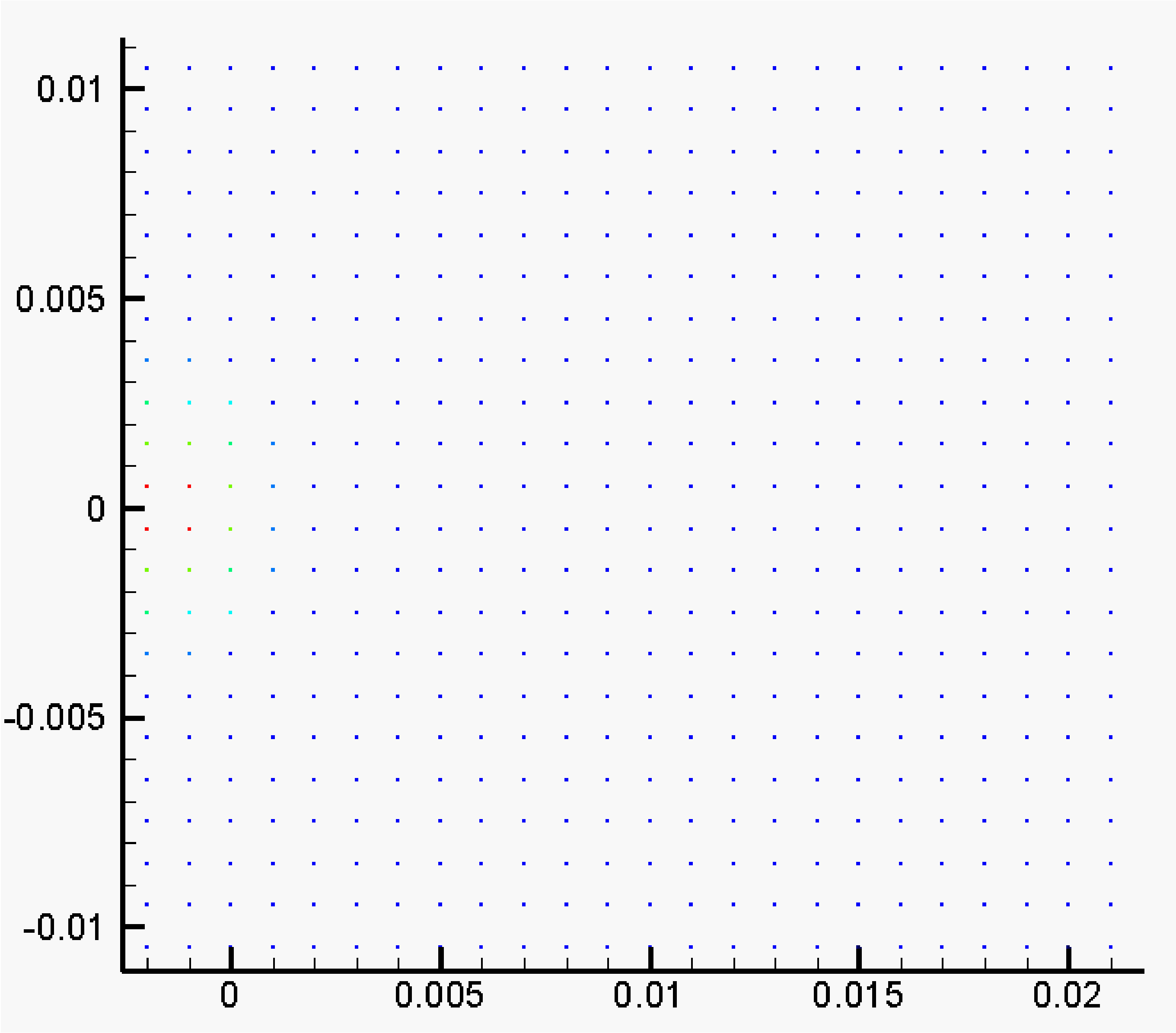
Reflected waves interact before branching

Branching before reflected waves return



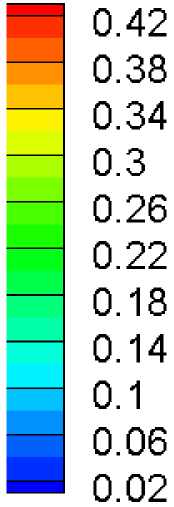
homalite

At low stress levels: straight crack

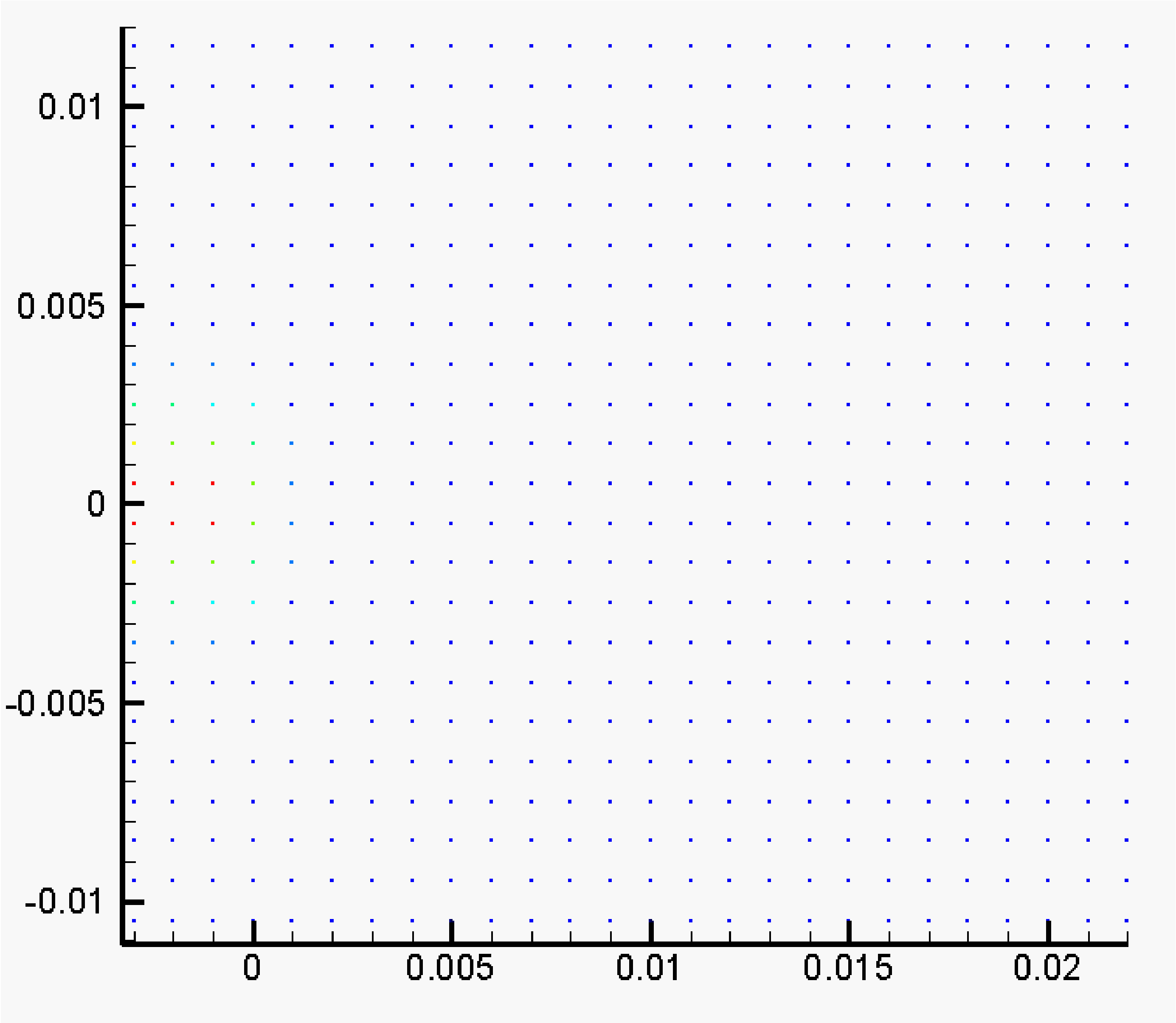


Arrows: nodal velocity vectors

Arrow Color:
nodal damage index (red>50%)

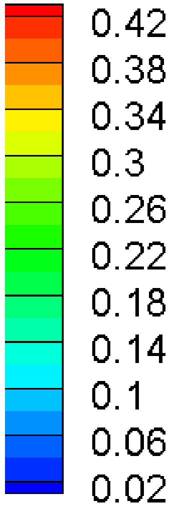


Higher applied amplitude loading



Arrows:
nodal velocity vectors

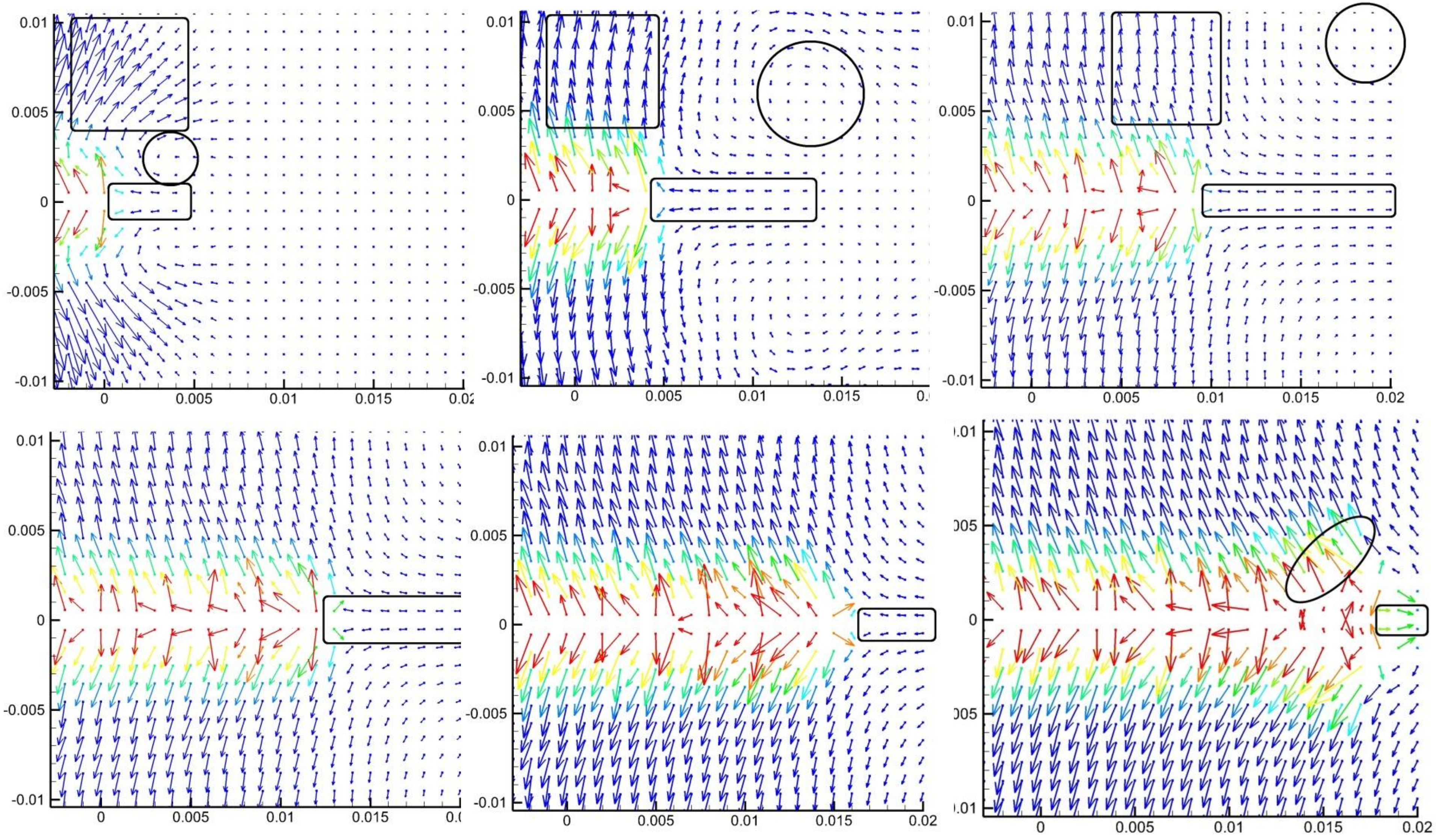
Arrow Color:
nodal damage index (red>50%)



“pile-up” of crack surface waves deflected by **material moving strongly against the propagating crack**

Bobaru and Zhang, Int. J. Fracture (2015)

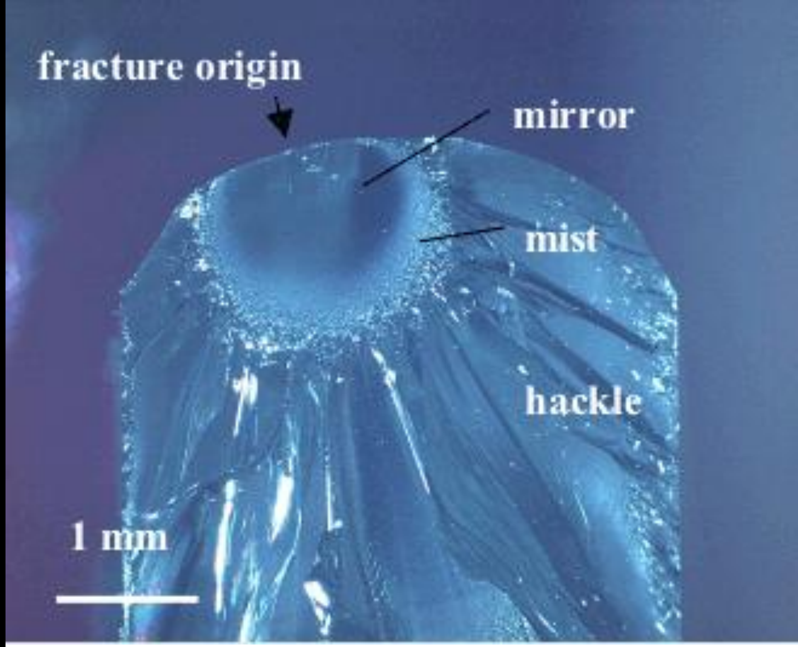
Migration of damage away from the crack line = surface roughening

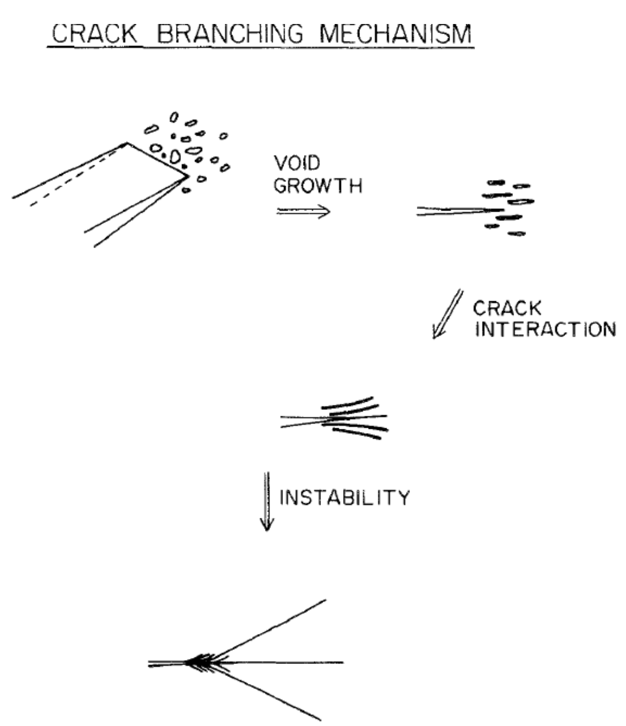


F. Bobaru and G. Zhang, “Why do cracks branch? A peridynamic investigation of dynamic brittle fracture”, *Int. J. of Fracture*, **196**(1): 59-98 (2015).

Need model flexibility to capture the actual “geometry” of crack growth

- Roughness on crack surfaces
- Dynamic cracks may branch
- Micro-damage in the process zone





Crack versus Damage

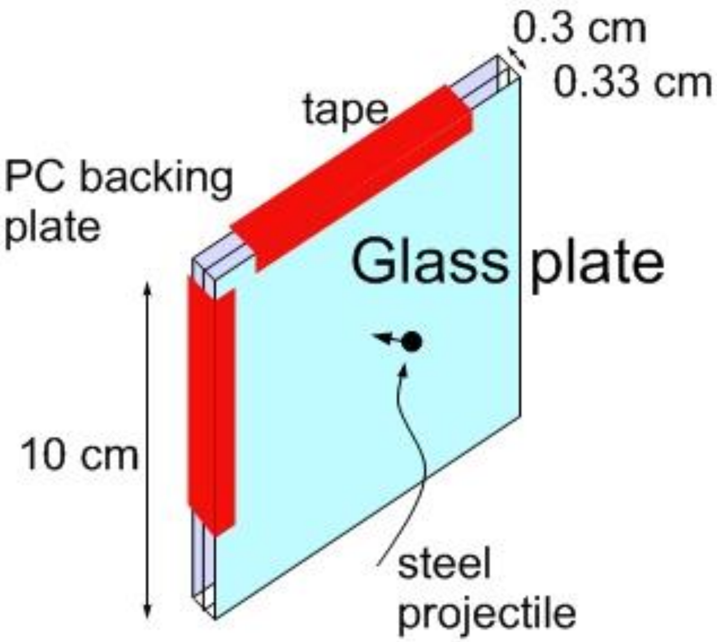
In peridynamics, they are the same!

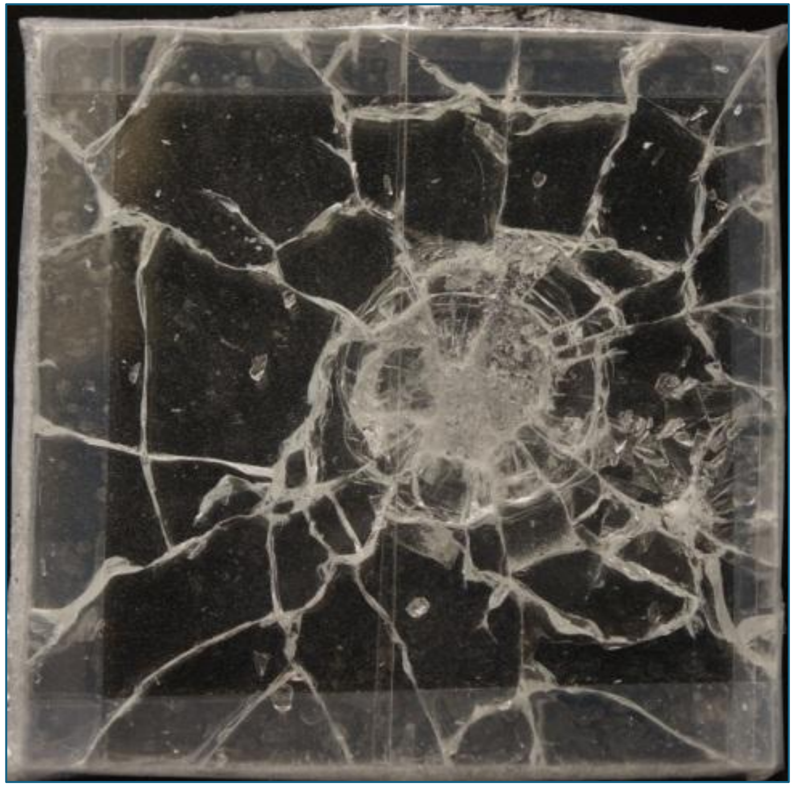
In PD, the solution decides if damage is “diffuse” or “localizes” into a crack

“in PD cracks are part of the solution, not part of the problem.”

Impact-damage in glass

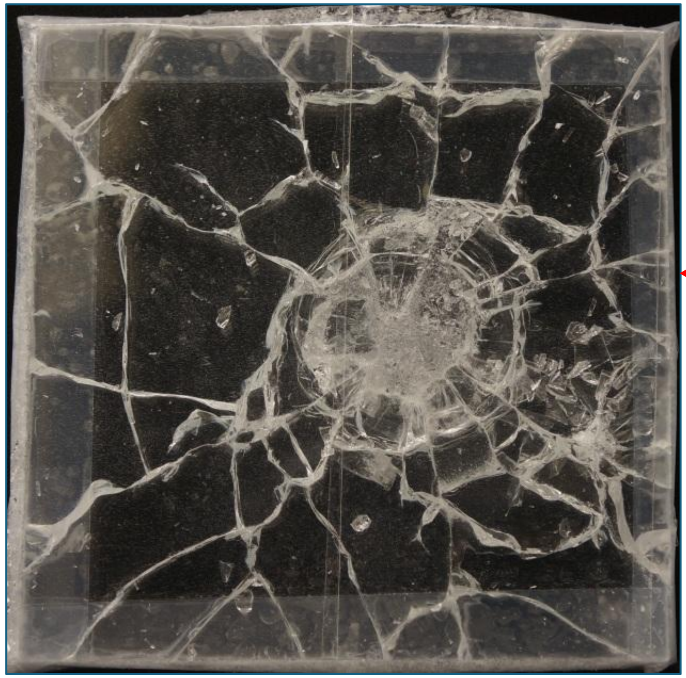
- Plates suspended to mimic “free boundary conditions”.
- Impact speeds of up to 150m/s: no damage observed in the PC plate.
- Tape used along the boundaries (to recover fragments after impact).
- Impact location is off-center (1 cm closer to the right).





Strike and back faces of glass at 150m/s

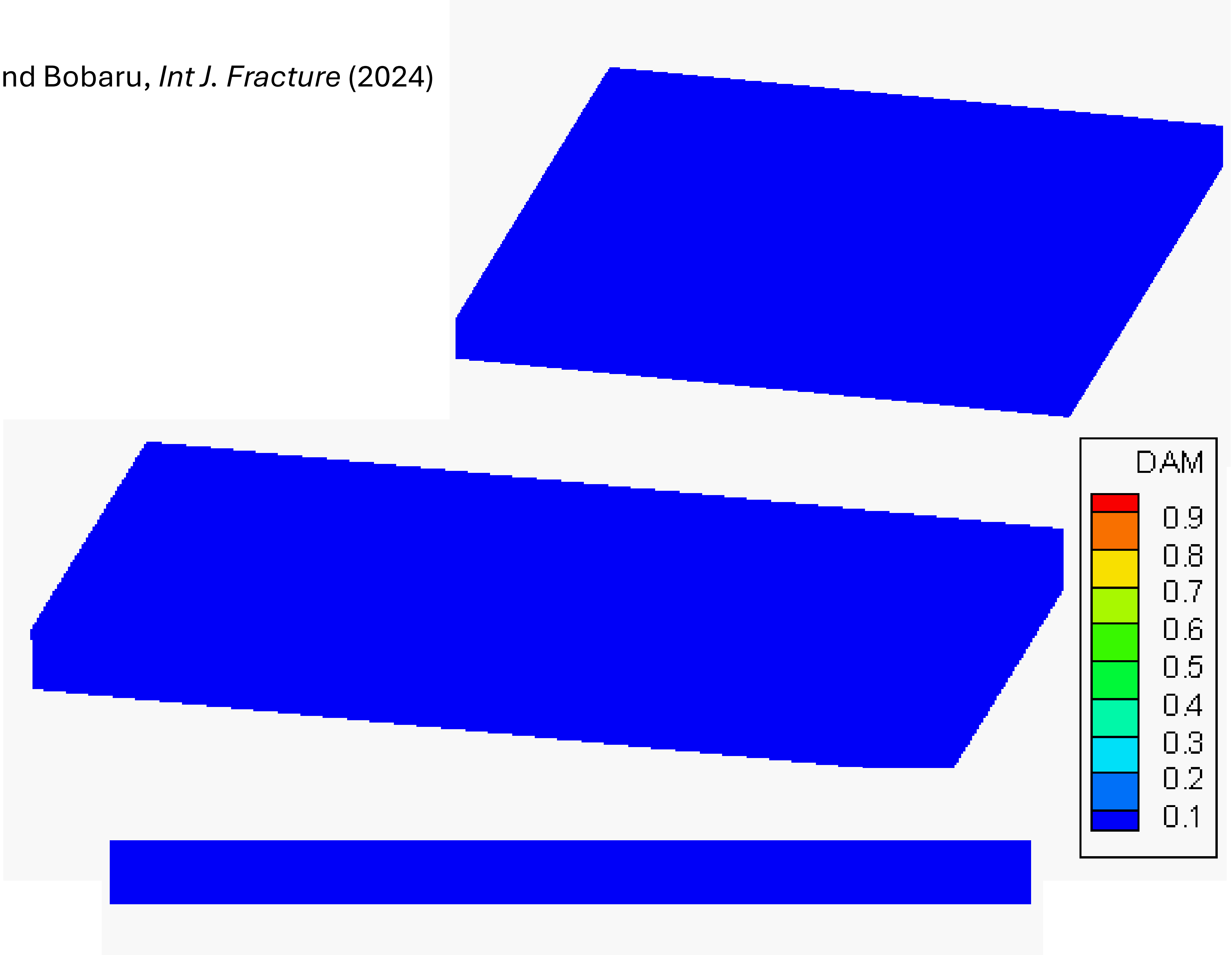
- About 33-35 major fragments; many through-thickness cracks tilted.
- Major radial cracks, some “branch” before reaching boundaries.
- Impact cone: small region of comminuted material on strike face, more damage on the back face of the plate.
- Major circumferential cracks, and some very fine, wispy lines/”cracks” up to 3.8-4 cm diameter around impact center.
- Some cracks are parallel to boundaries.

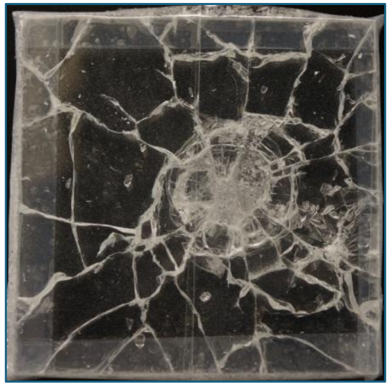


Strike face

Back face

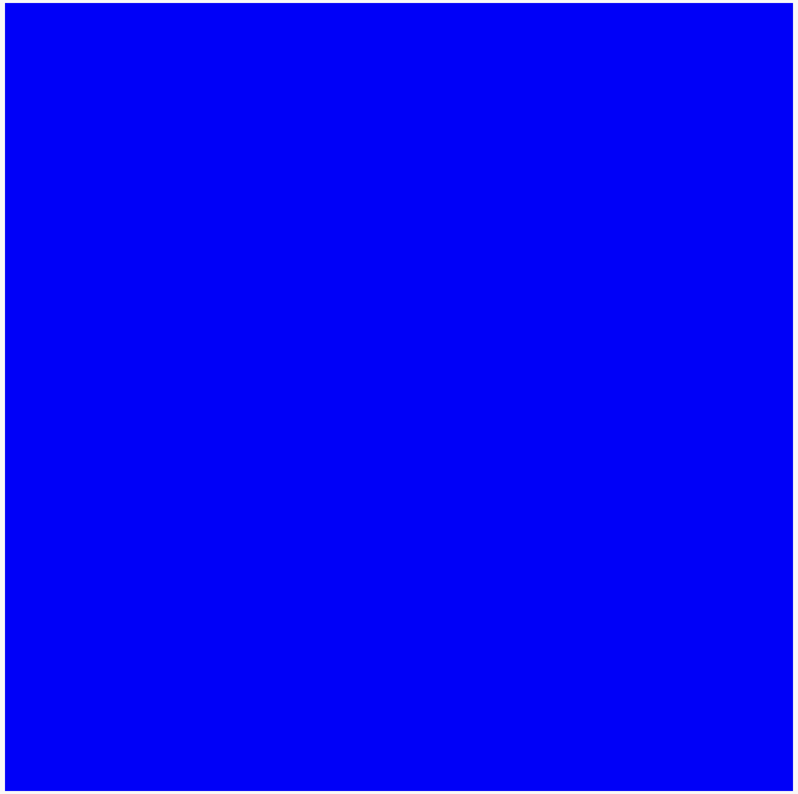
Wang, Yu, Yen, and Bobaru, *Int J. Fracture* (2024)

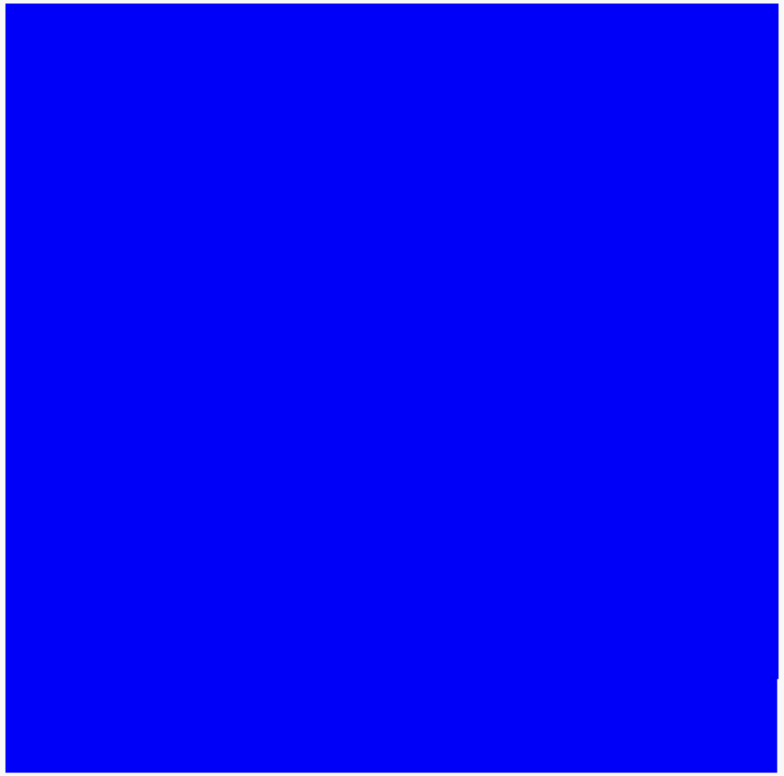




Strike face

Back face



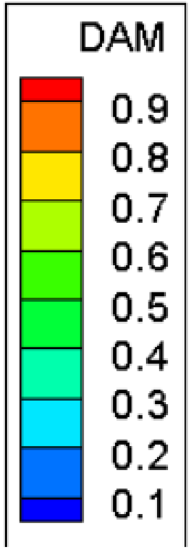


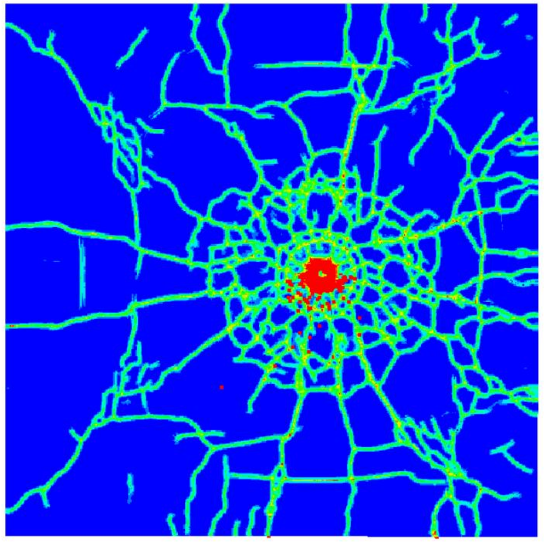
Strike face

Back face

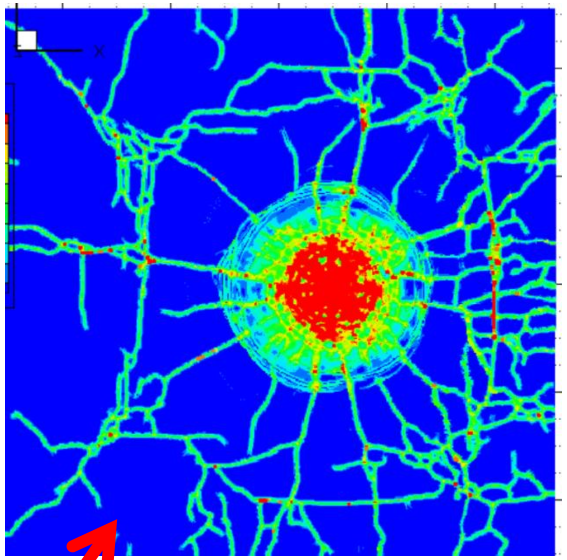
PD results: impact speed 150m/s; damage at 100 μs after impact

- Similar number of major fragments as in experiments (~33-35)
- Similar structure of cone fracture, radial cracks, and circumferential cracks as in exp.
- Some cracks parallel to the side boundaries.
- Some cracks "branch" near boundaries.
- Set of wispy "cracks" seen on back face: same outer diameter as in experiments (~3.8-4 cm), non-symmetrical.



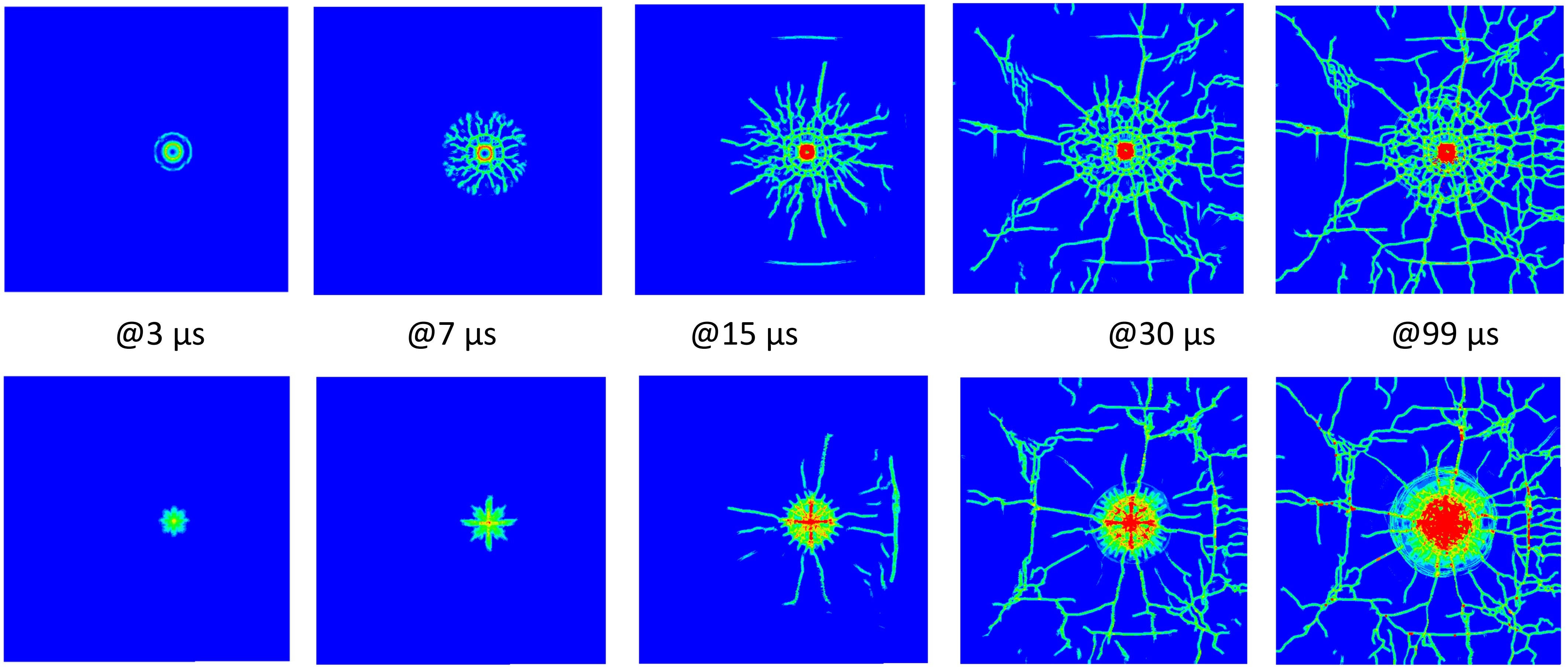


Strike face



Back face

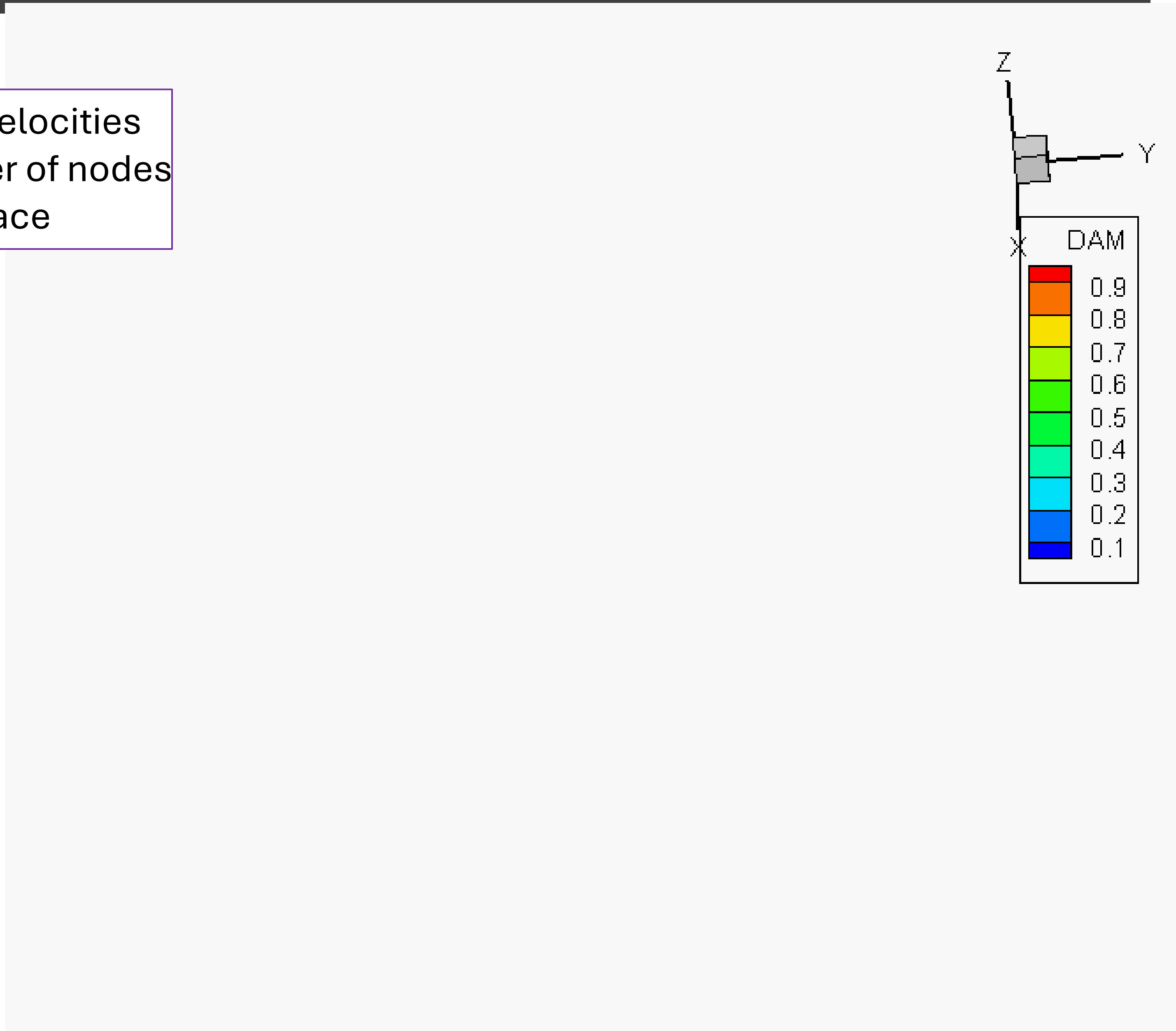
The evolution of damage



See 16 simulation movies in Wang, Yu, Yen, and Bobaru, *Int J. Fracture* (2024)

Understanding what “drives” the propagation of radial cracks

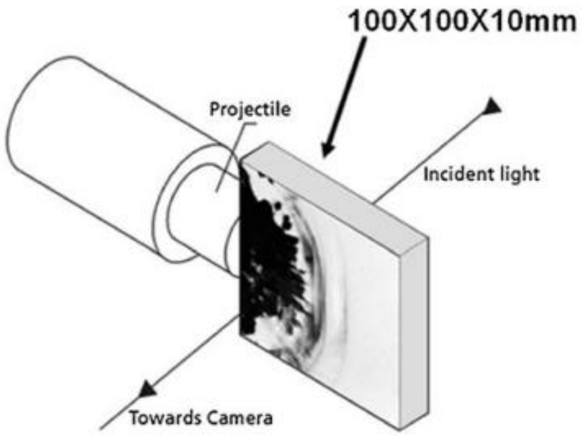
Out-of-plane nodal velocities for a section of a layer of nodes near the impact surface



Edge-on impact on polycrystalline ceramics

Experiment

McCauley, J. W., et al. "Experimental observations on dynamic response of selected transparent armor materials." *Experimental Mechanics* 53.1 (2013): 3-29.



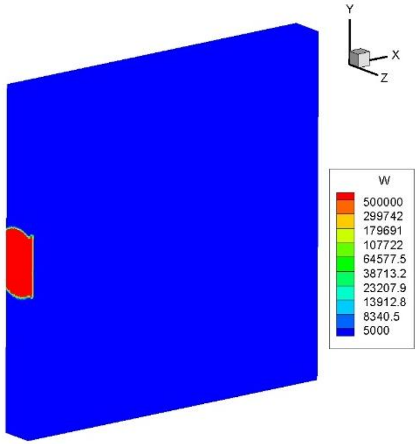
- Sample size 10x10x1 cm
- 4-30 GPa pressure imparted by impactor
- 10μs needed for p-wave to arrive right boundary

PD simulation

PD simulation:

- Sample size 2.5x2.5x0.25 mm

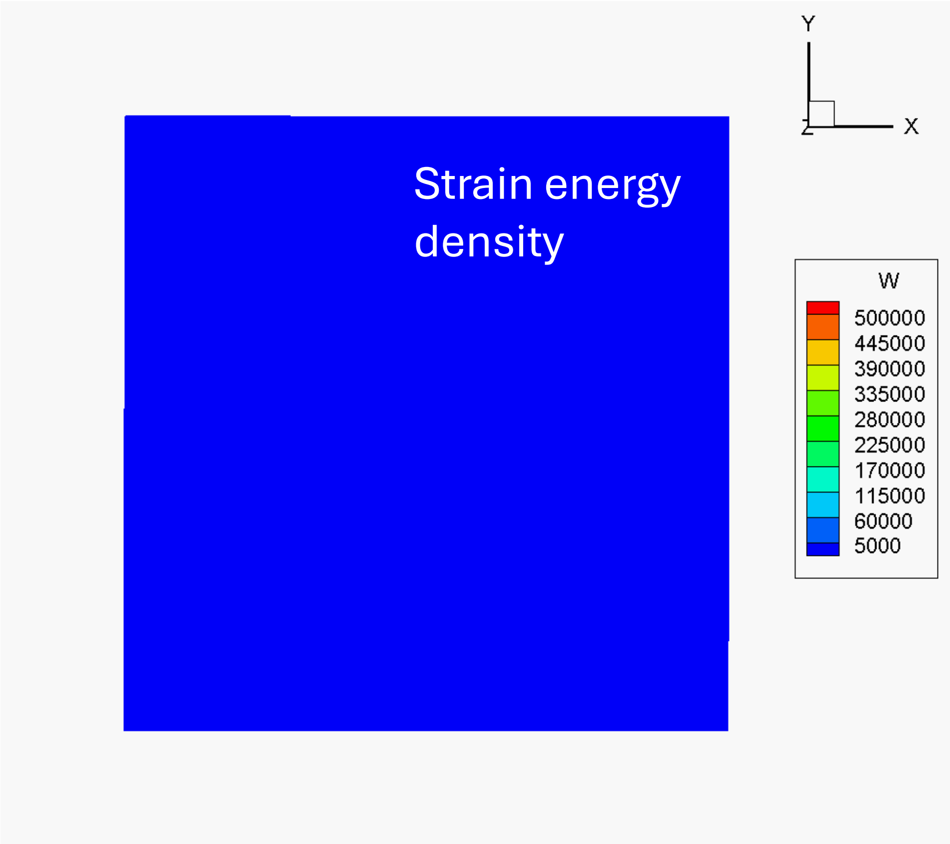
195 grains of actual size

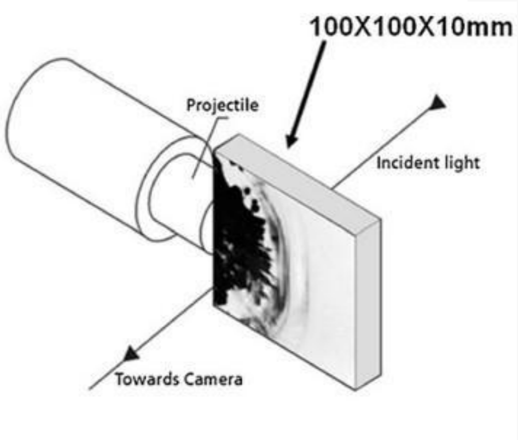


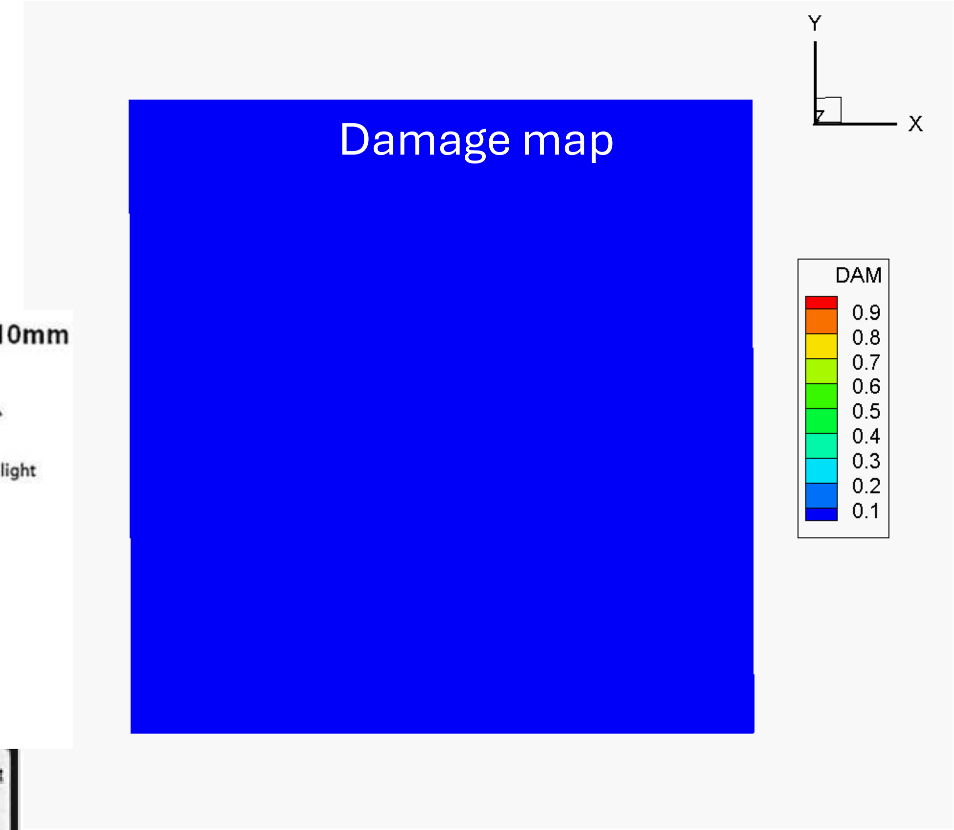
4GPa applied on a circular region (radius = 0.24mm) of left surface (x = -1.25mm)

Super-shear damage front and sub-sonic cracks

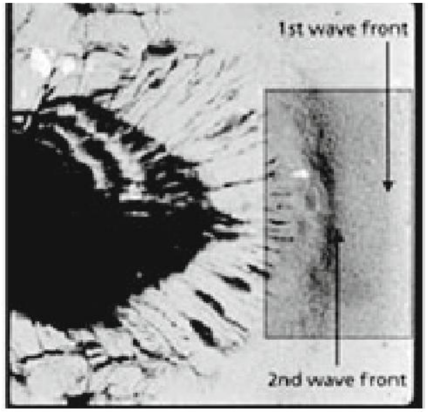
Zhang, Gazonas, and Bobaru. *Int. J. Impact Engineering* (2018)







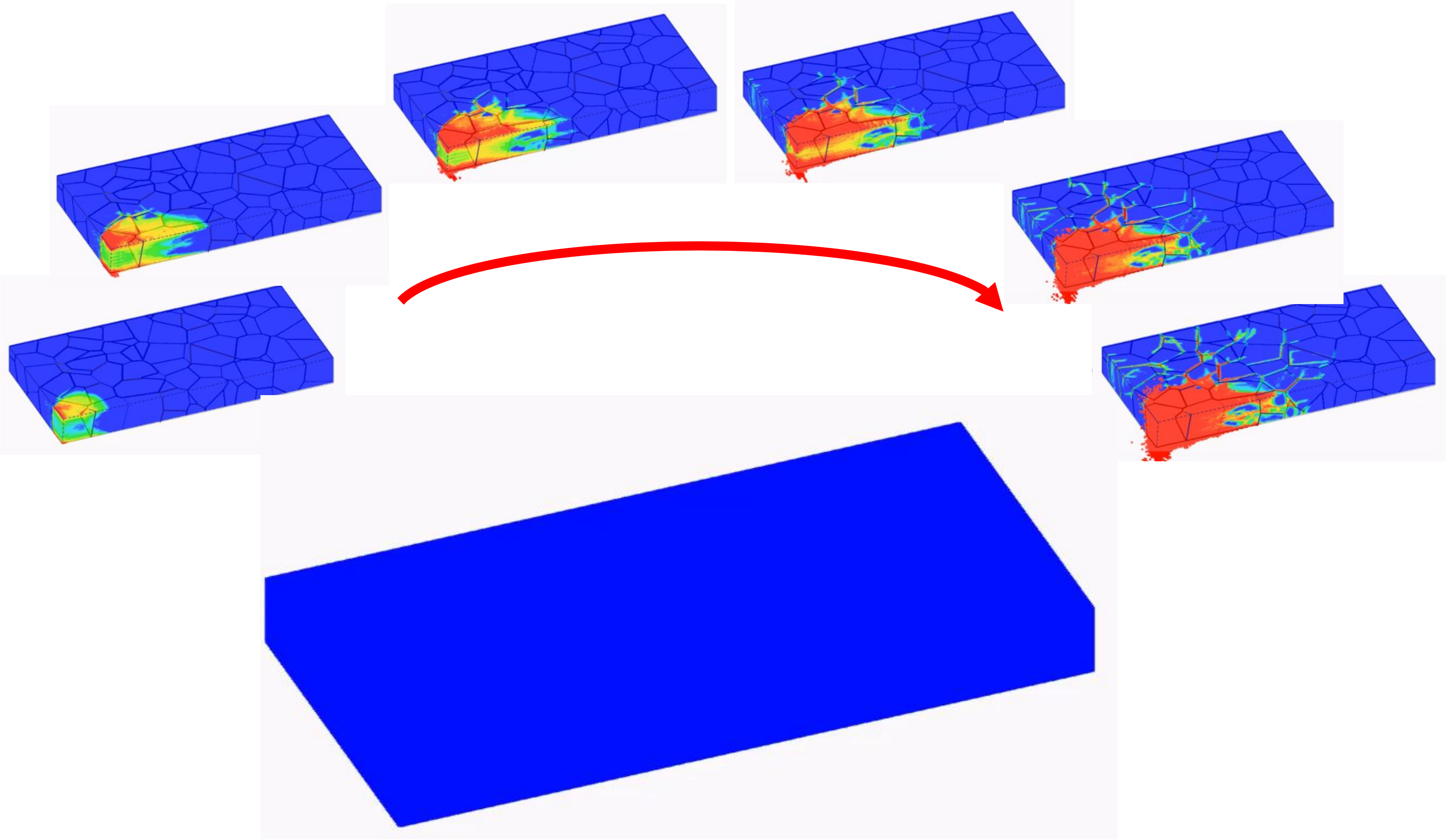
Surface damage in experiment (380m/s impact velocity)



Shape of computed failure zone is similar to that in experiment.

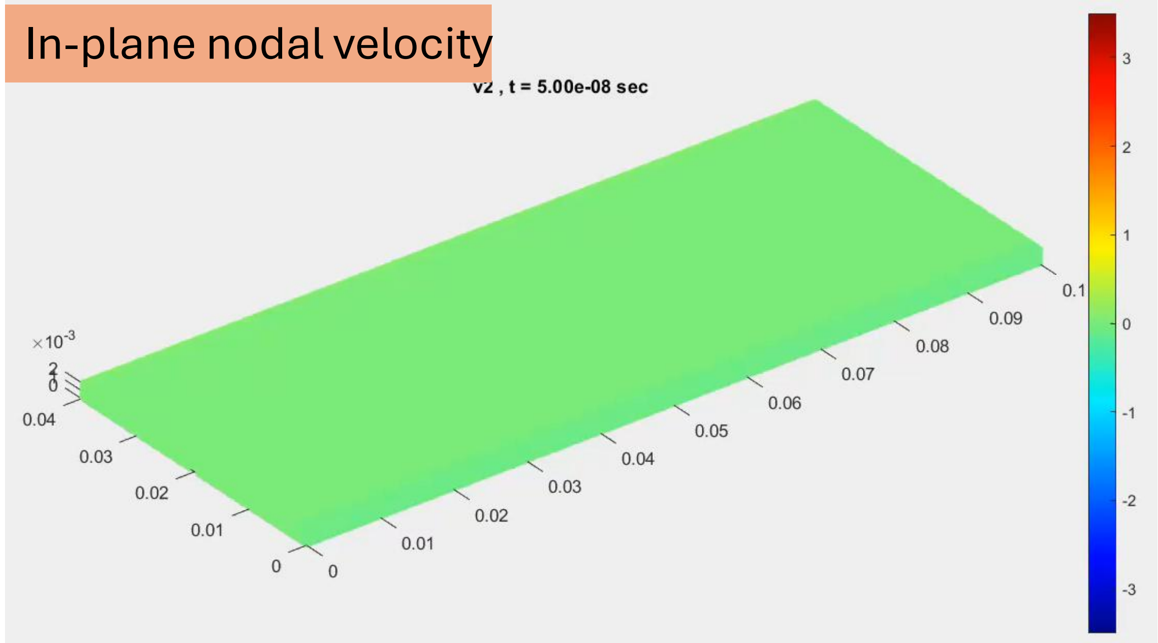
McCauley, J. W., et al. *Experimental Mechanics* **53**(1):3-29, 2013.

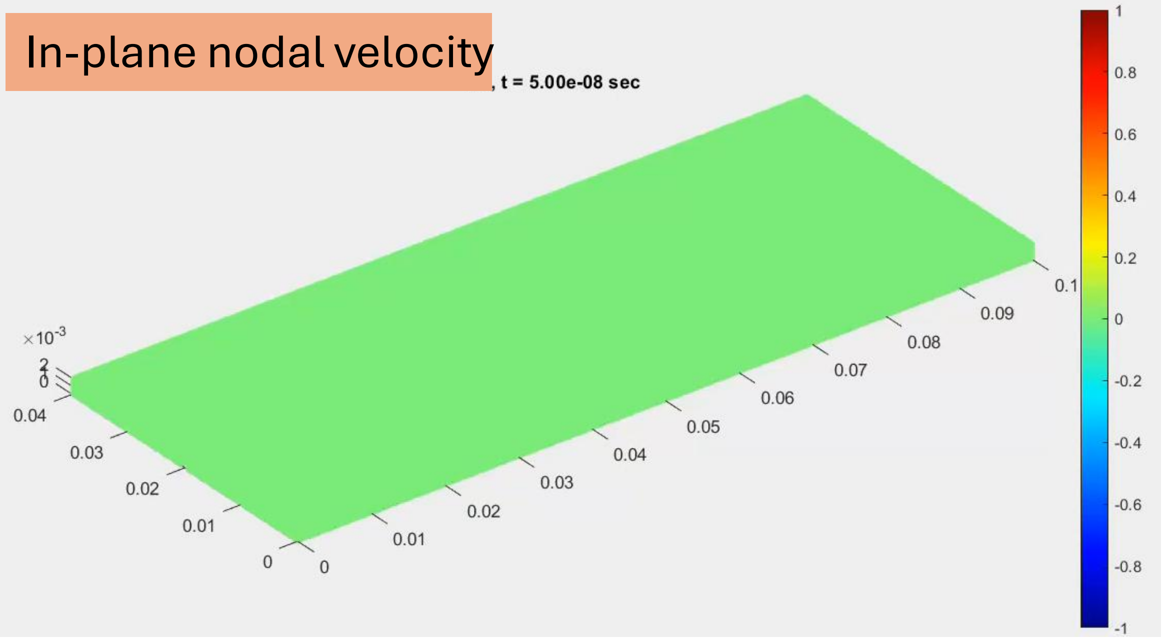
Autonomous Evolution of Damage

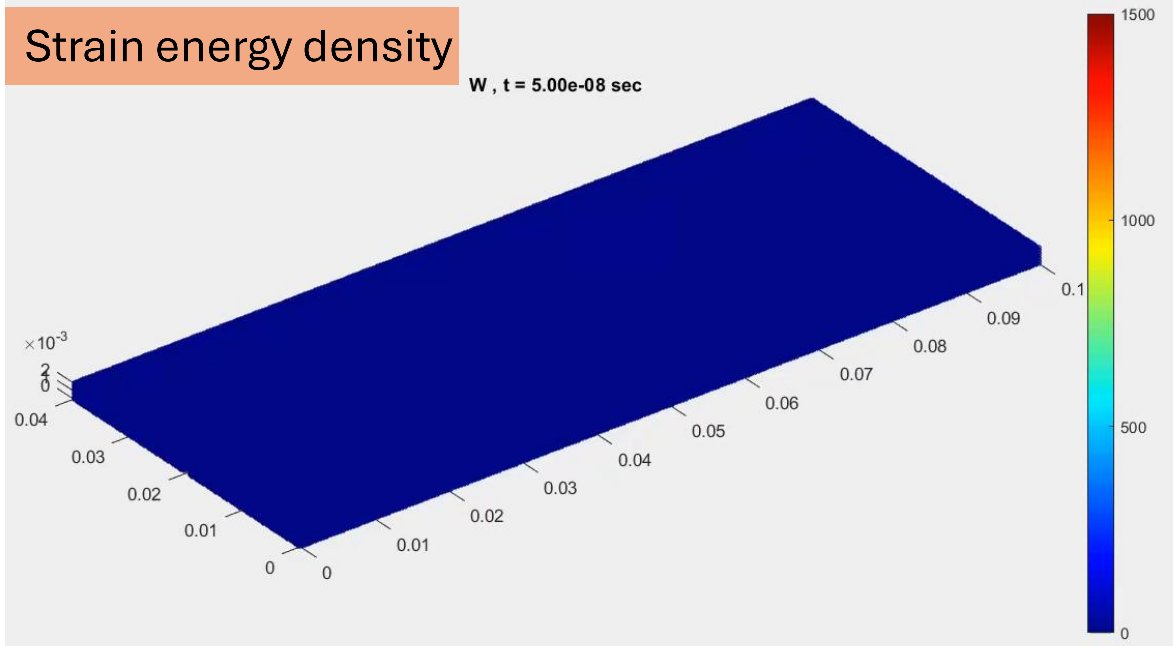


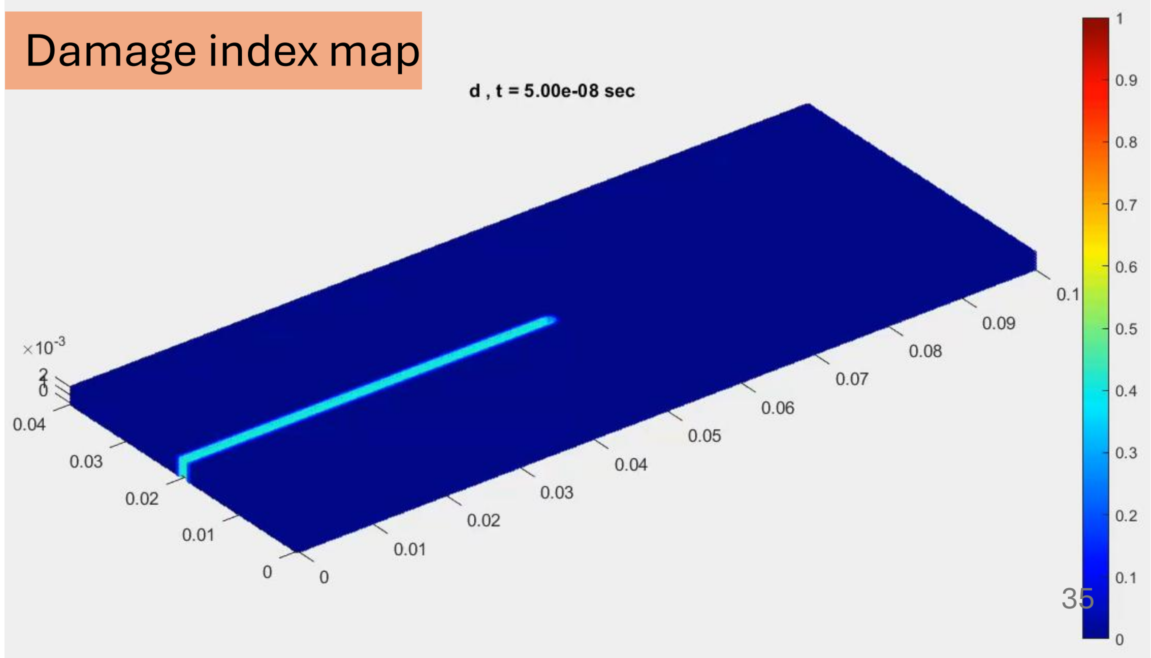
Zhang, Gazonas, and Bobaru, *Int. J. Impact Eng.* (2018)

PeriFast/Dynamics (Matlab-based on GitHub)









PeriFast (Matlab code on GitHub)

- Perifast/Dynamics
- Perifast/Corrosion

Jafarzadeh, Larios, & Bobaru, (2020). *Journal of Peridynamics and Nonlocal Modeling 2,* 85-110.
Jafarzadeh, Wang, Larios, & Bobaru, (2021). *Computer Methods in Applied Mechanics and Engineering 375,* 113633
Jafarzadeh, Mousavi, Larios, & Bobaru, (2022) *Computer Methods in Applied Mechanics and Engineering* 392, 114666.
Jafarzadeh, Mousavi, Wang, Bobaru, (2024) *Journal of Peridynamics and Nonlocal Modeling* 6 (1), 33-61
Wang, Jafarzadeh, Mousavi, Bobaru (2024) *Journal of Peridynamics and Nonlocal Modeling* 6 (1), 62-86

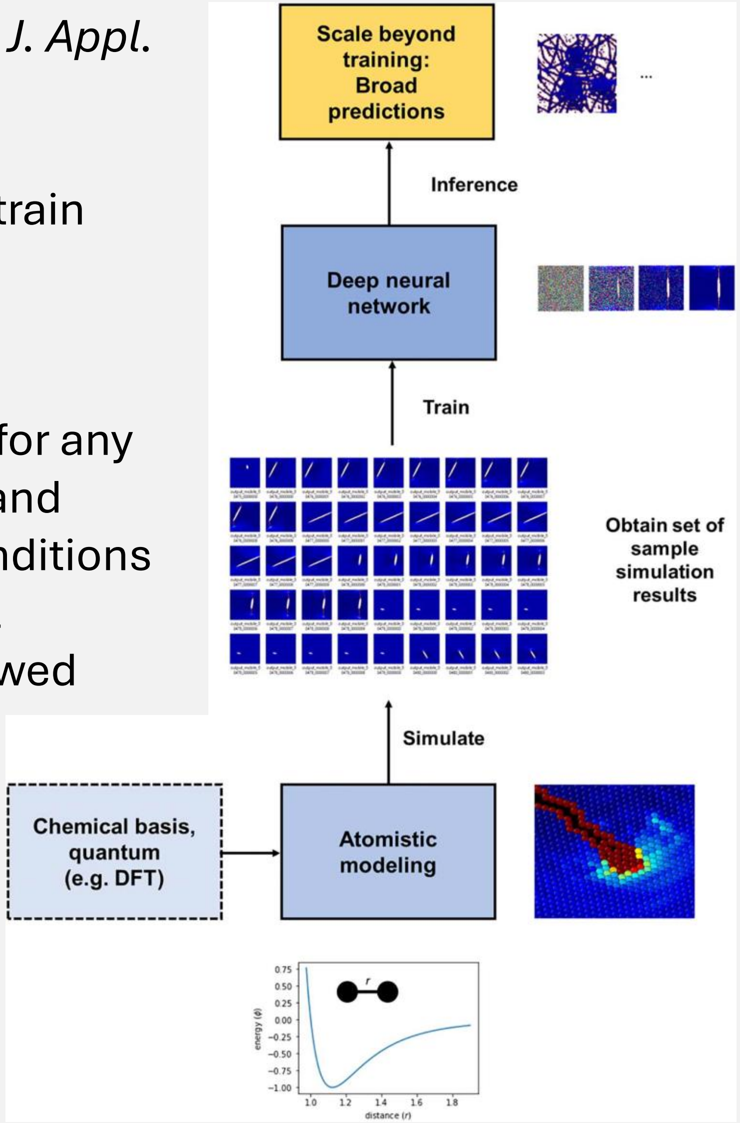
Recent work on AI for fracture

Markus Buehler, *J. Appl. Mech*, (2022)

Cost function: strain energy density

Limitations:

- need to train for any new loading and boundary conditions
- Non-physical behavior allowed



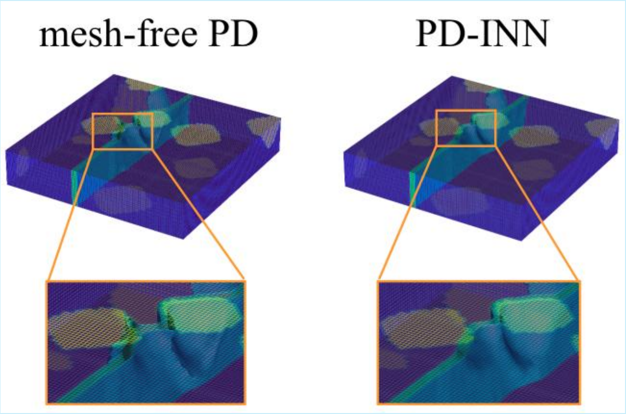
PINNs

Eghbalpoor, Sheidaei,. *Theor. Appl. Fract. Mech.* (2024)

Cost function: PD equations

Limitations:

- Costly to train
- Any new material needs new kernel



Promising paths for AI in fracture and damage

- **Operator learning**: use high-fidelity PD models to generate training data

- Use DNNs to discover/learn **the PD kernel** for models of fracture and damage in materials with complex microstructure.