Particle-base Simulations

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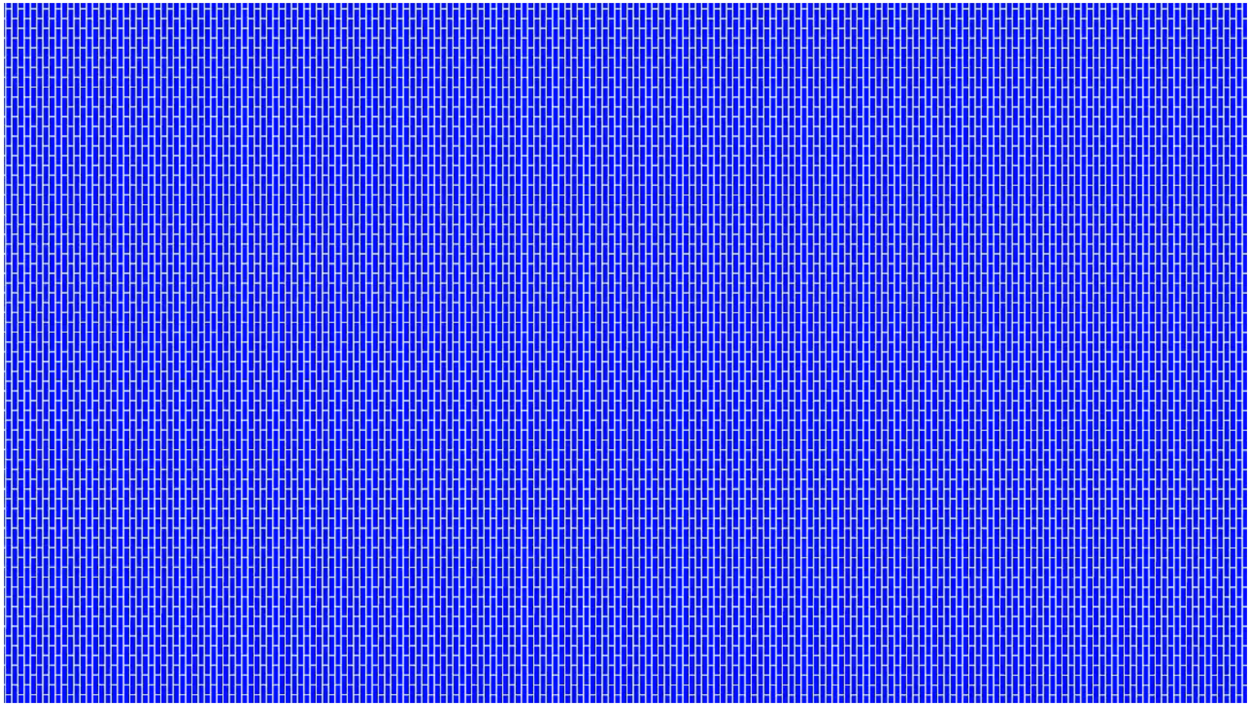
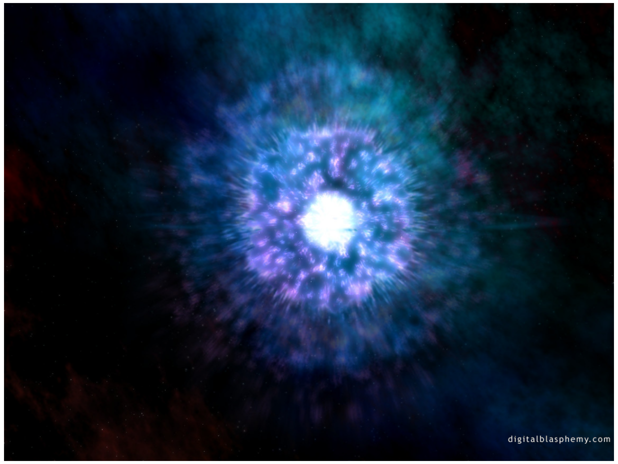


Introduction



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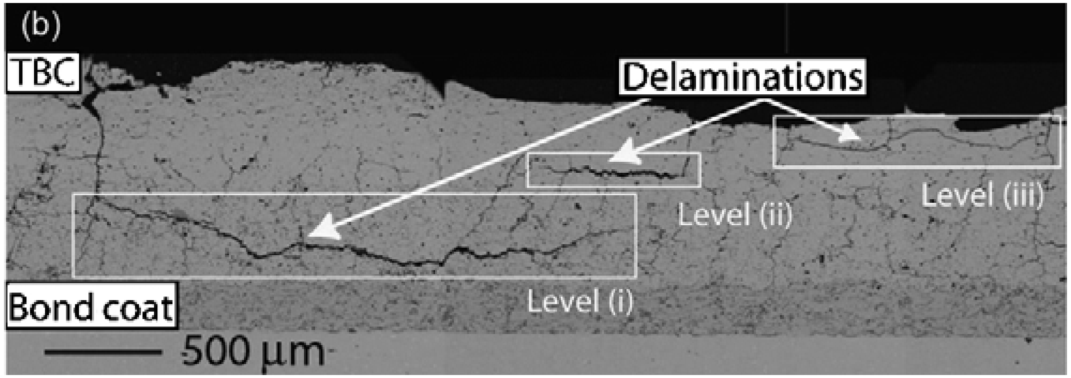
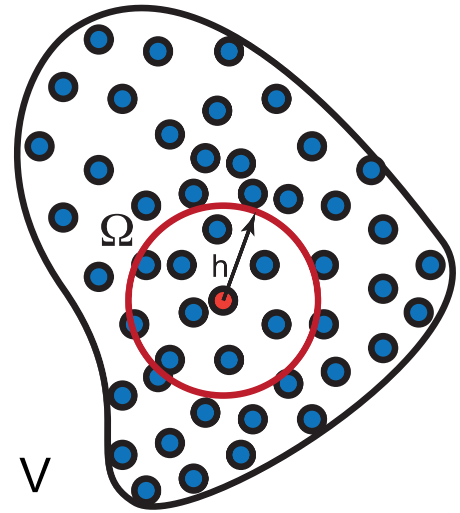


Kramer et al., Mat. Sci. Eng. A, 2008

What? Why? How?



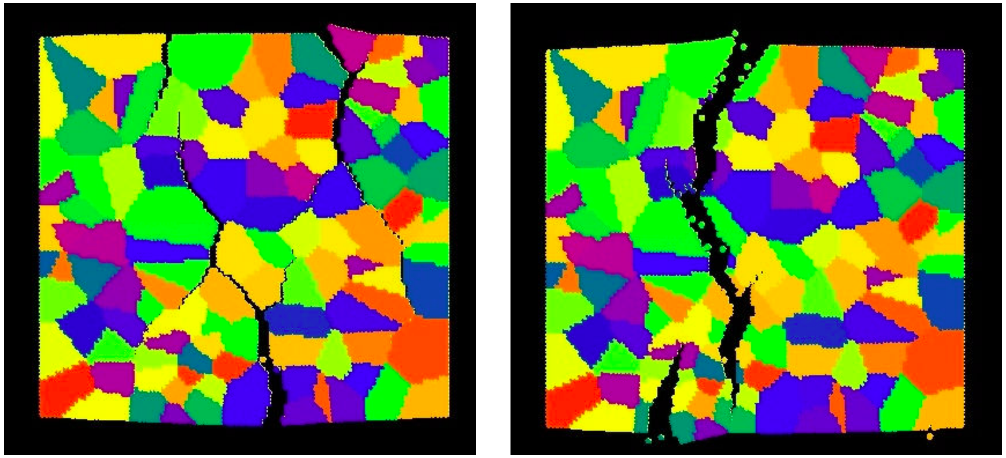
- Smoothed-particle hydrodynamics (SPH)
- Peridynamics
- Moving Least Squares (MLS)
- Discrete Element Method (DEM)

- Same equations apply regardless of cracks
- Cracks/damage “just happen” as a result of properties/loading

- All reduce to collection of interacting particles.
- “Meshless” = nodes, but no elements (i.e. no predefined connectivity)
- All involve intrinsic length scale (element size?)
- Involve calculation of derivatives (except for ν = ¼)
- **Most** utilize dynamic integration of equations of motion.

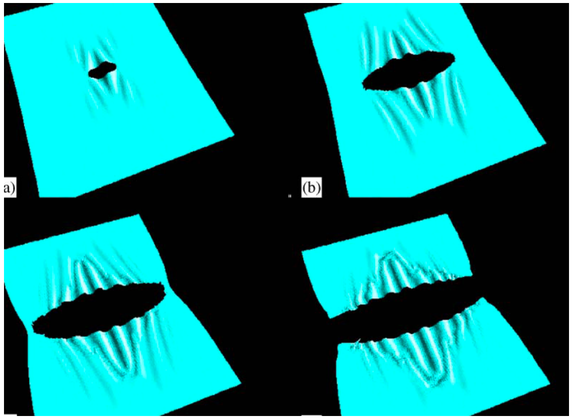
Examples: Silling's peridynamics

Inter/transgranular fracture

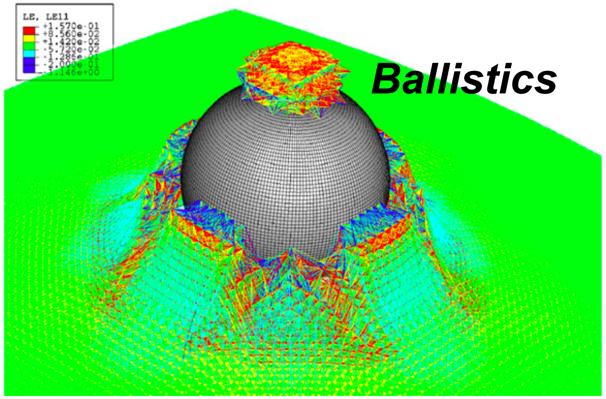


Askari, et al. JOP, 2008

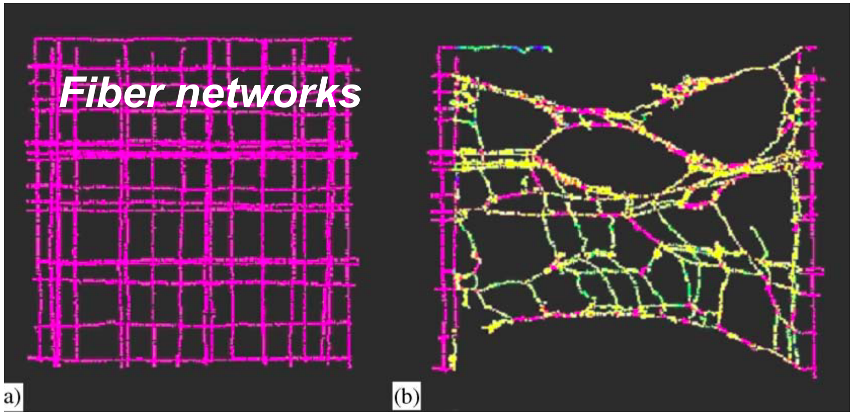
Cracking (plates, membranes)



Silling and Bobaru, IJNLM, 2005



Macek and Silling, FE Anal. Des., 2007

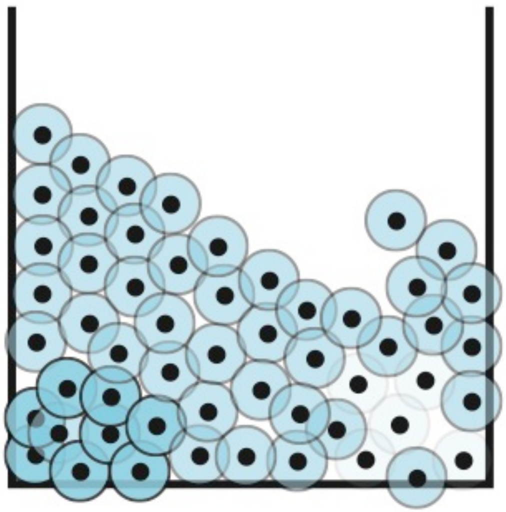


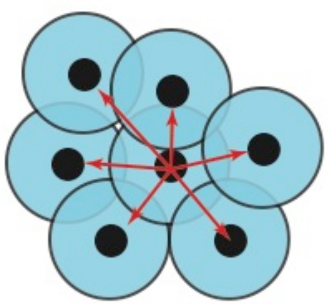
Outline

- Smoothed Particle Hydrodynamics (SPH)
- Peridynamics
- Peristatics* with GPUs (and weird particles)
- Concluding Remarks

***Caution: term has just been coined. Object or you are complicit. Thomas Moore, 1535 (ACE)**

Smoothed Particle Hydrodynamics





- Navier-Stokes: equilibrium & linear viscous fluid:

$$\rho \frac{d\underline{v}}{dt} = -\nabla p + \mu \nabla^2 \underline{v} + \underline{f}$$

- Want collection of particles to represent fluid:

$$\underline{a}_i = \frac{d\underline{v}_i}{dt} = \frac{\underline{F}_i}{\rho_i}; \qquad \ddot{\underline{r}}_i = \frac{\underline{F}_i(\underline{r}, \dot{\underline{r}})}{\rho_j(\underline{r})}$$

Smoothed Particle Hydrodynamics: SPH

- The key to it all: (volume) smoothed (**interpolated**) quantities:

$$A(\underline{r}) = \int_{\Omega(h)} A(\underline{r}')W\left(\underline{r} - \underline{r}'\right) d\underline{r}$$

$$A(\underline{r}) = \sum_j A_j V_j W(\underline{r} - \underline{r}_j) \qquad V = \frac{m}{\rho} \qquad A(\underline{r}) = \sum_j A_j \frac{m_j}{\rho_j} W(\underline{r} - \underline{r}_j)$$

- For example, density:

$$\rho_i = \rho(\underline{r}_i) = \sum_j \rho_j \left(\frac{m_j}{\rho_j}\right) W(\underline{r}_i - \underline{r}_j) = \sum_j m_j W(\underline{r}_i - \underline{r}_j)$$

Smoothed Particle Hydrodynamics: SPH

- Kernel (interpolation) function properties:

$$\int_{\Omega(h)} W(\underline{r})d\underline{r} = 1; \qquad \lim_{h\to 0} W(\underline{r}) = \delta(\underline{r}); \qquad W(\underline{r}) \geq 0$$

- ***h*** is critical, defines length-scale over which pressure/density are computed.

pressure $$W(\underline{r},h) = \frac{315}{64\pi h^9}\left(h^2 - |\underline{r}|^2\right)^3; \qquad 0 \leq |\underline{r}| \leq h$$

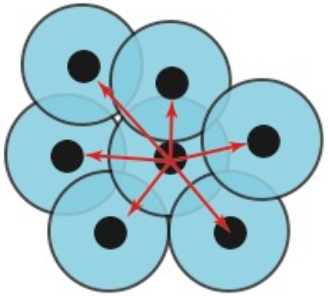
viscosity $$W_\mu(\underline{r},h) = \frac{15}{2\pi h^3}\left(-\frac{|r|^3}{2h^3} + \frac{|r|^2}{h^2} + \frac{h}{2|r|} - 1\right)$$

Smoothed Particle Hydrodynamics: SPH

$$\rho \frac{d\underline{v}}{dt} = -\nabla p + \mu \nabla^2 \underline{v} + \underline{f}$$

- Need to compute gradients:

$$\nabla A(\underline{r}) = \sum_j A_j \left(\frac{m_j}{\rho_j}\right) \nabla W(\underline{r} - \underline{r}_j)$$



$$\begin{aligned} \underline{f}_i^p &= -\nabla p(\underline{r}_i) \\ &= -\sum_{j \neq i} p_j \left(\frac{m_j}{\rho_j}\right) \nabla W(\underline{r}_i - \underline{r}_j) \end{aligned}$$

Note: p_j, ρ_j are functions of particle position!

- Gradients 'pushed' onto kernal functions, similar to FEA

Smoothed Particle Hydrodynamics: SPH

- More accurate way to compute derivatives:

$$\rho \nabla A = \nabla(\rho A) - A \nabla \rho \rightarrow \nabla A = \frac{1}{\rho}\left(\nabla(\rho A) - A \nabla \rho\right)$$

- Force on particle due to pressure:

$$\underline{f}_i^p = -\rho_i \sum_{j \neq i} \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) m_j \nabla W \left(\underline{r}_i - \underline{r}_j \right)$$

Bulk modulus:

$$p_i = \kappa \left(\rho_i - \rho_o \right)$$

- Force on particle due to visocity:

$$\underline{f}_i^\mu = \mu \sum_j \left(\frac{m_i}{\rho_j} \right) \left(\underline{v}_j - \underline{v}_i \right) \nabla^2 W \left(\underline{r}_i - \underline{r}_j \right) = \mu \sum_j \left(\frac{m_i}{\rho_j} \right) \left(\dot{\underline{r}}_j - \dot{\underline{r}}_i \right) \nabla^2 W \left(\underline{r}_i - \underline{r}_j \right)$$

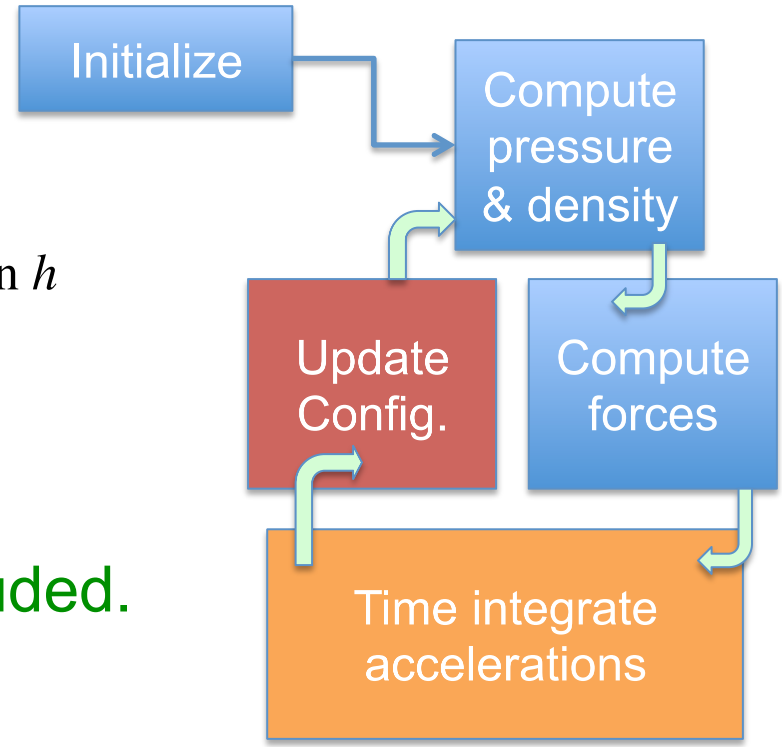
Smoothed Particle Hydrodynamics: SPH

$$\underline{a}_i = \frac{1}{\rho_i}\left(\underline{f}_i^p + \underline{f}_i^\mu\right)$$

$$\rho_i = f(\underline{r}_K) \quad \text{for all } K \text{ particles in } h$$

$$\underline{f}_i^p = f(\rho_i) = f(\underline{r}_K) \quad \text{for all } K \text{ particles in } h$$

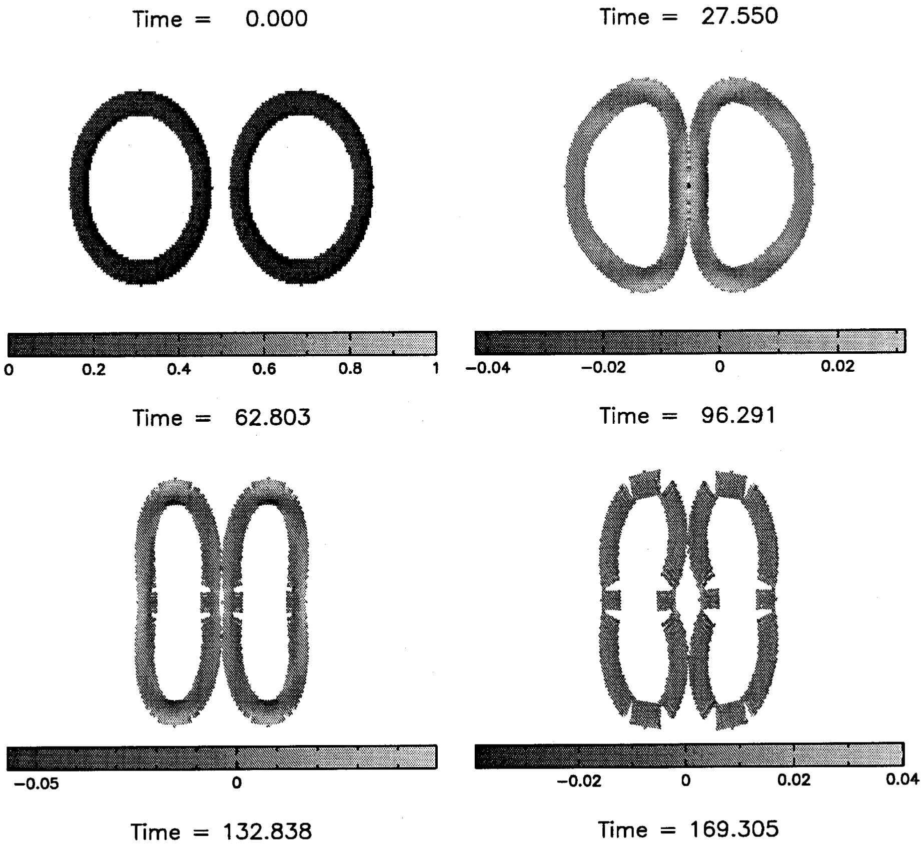
$$\underline{f}_i^\mu = f(\dot{\underline{r}}_K, \underline{r}_k) \quad \text{for all } K \text{ particles in } h$$



- Surface tension must be included.
- Must have enough particles.
- For any time step, ‘neighbors’ must be identified.
- Collision detection is needed for boundaries.

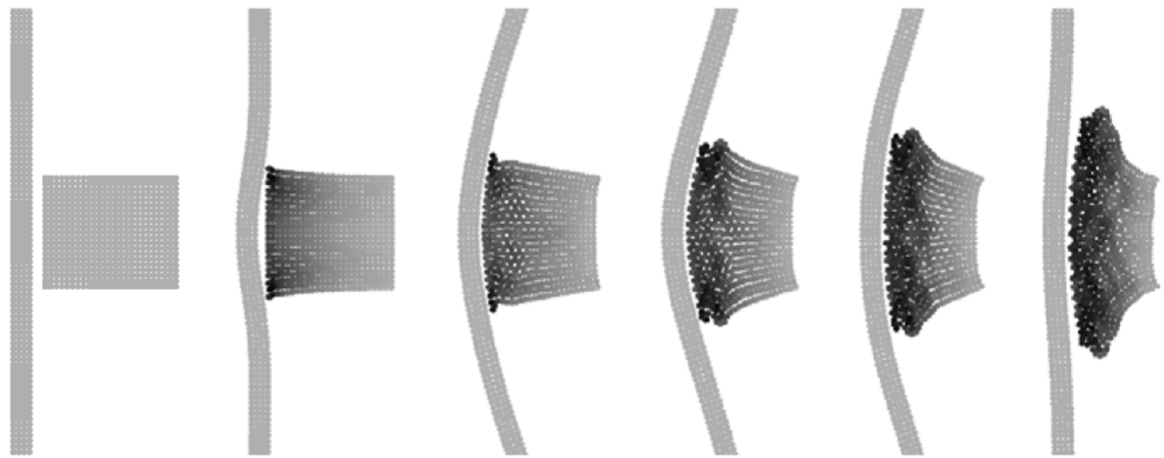
Smoothed Particle ***Elastodynamics***: SPE

- Work through formalism for different constitutive law (different gradient terms)
- Time-stepping stepping slow: implicit algorithms slow.
- ‘Neighbors’ can be fixed for brittle materials (use cohesive laws to account for fracture)

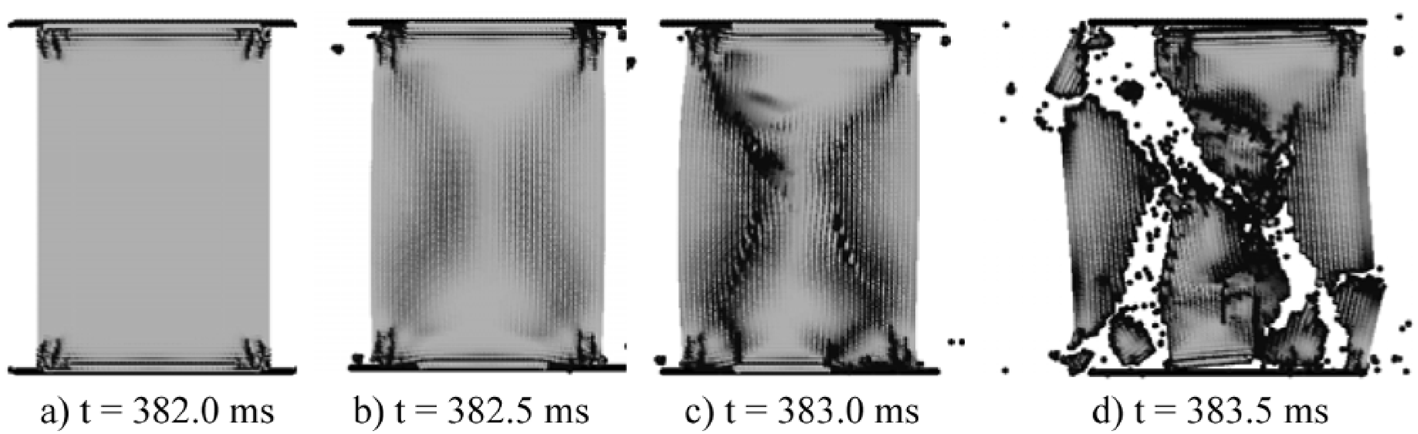


Gray, Monaghan, Swift, Comp. Struc., 2001

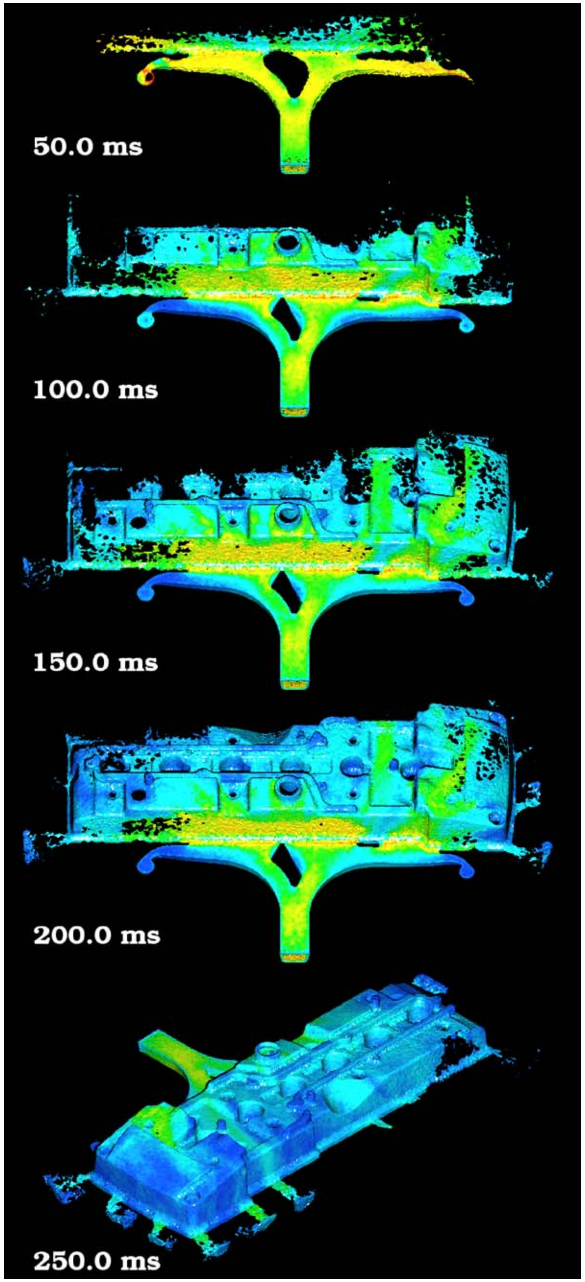
Examples of SPH for elastodynamics:

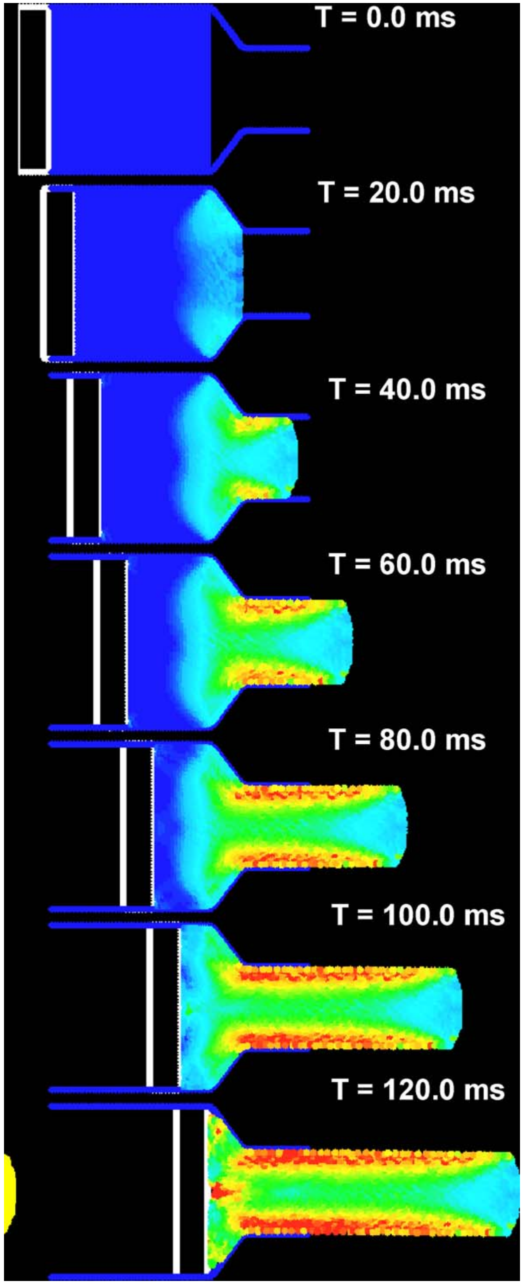


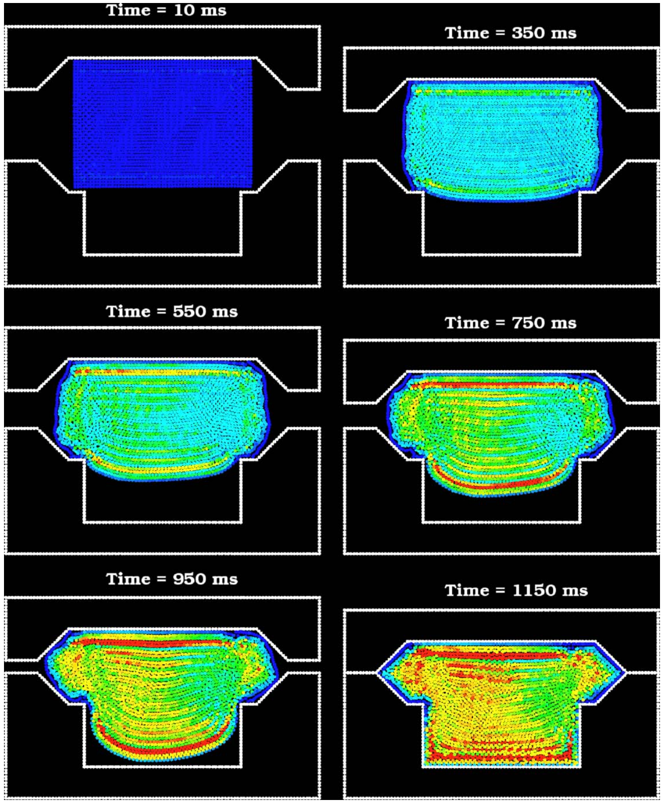
Cleary and Das, IUTAM Syposium, 2008: elastic-plastic projectile



Cleary and Das, IUTAM Syposium, 2008: brittle compression



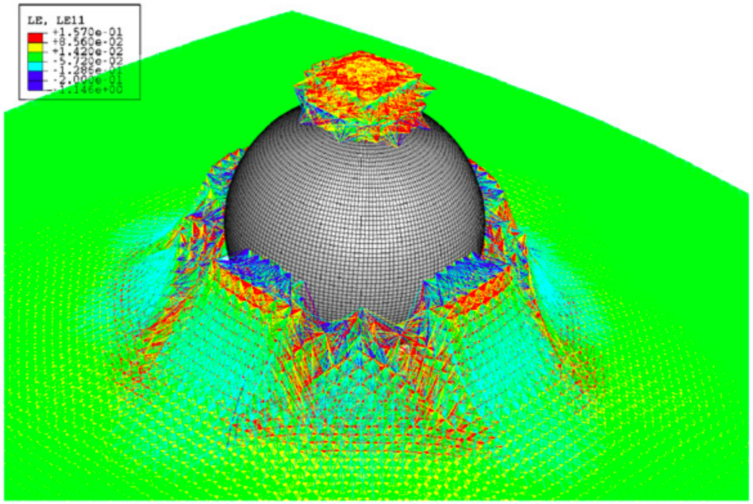




Cleary, Prakash and Ha, J. Mat. Proc. Tech., 2006

Peridynamics (Silling)

- Two ‘flavors’:
  - **Bond-based:** simply pair interactions, ν = ¼.
  - **State-based:** peridynamic stress and deformation tensors allow arbitrary constitutive models.
- Note based on PDEs (distinction with SPH) but reduces to PDEs in limit of refinement.



Macek and Silling, FE Anal. Des., 2007x

[1]Note that the notation $\boldsymbol{f} = \boldsymbol{f}(\boldsymbol{\xi}, \boldsymbol{\eta})$ is somewhat ambigious. Indeed, for a given function $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x}, t)$ the mathematical correct way to describe $\boldsymbol{f}$ is using the Nemytskii operator $F : \boldsymbol{u} \mapsto F\boldsymbol{u}$ with $(F\boldsymbol{u})(\boldsymbol{x}, \hat{\boldsymbol{x}}, t) = \boldsymbol{f}(\hat{\boldsymbol{x}} - \boldsymbol{x}, \boldsymbol{u}(\hat{\boldsymbol{x}}, t) - \boldsymbol{u}(\boldsymbol{x}, t))$.

Peridynamics

- The peridynamic equation of motion:

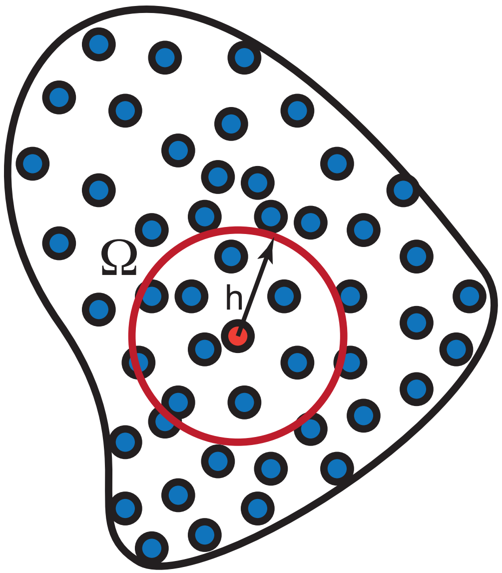
$$\rho \underline{\ddot{u}}(\underline{x},t) = \int_{\Omega(h)} \underline{f}\left[\underline{u}(\underline{x}',t) - \underline{u}(\underline{x},t), \underline{x}' - \underline{x}\right] dV_{\underline{x}'}$$

- The discretized form:

$$\rho \underline{\ddot{u}}_i = \sum_p \underline{f}\left(\underline{u}_p - \underline{u}_i, \underline{x}_p - \underline{x}_i\right) V_p$$

- A sensible statement:

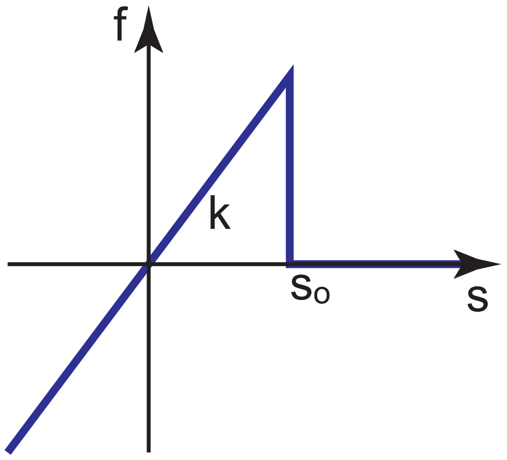
$$\rho \underline{\ddot{u}}_i = \underline{f}_{ip}\left(\underline{dx}^{ip}, \underline{du}^{ip}\right) V_p$$



Peridynamics

- Bond stretch between particle "i" and particle "p":

$$s_{ip} = \frac{|\underline{dx}^{ip} + \underline{du}^{ip}| - |\underline{dx}^{ip}|}{|\underline{dx}^{ip}|}$$



- The constitutive law:

$$|\underline{f}_{ip}| = k \cdot s_{ip}$$

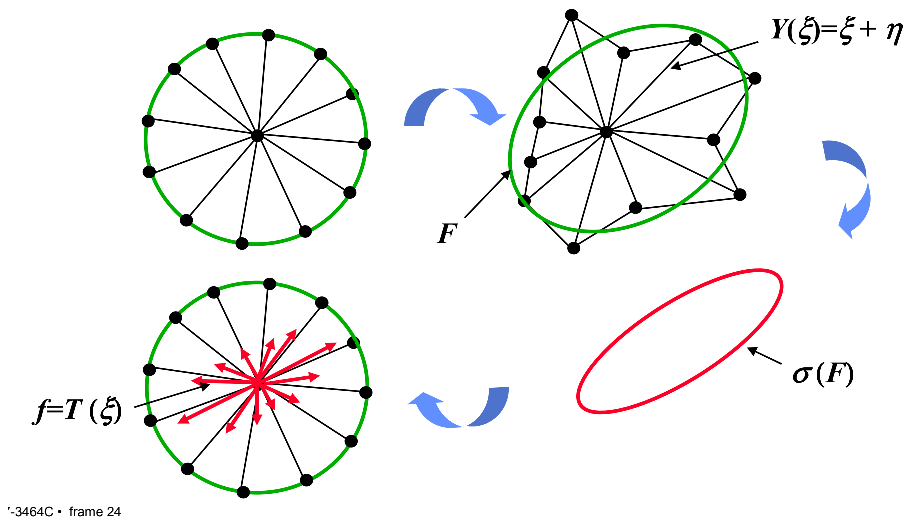
- Equivalent continuum properties:

$$\kappa = \frac{\pi h^4 k}{18}; \qquad \nu = \frac{1}{4} \qquad G_c = \frac{9 s_o^2 \kappa \delta}{5}$$

Peridynamics

- State-based model: compute peridynamic deformation and stress states

- Map motion onto deformation gradient
- Conventional stress-strain to get stress
- Map stress onto bond forces

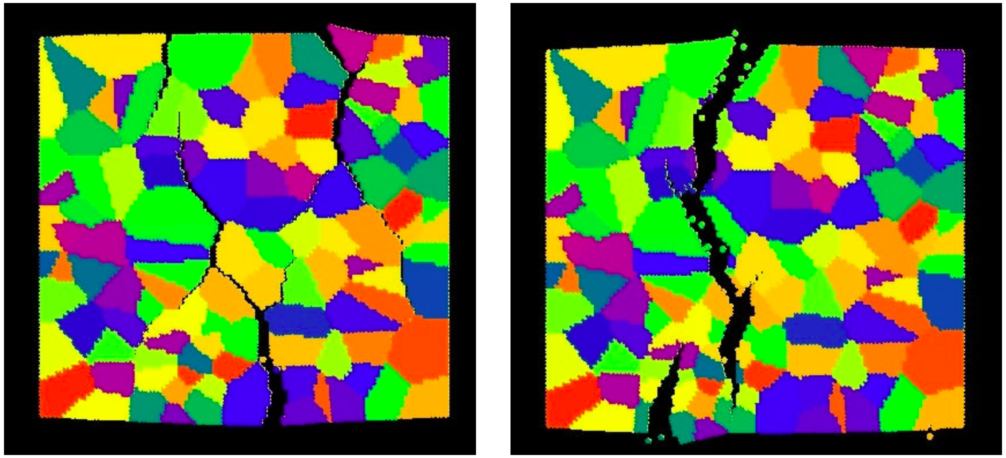


Sandia National Laboratories

Silling, McMat07 (his website)

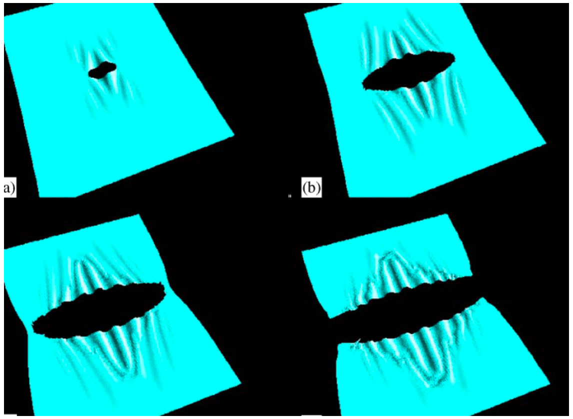
Examples: Silling’s peridynamics

Inter/transgranular fracture

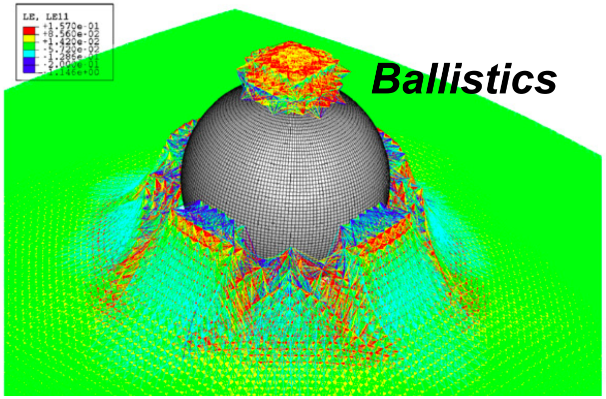


Askari, et al. JOP, 2008

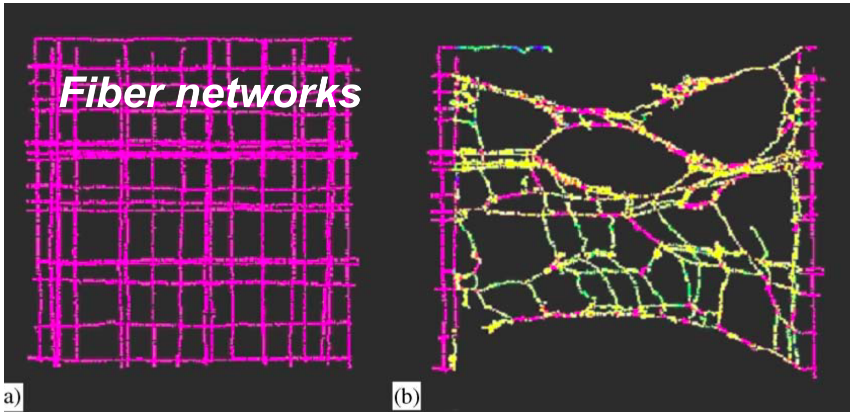
Cracking (plates, membranes)



Silling and Bobaru, IJNLM, 2005

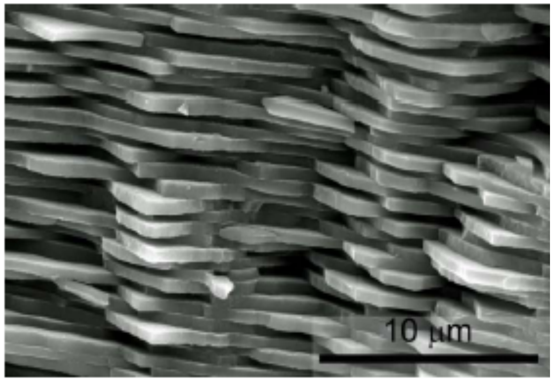


Macek and Silling, FE Anal. Des., 2007



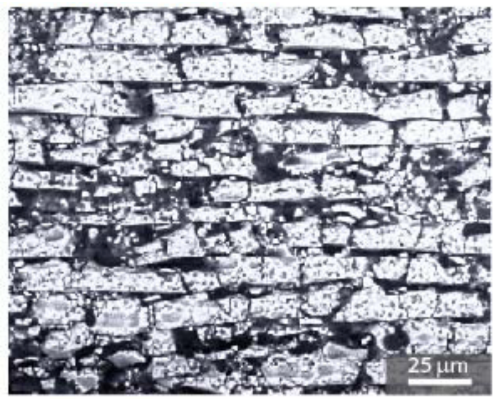
Peristatics* (with weird particles)

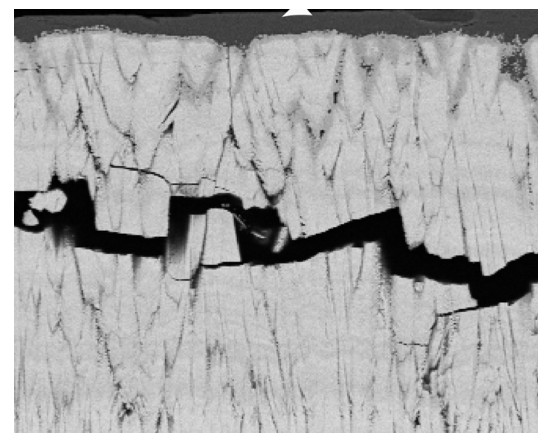
Rone Kwei Lim, William Pro, Professor Linda Petzold & Professor Marcel Utz (Southampton)



Nacre (abalone): Barthelat, et al., JMPS, 2007

Synthetic Al_2O_3/PMMA: Munch, et al., Science, 2008



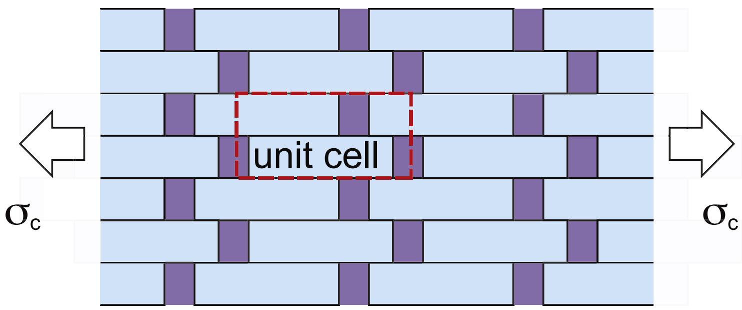


Thermal barrier coating: Donohue, et al., Mat. Sci. Eng. A, 2013

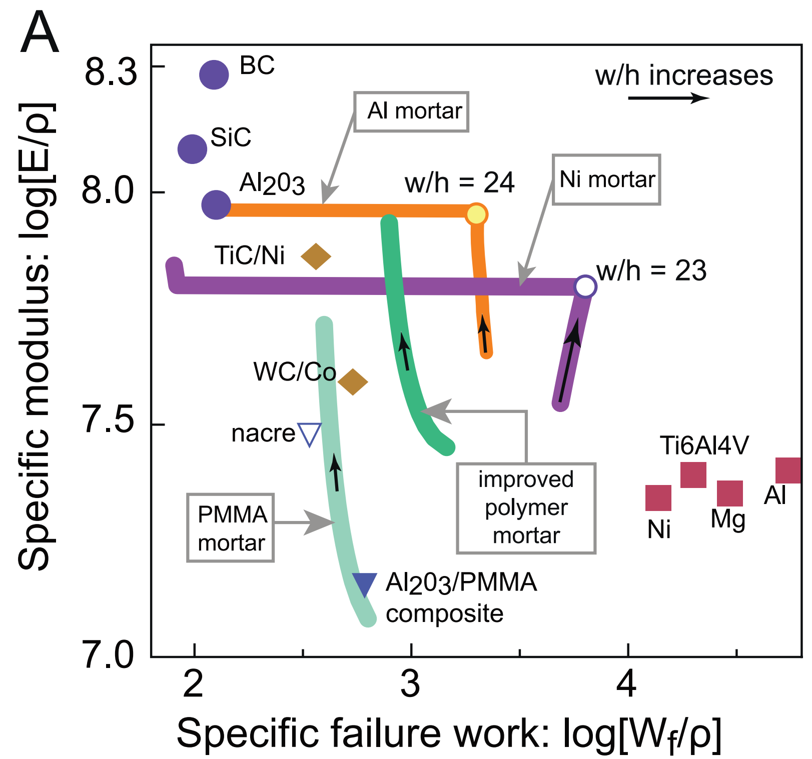
***(Most of) you are complicit.**

Brick and mortar 'particle' modeling

Deformed composite:



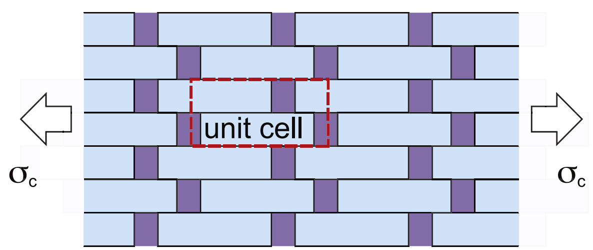
- Small volumes of ceramics are strong.
- Small fractions of ductile phase limits compliance.
- Interlocking, ordered architecture transfers loads to bricks and diffuses damage.

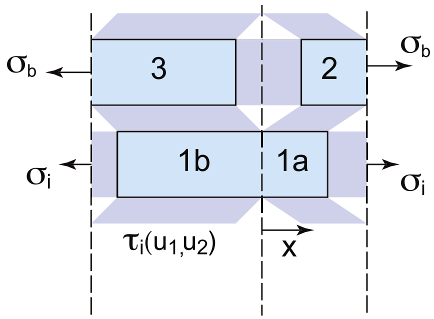


Begley, et al., "Micromechanical models to guide the development of brick and mortar composites", JMPS, 2012

Brick and mortar particle modeling

$$\overline{E}_c = \frac{\overline{E}_c}{\overline{E}_b} = \frac{2(\sinh[\kappa_2]\kappa_1 - 2\sinh[(-1+\overline{s})\kappa_2]\sinh[\overline{s}\kappa_2]\kappa_2)}{2\sinh[\kappa_2](1+\kappa_1)+(\cosh[\kappa_2]-\cosh[(-1+2\overline{s})\kappa_2])\kappa_2}$$





$$\kappa_1 = \frac{\overline{E}_m w}{\overline{E}_b t_1} \qquad \kappa_2 = \sqrt{\frac{(1-\nu_m)\overline{E}_m w^2}{2\overline{E}_b t_2 h}}$$

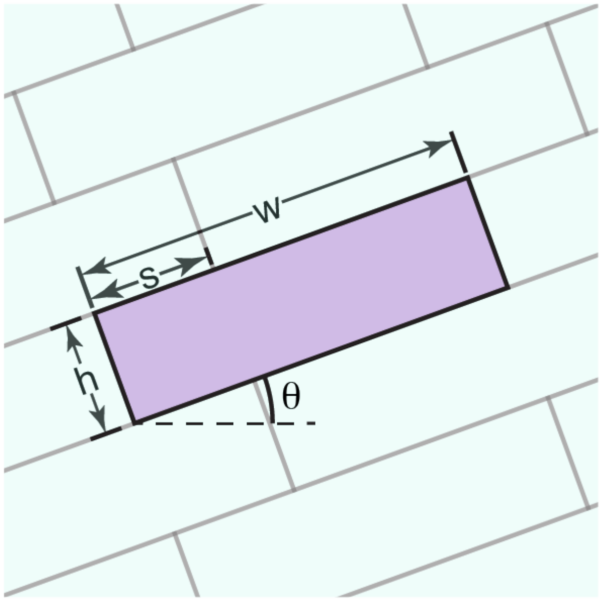
- Subtle asymptotic limits: both small and large stiffnesses can be relevant

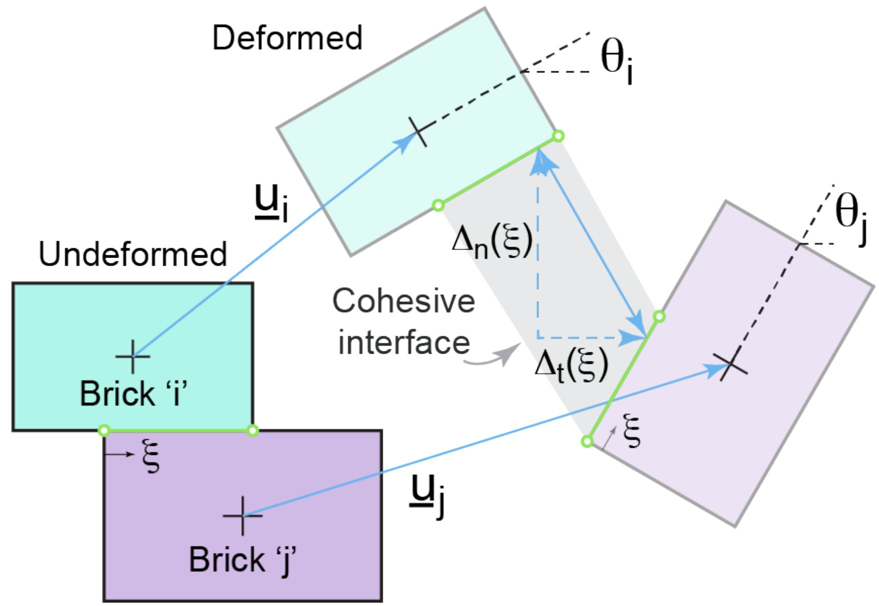
$$\kappa_1 \sim 0.1; \qquad \kappa_2 \sim 0.3$$

$$\bar{E}_c = \frac{\bar{E}_m w}{t}\left(1 + \frac{w}{12h}\right)$$

Begley, et al., "Micromechanical models to guide the development of brick and mortar composites", JMPS, 2012

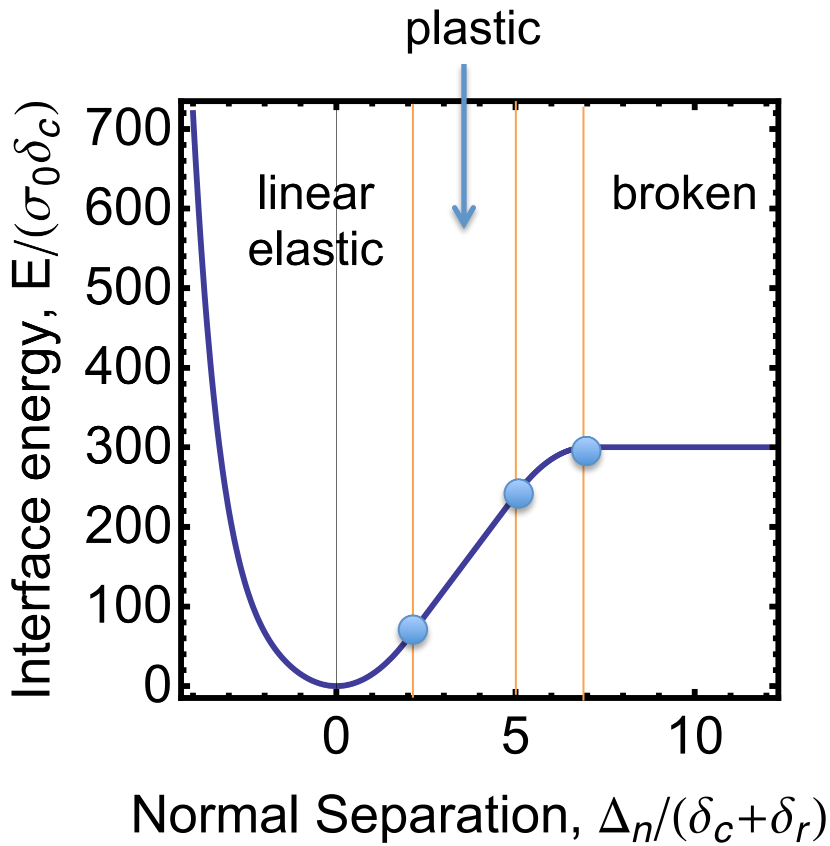
Brick and mortar particle modeling

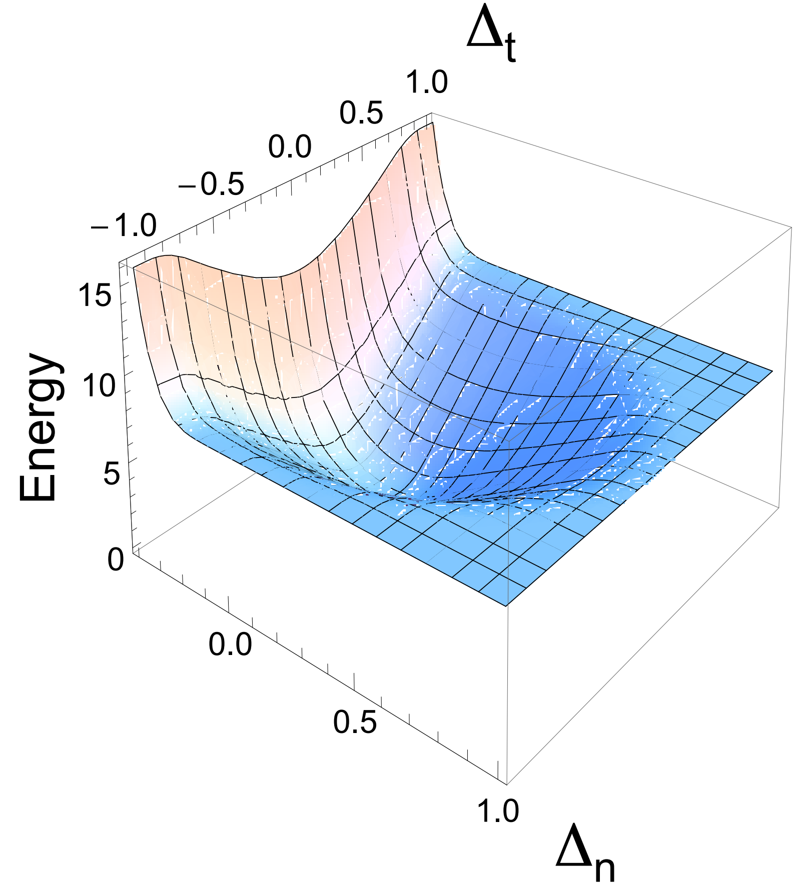




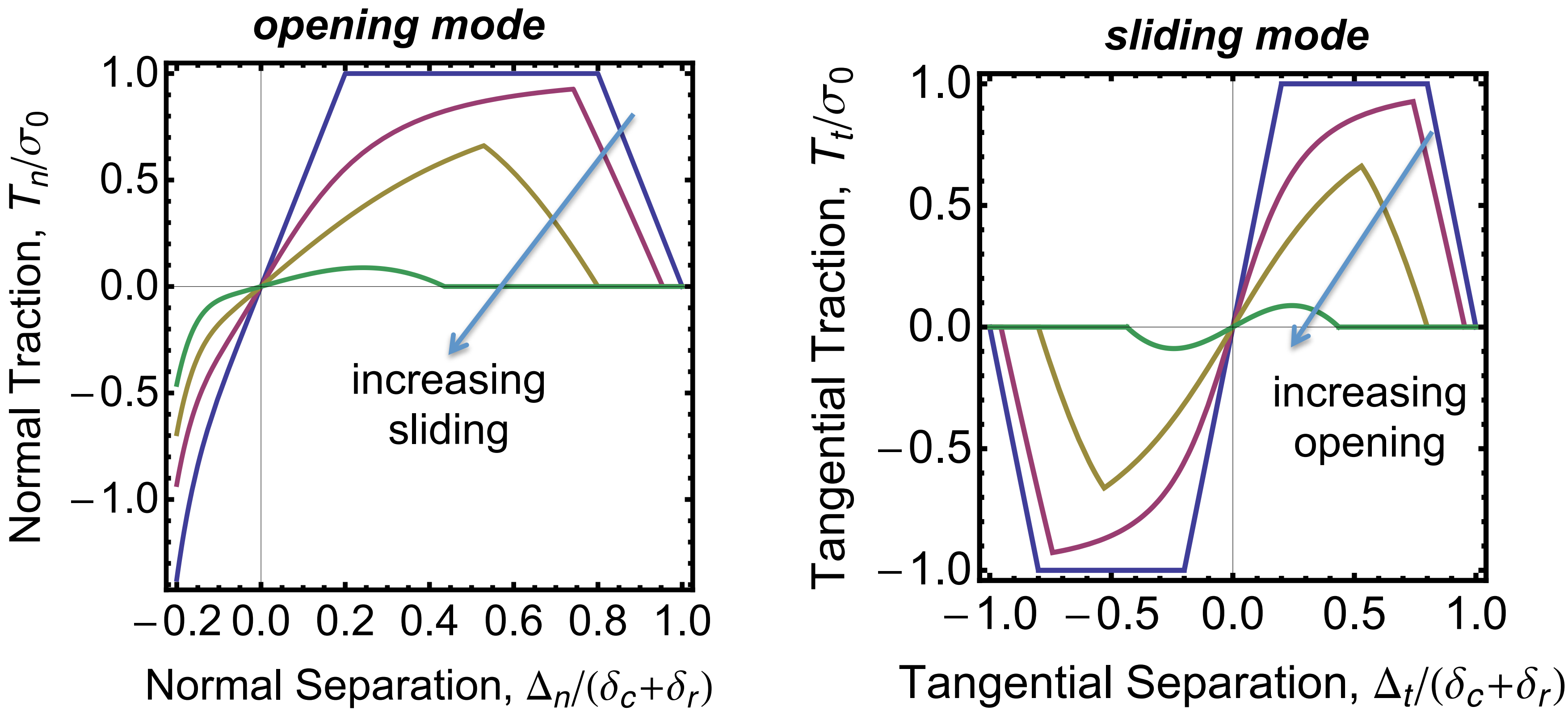
- Only brick displacements & rotation matter.
- All energy at the system is in the interface.
- Cohesive law describes energy of the interface in terms of relative motion.

Brick and mortar particle modeling





Brick and mortar particle modeling

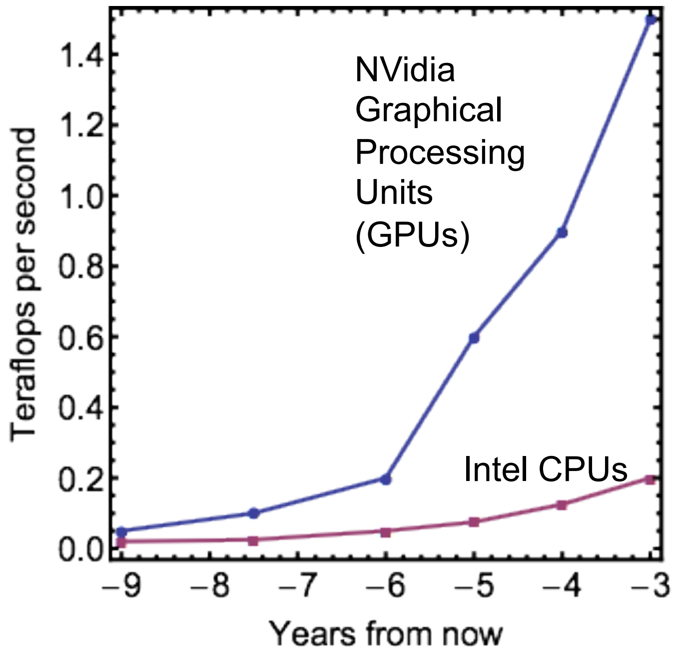


Brick and mortar particle modeling

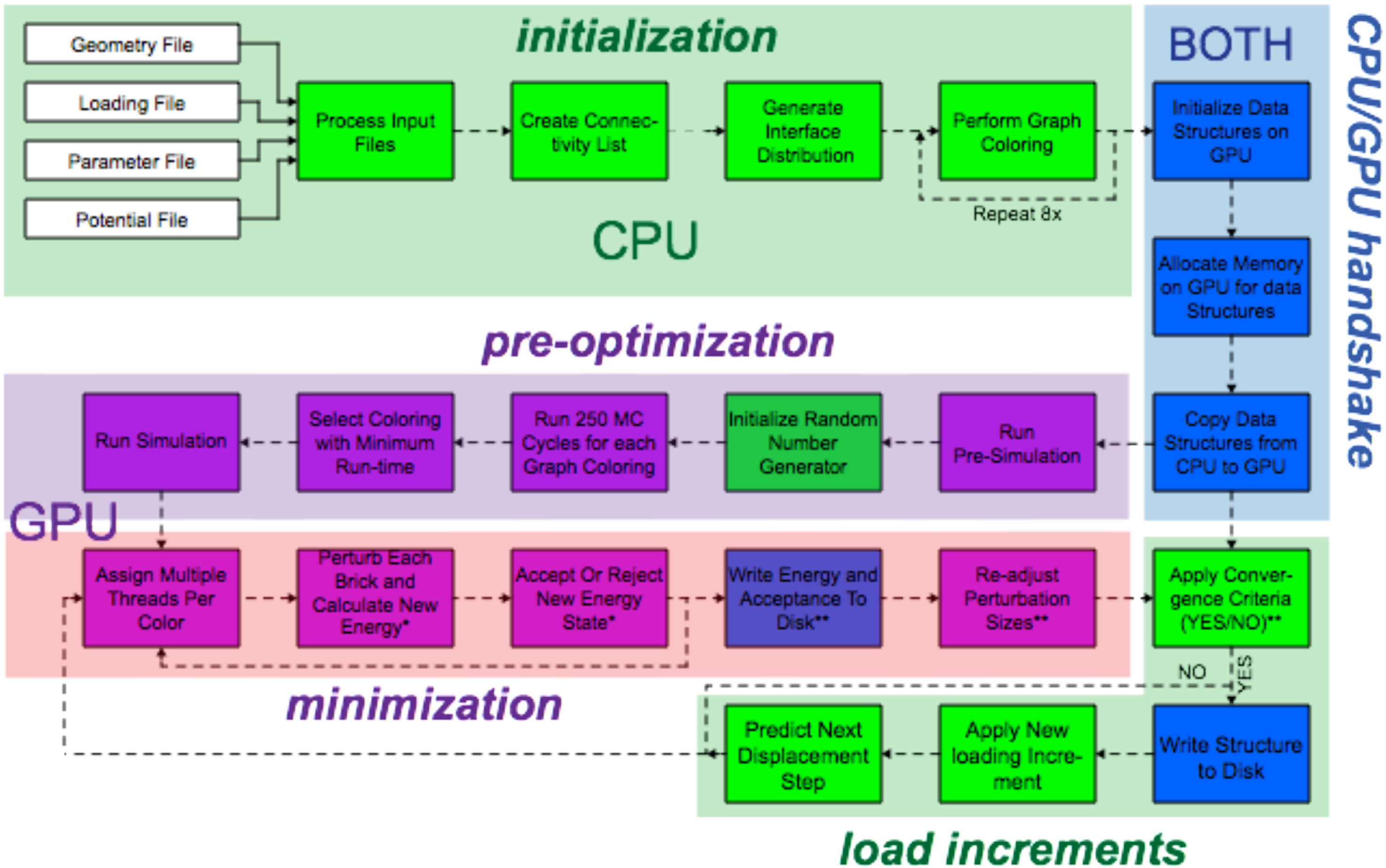
- Derivatives are expensive and localization is tough to capture.
  (---, ---)

- Connectivity is nearest neighbor and parallel function calls are cheap.
  (+++,+++)

- Monte Carlo minimization (direct search)
- Calculate energy for new positions, accept lower energy states (and a small fraction of higher ones)

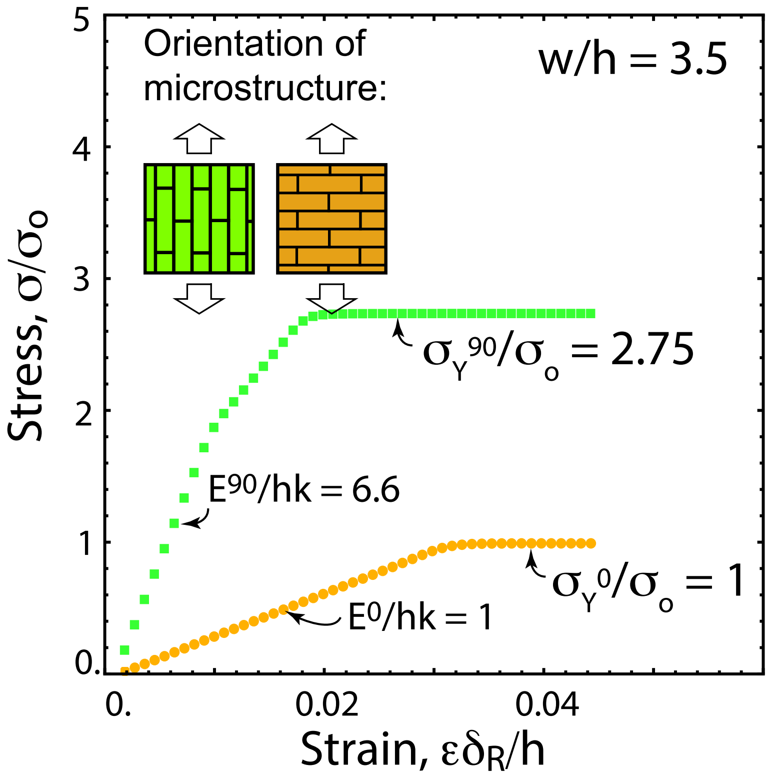


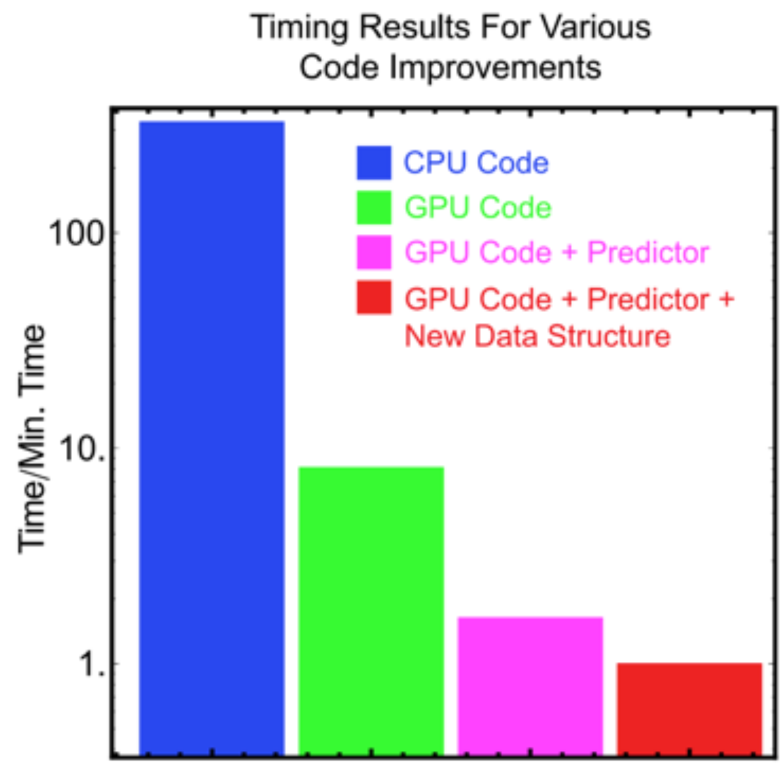
Brick and mortar particle modeling



Rone Kwei Lim, William Pro, Professor Linda Petzold

Brick and mortar particle modeling

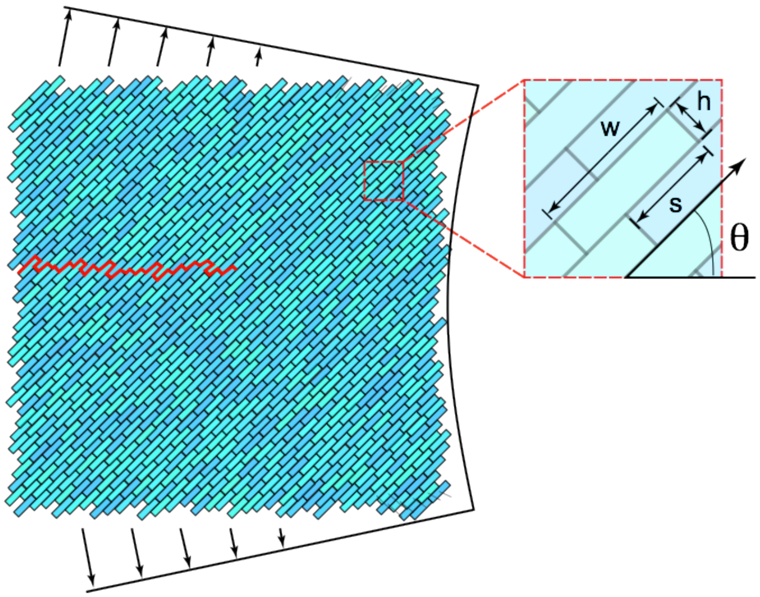




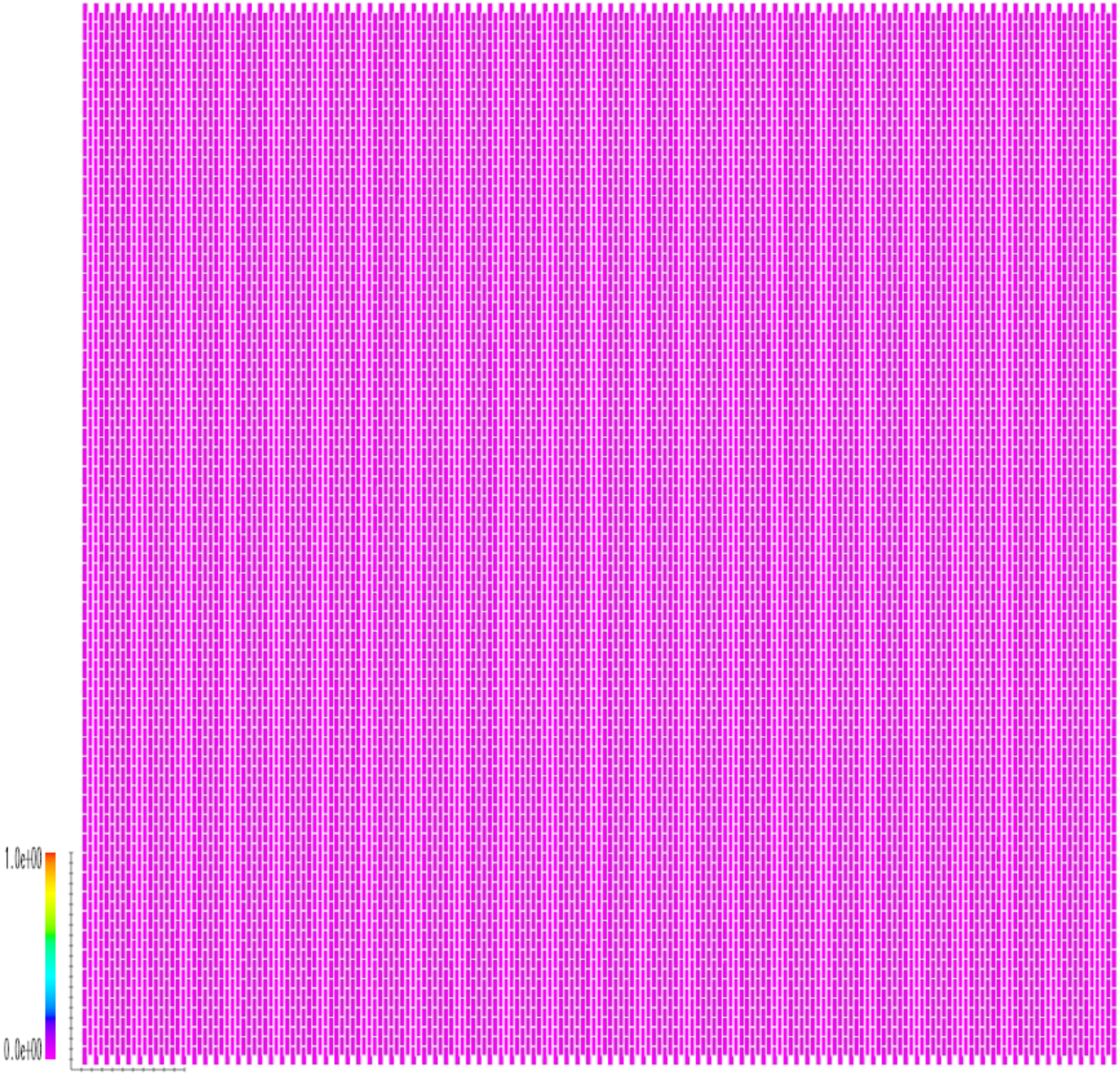
Brick and mortar particle modeling

The computer version of Begley & Landes, 1972, ASTM STP 514

- Compute elastic energy (as a function of crack length, loading, geometry, etc.)
- Calculate the macroscopic energy release rate for the anisotropic elastic solid.
- Determine loads to initiate fracture, Infer initiation toughness.
- If toughness is actually a property, it should be independent of geometry and loading



bending displacements



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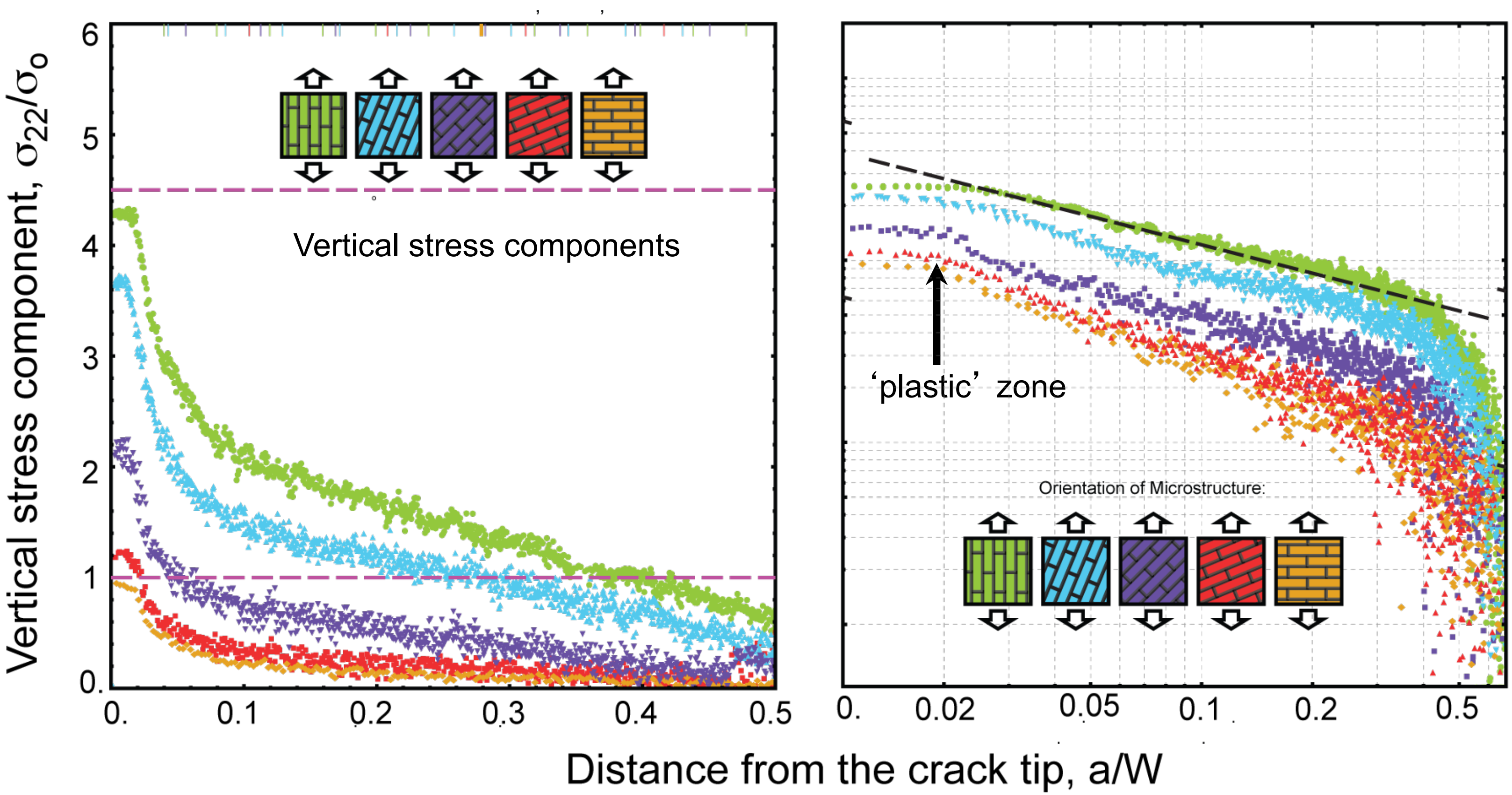
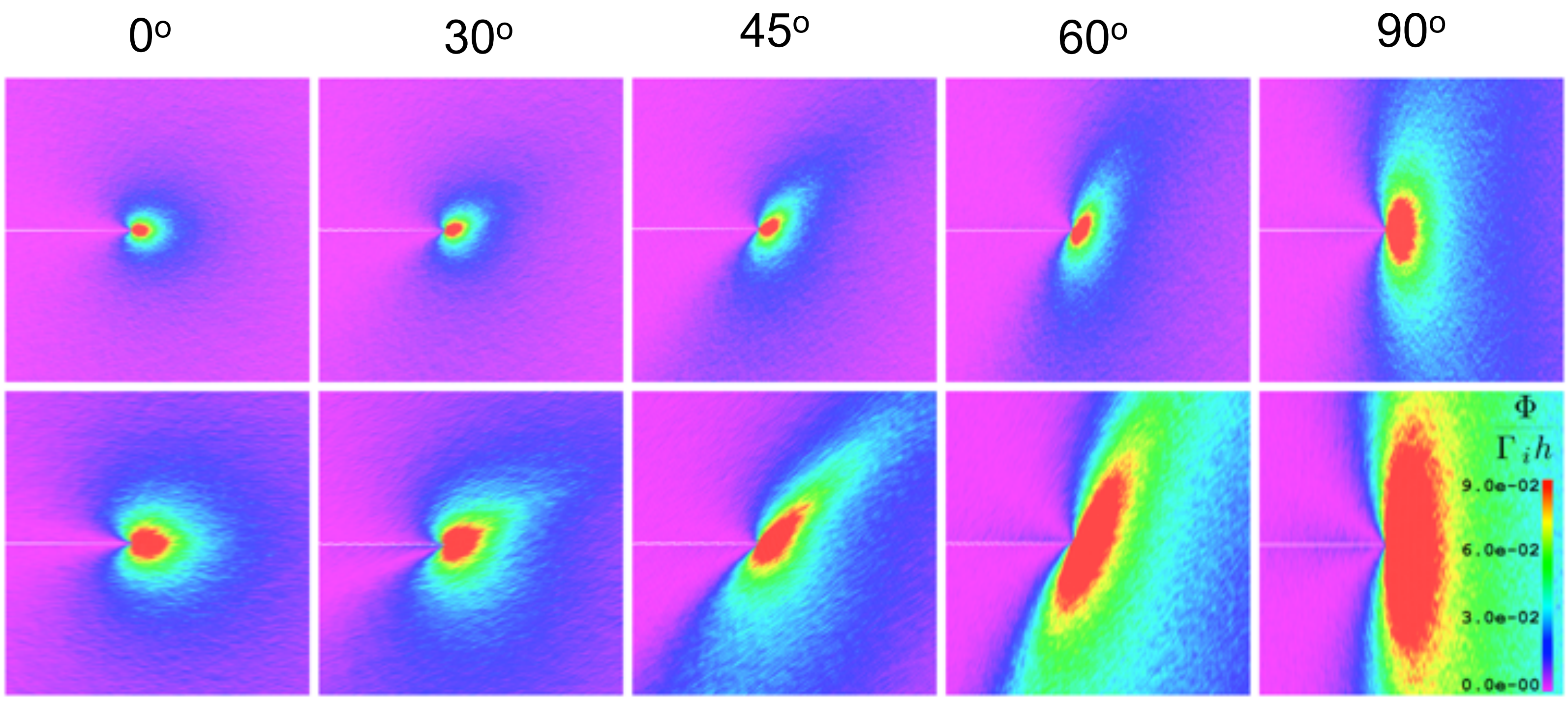
Brick and mortar particle modeling



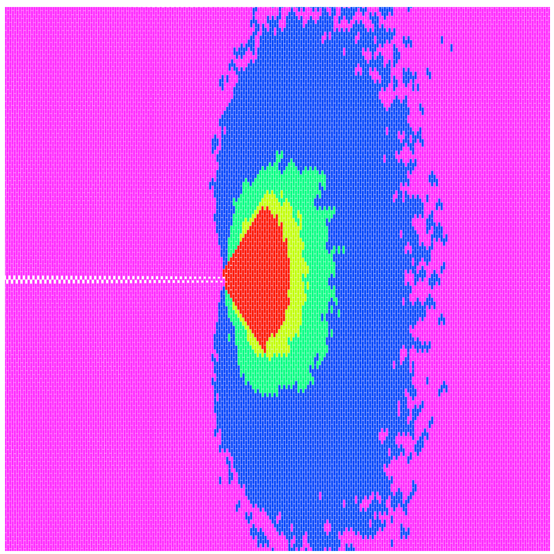
Brick and mortar particle modeling

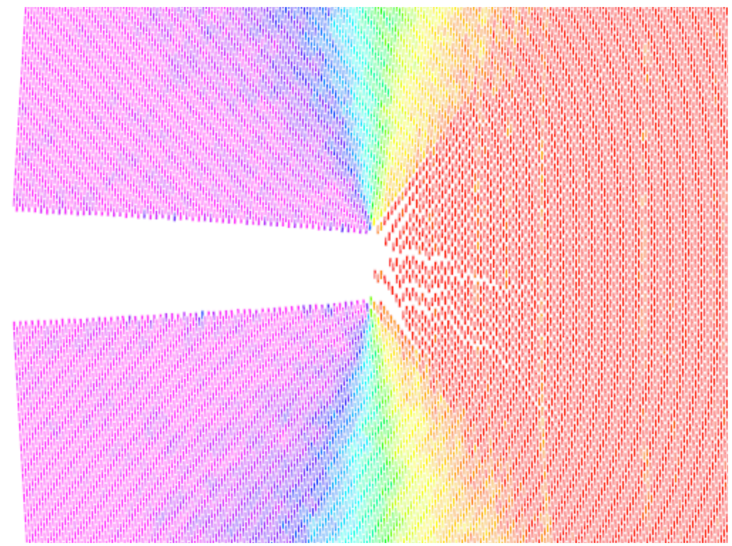


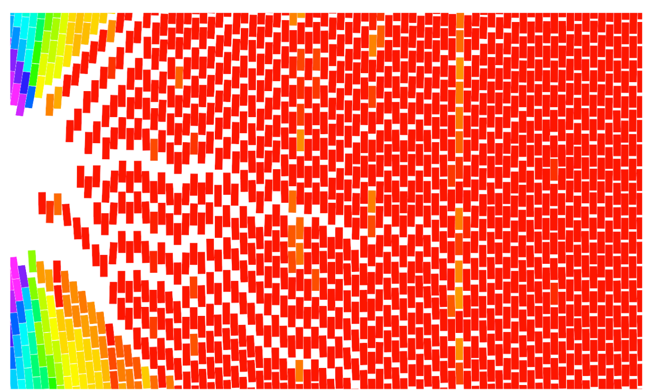
Energy distribution

Brick and mortar particle modeling

Energy distribution: 90 degree case





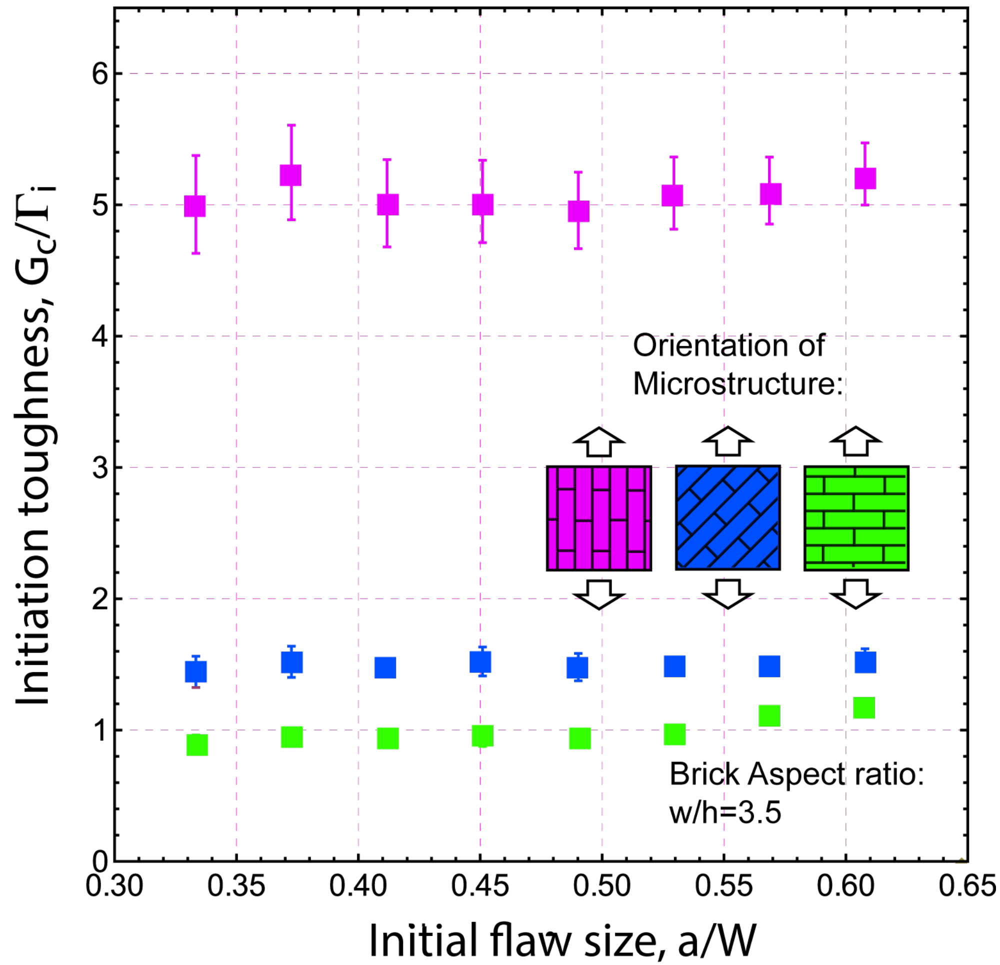


Brick and mortar particle modeling

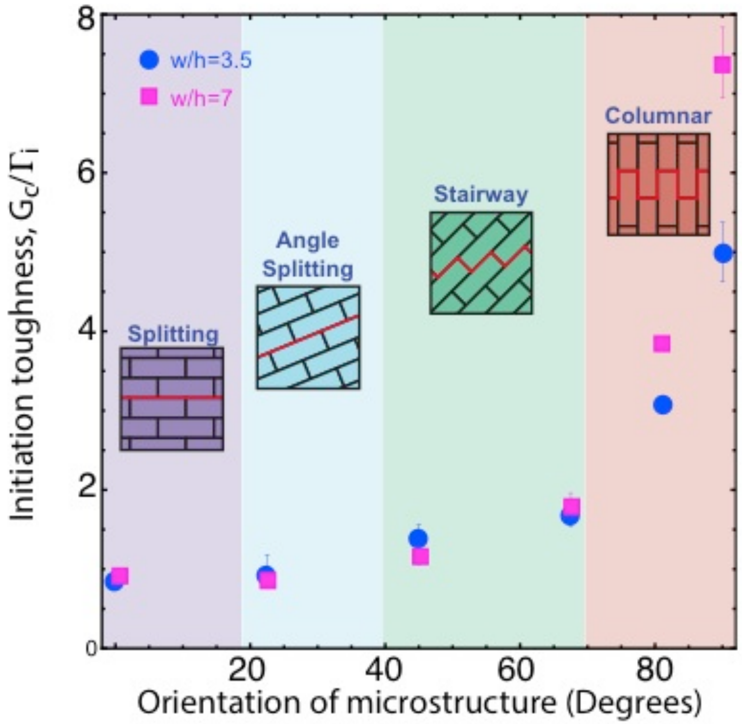
"An Academic Life"

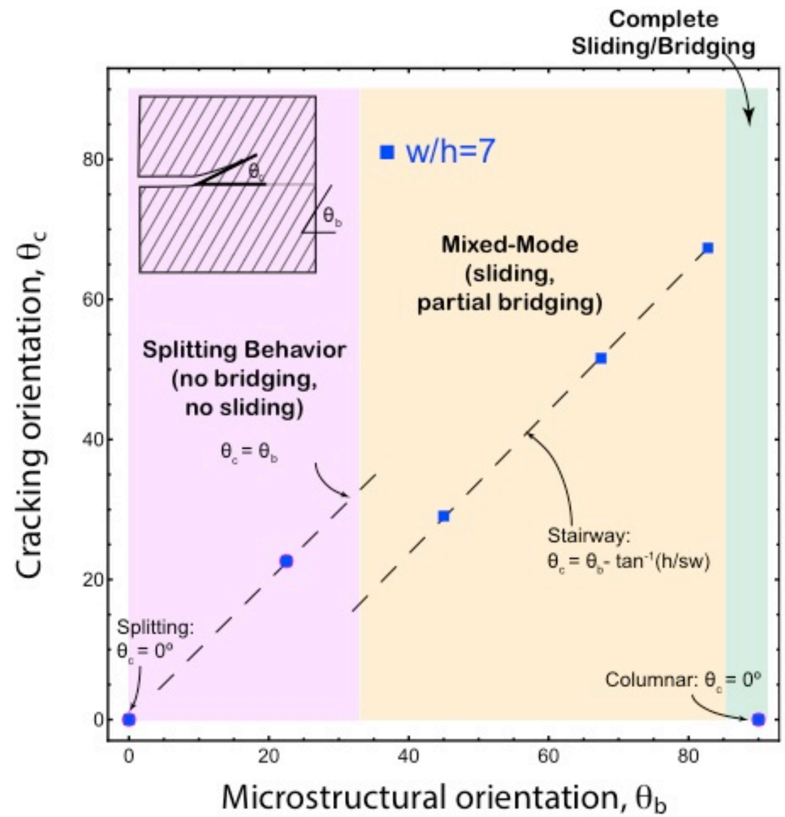
Screenplay by M.R. Begley & W. Pro

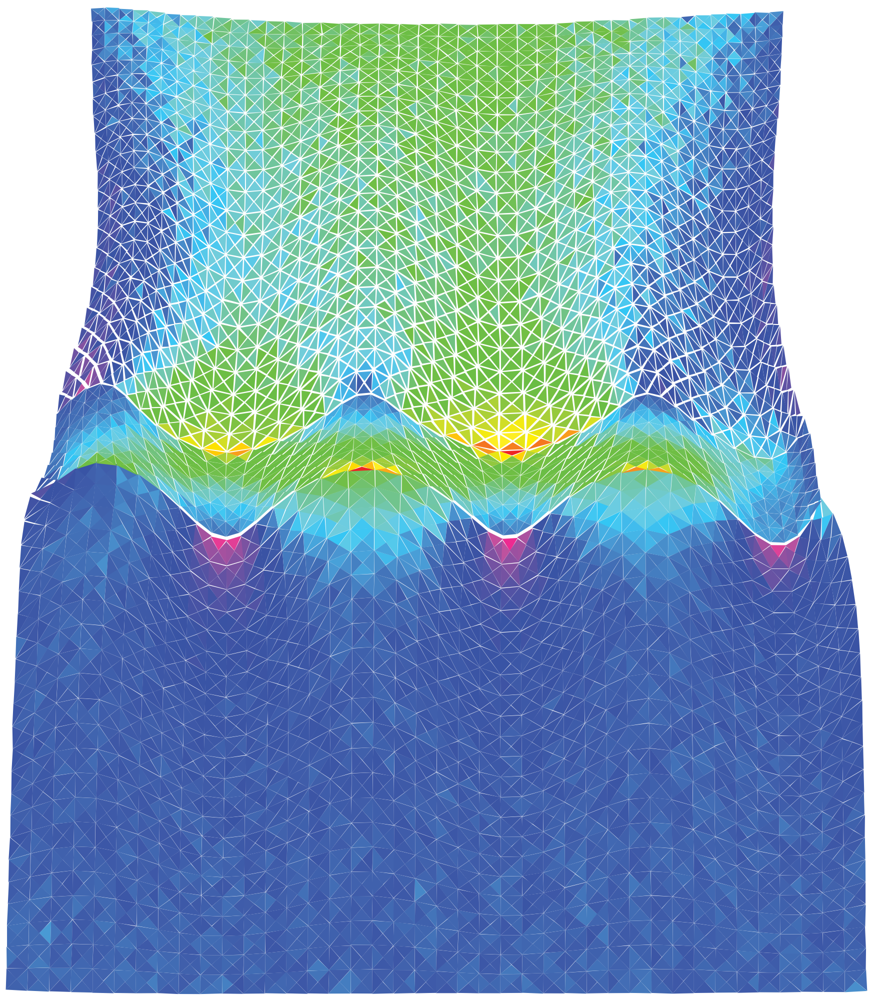
- Begley: "Plot the initiation toughness for all your specimens and loading conditions on a single plot."
- (Pause for figure.)
- Begley: "Is this it?!?! I thought you ran like 100 cases. Plot them all."
- William: "Why? They're all pretty much identical."
- (Pause for dumfounded stare.)
- William: "Oh. Yeah. We should do that."

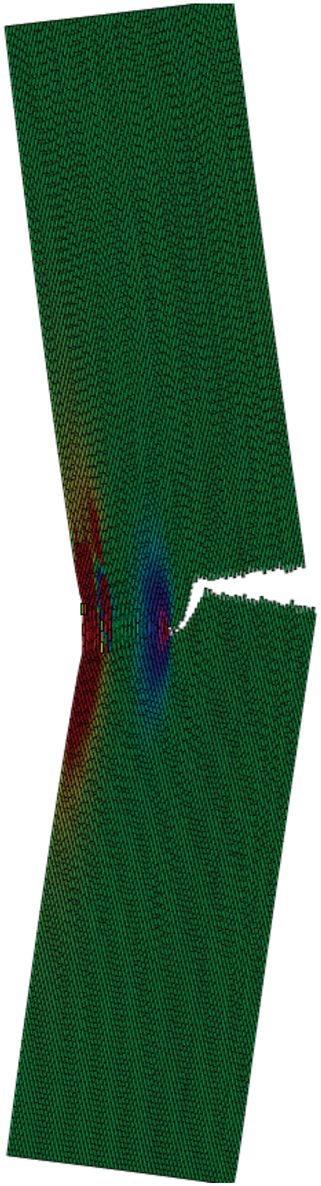


Brick and mortar particle modeling

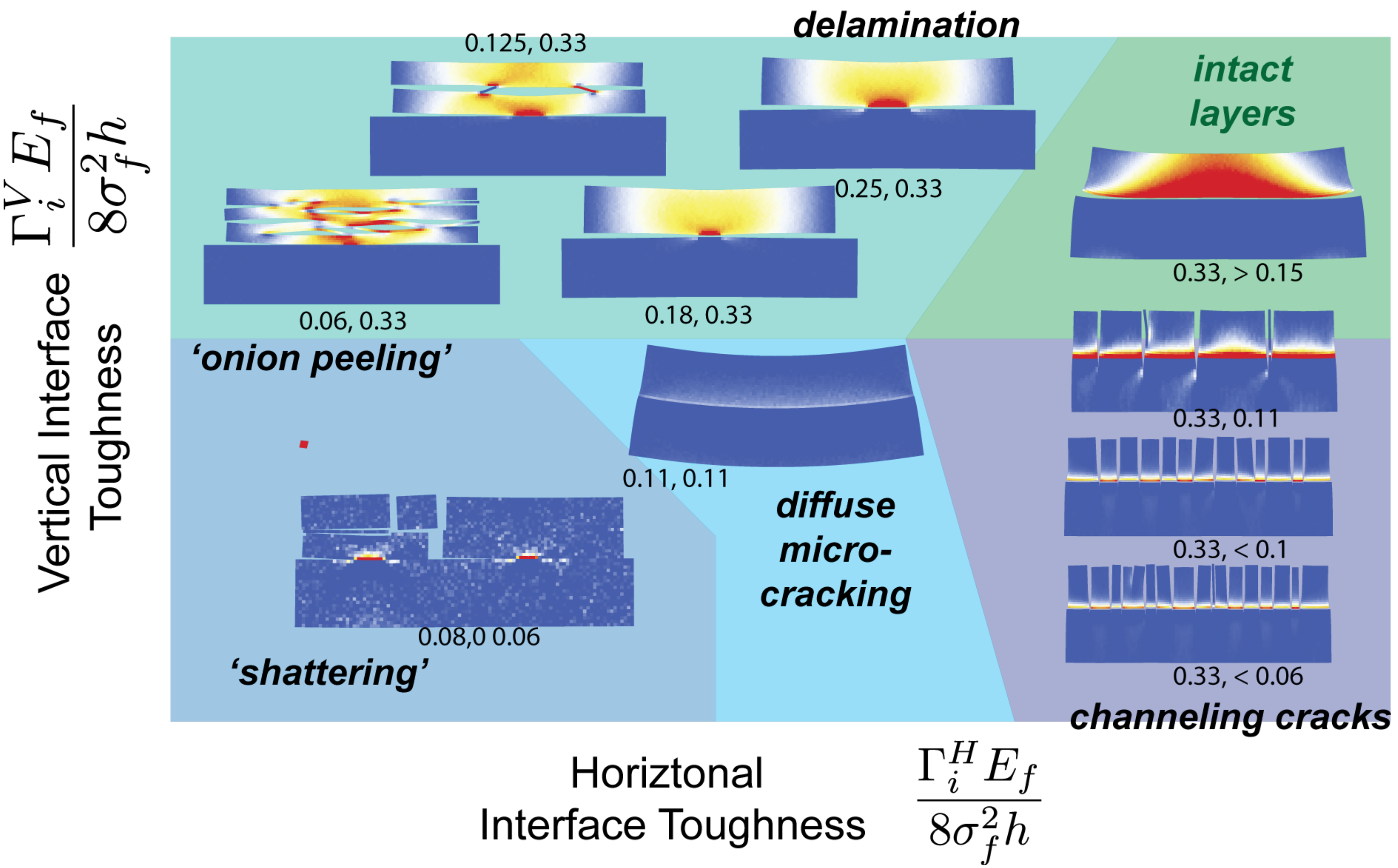








Elastic brick and mortar particle modeling



Concluding Remarks

Particle methods:

- Reduce complexity of meshing.
- Allow for discontinuities, geometry evolution.
- Can be adapted to a wide variety of constitutive models.
- Involve internal length scale: strongly impacts accuracy, speed.
- ***Calibration?!?!?***