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Computational Methods for Pervasive Failure Simulations in Sierra Mechanics

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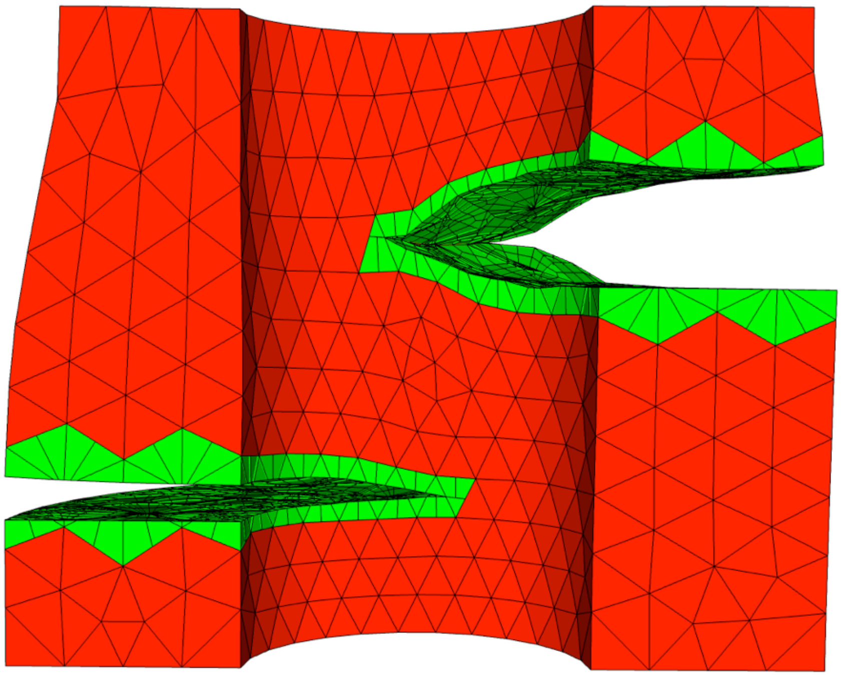
Outline

- Fragmentation, Motivating Example
- Finite Element Approaches
- X-FEM in Sierra
- Gradient-Based Damage Models
- Conclusions



Fragmentation

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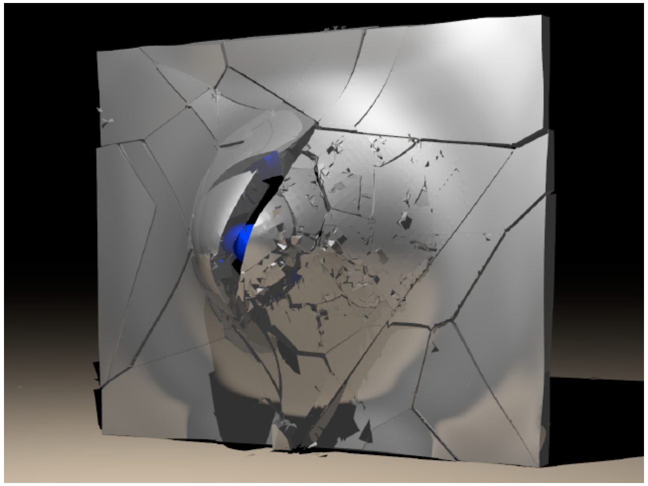
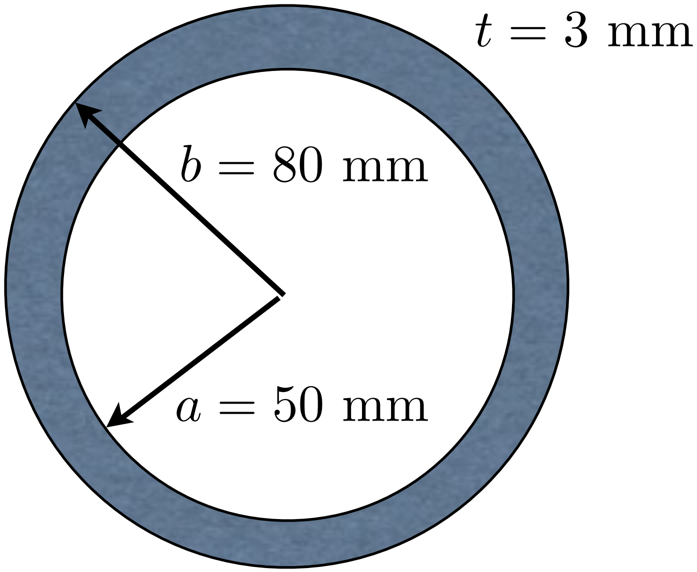
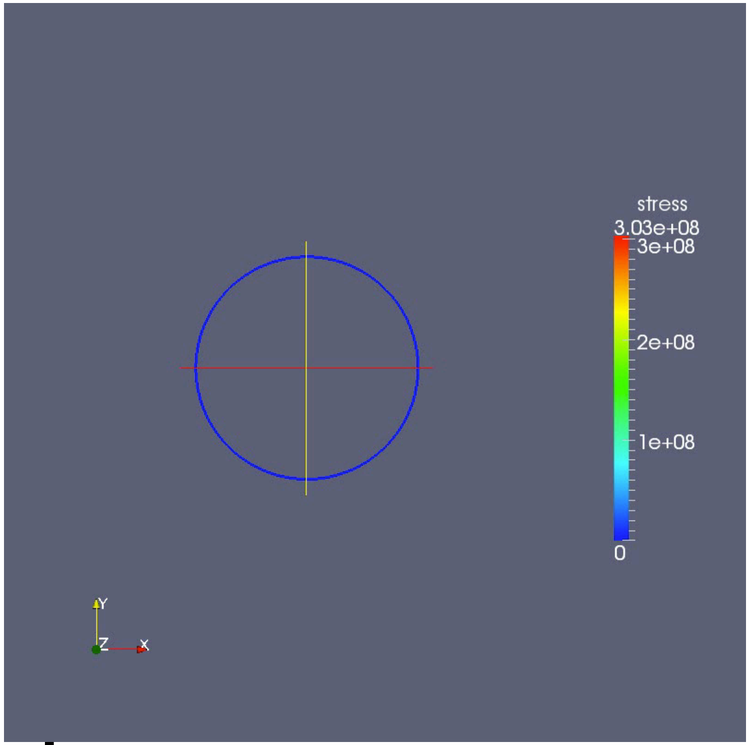
- **Massive, pervasive failure of a structure due (typically) to rapid loading**
- **Dramatic change in the topology of the domain**
- **Simulation challenges: capturing length and time scales, representing the complex geometry**
- **Contact between fragments is also deemed vital for many applications**
- **Typical quantities of interest include fragment distributions, minimum fragment sizes, etc.**



Canonical Problem

- **Ceramic ring subjected to angular rotation**

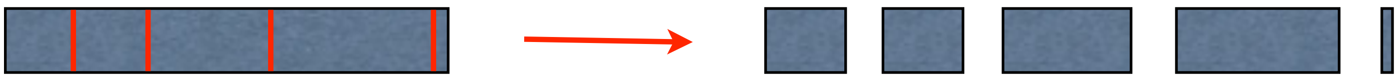




- **Similar to early experiments by Mott.**
- **Of interest because it lends itself to simple (i.e. one-dimensional) representations**

Options for Finite Element Simulations

- **Connected domain to highly disconnected domain?**



- **Element "death"**

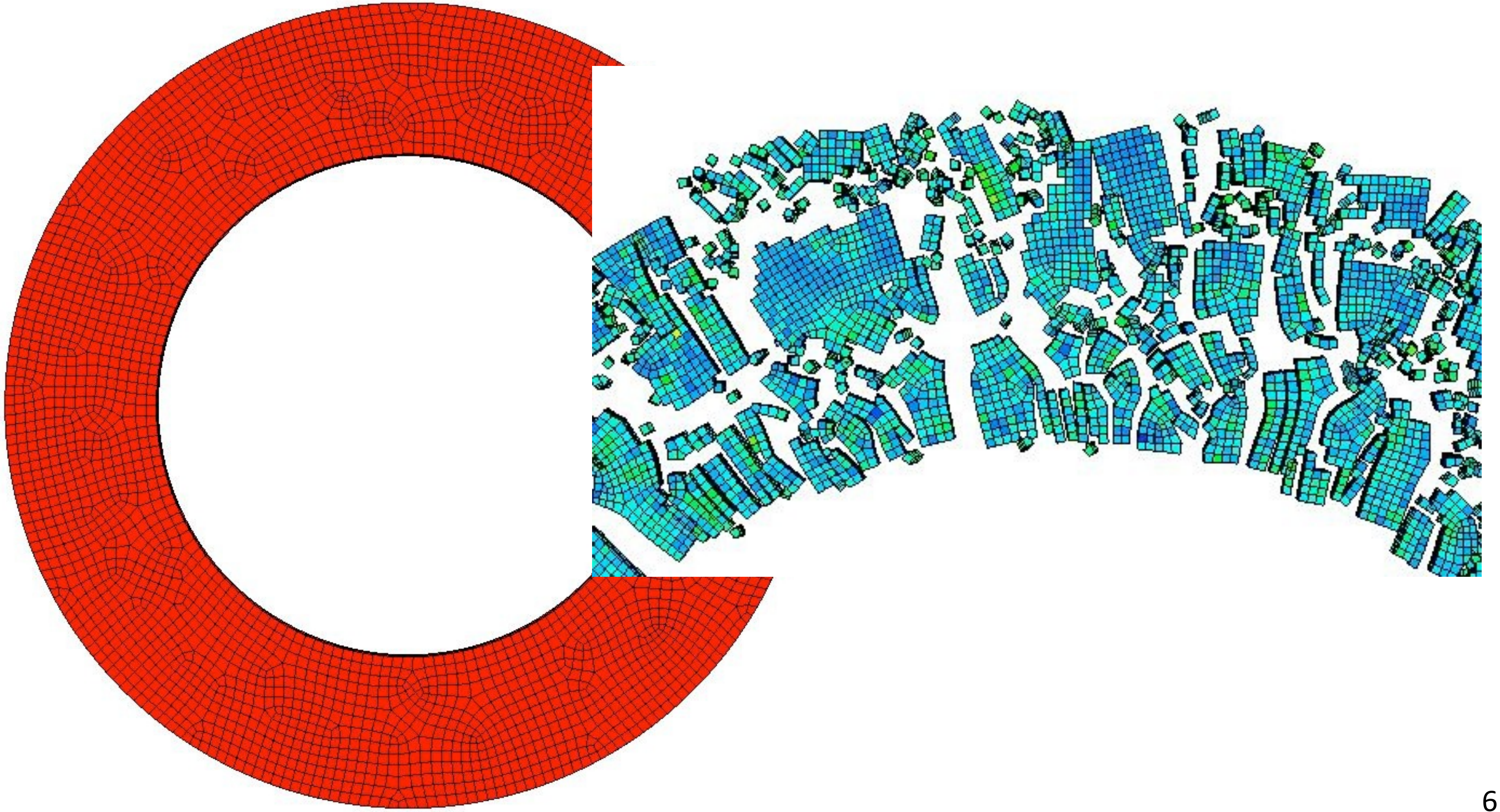
- **Cohesive networks (adaptive insertion)**

- **Embedded finite elements**

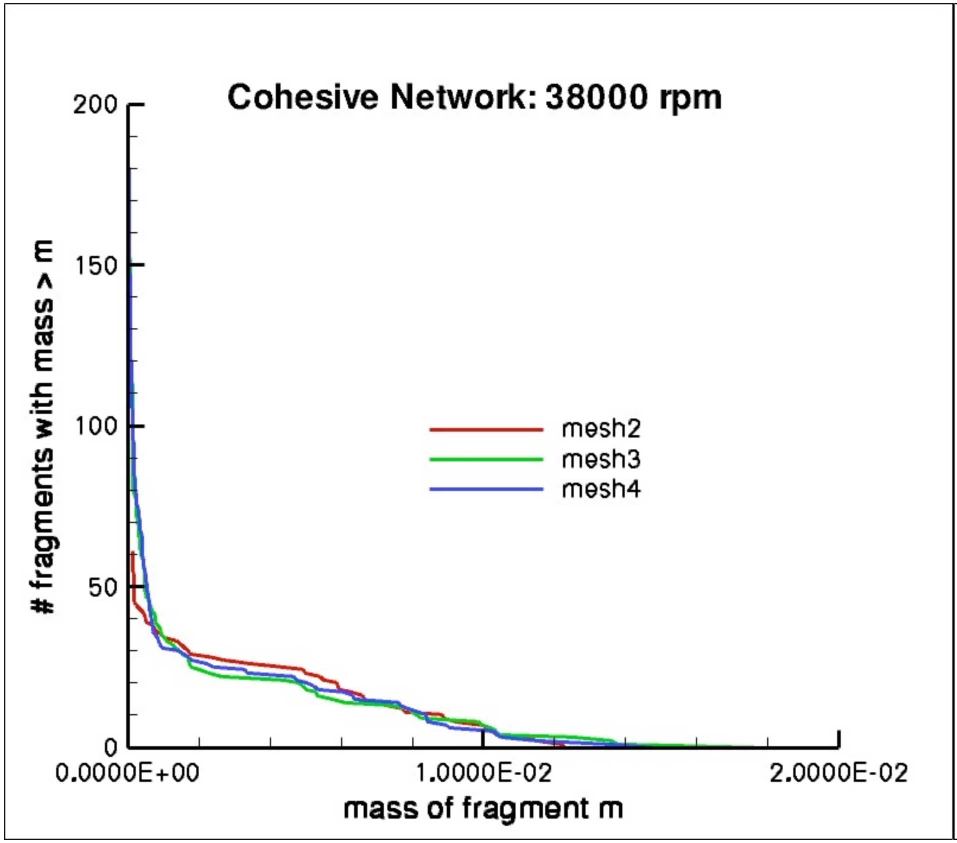
- **Continuous, adaptive remeshing**

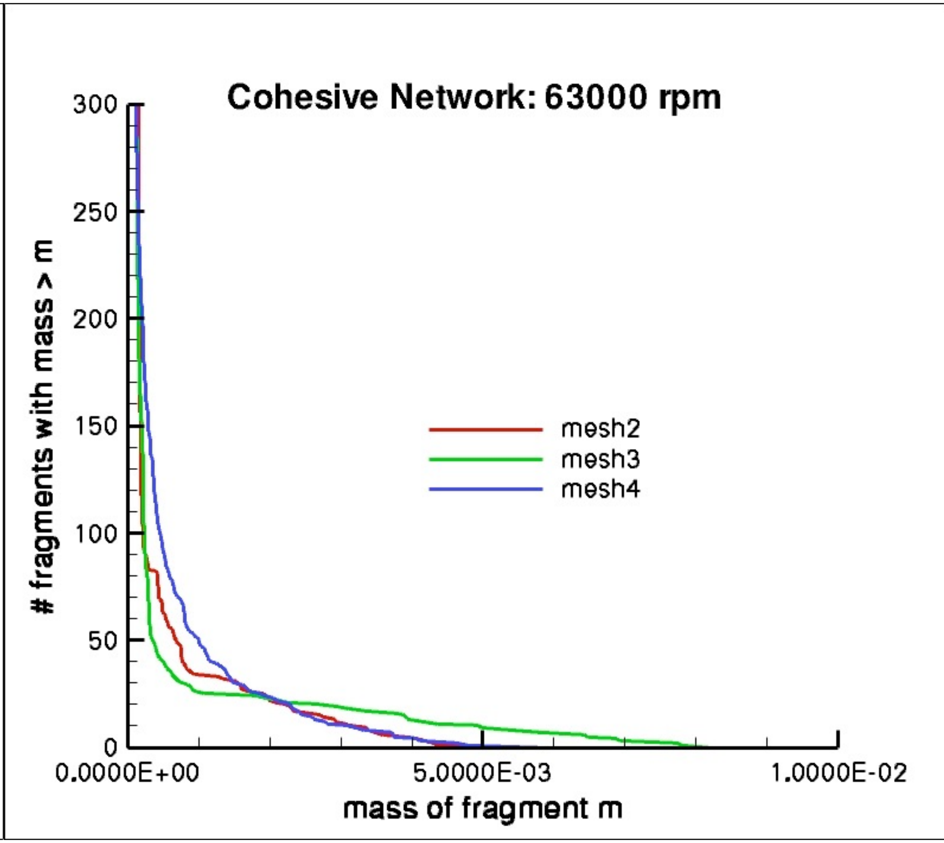
Ring Studies with Cohesive Network

- **Eight-node brick meshes (spatially perturbed)**



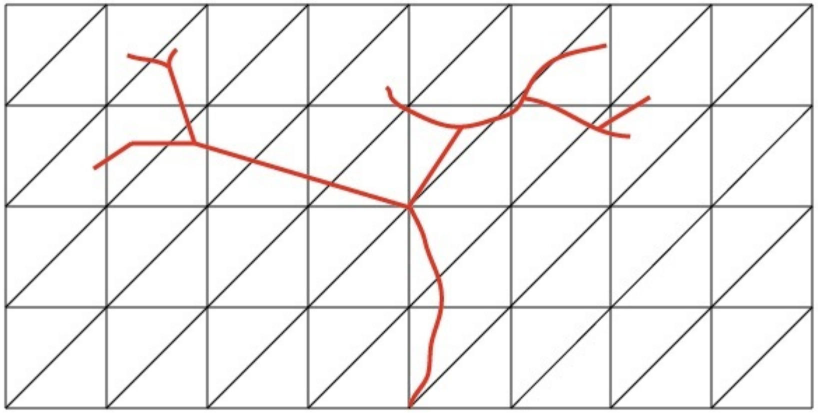
Fragment Statistics Over Refined Grids





X-FEM in Sierra

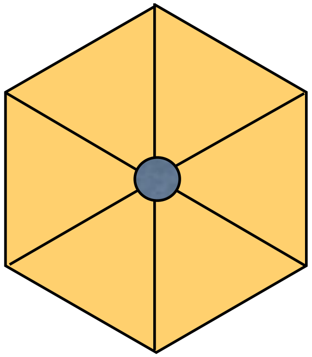
- **Allow for crack geometry to be represented independently of the underlying mesh:**



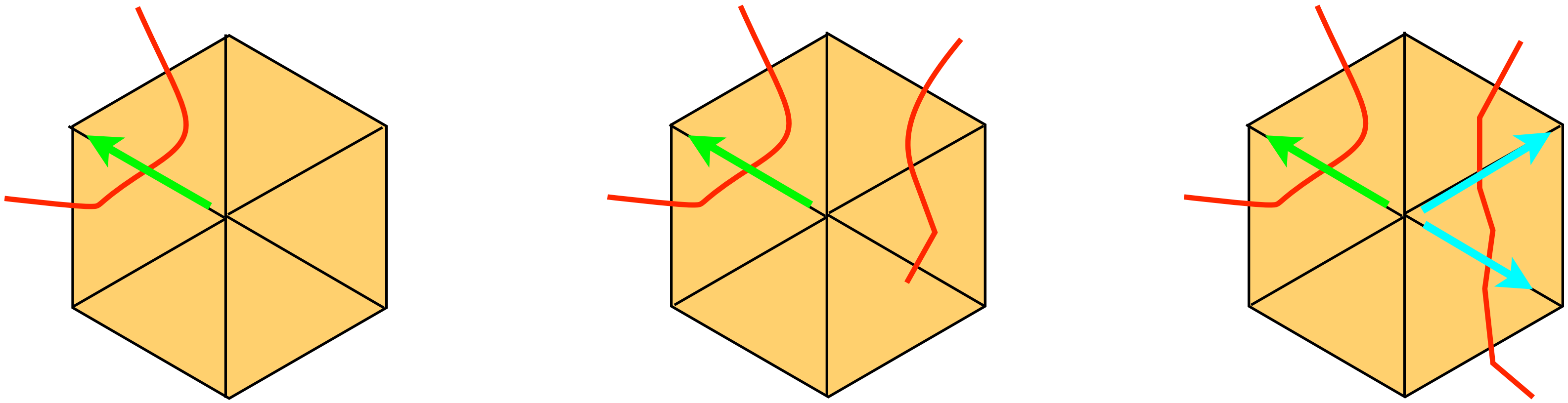
- **Meshes can be fixed, or adaptively refined.**

Embedded Approach to Fragmentation

- **Nodal patch**

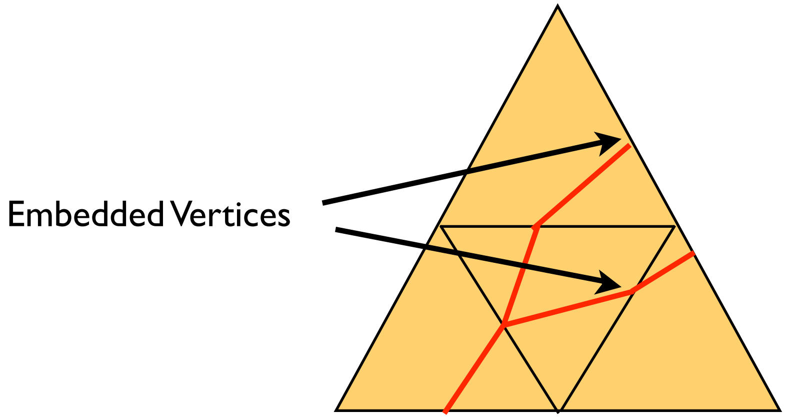


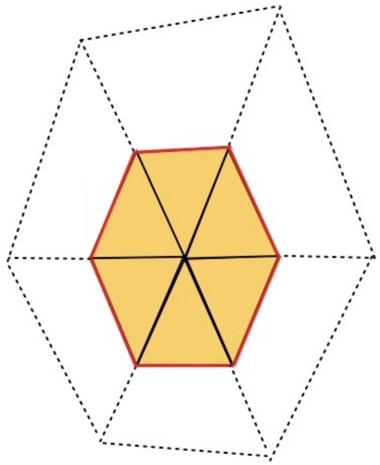
- **Creation of new "virtual nodes" based on complete scoops out of the patch formed by fracture surfaces:**



Restrictions on Topology

- **Necessary to make problem tractable within the resolution of the mesh**

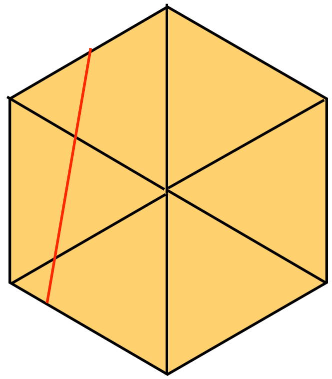




- **Use piecewise-linear cuts**
- **Crack surfaces only intersect element edges**
- **Triangles may contain up to three embedded vertices**

Insertion of Cohesive Zones (Nucleation,

- **Nucleation occurs across an entire patch**
- **Nucleation only permitted if no edges of patch have been intersected by an existing surface**
- **Algorithm grows existing cohesive zones first, then checks for nucleation.**
- **New surfaces inserted after velocity update. Virtual nodes inherit history values from their donors**



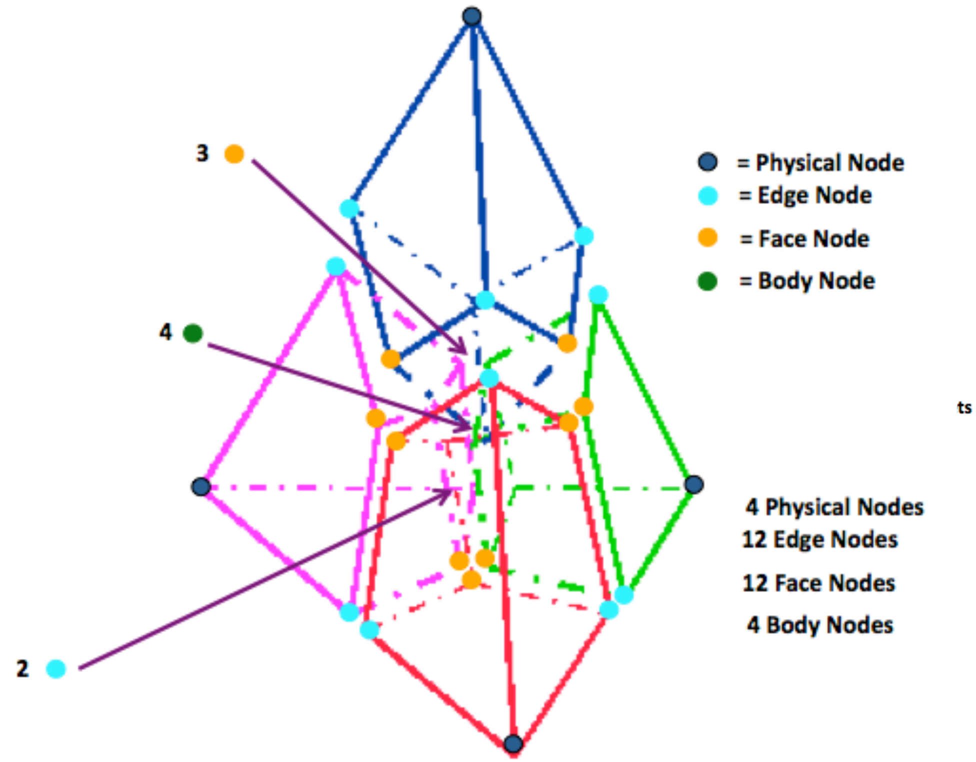
$$\mathbf{x}_{n+1} = \mathbf{x}_n + \Delta t \mathbf{v}_n + \frac{1}{2}\Delta t^2 \mathbf{a}_n$$

$$\mathbf{a}_{n+1} = \mathbf{M}^{-1}(\mathbf{F}^{ext}_{n+1} - \mathbf{F}^{int}_{n+1})$$

$$\mathbf{v}_{n+1} = \mathbf{v}_n + \frac{1}{2}\Delta t(\mathbf{a}_{n+1} + \mathbf{a}_n)$$

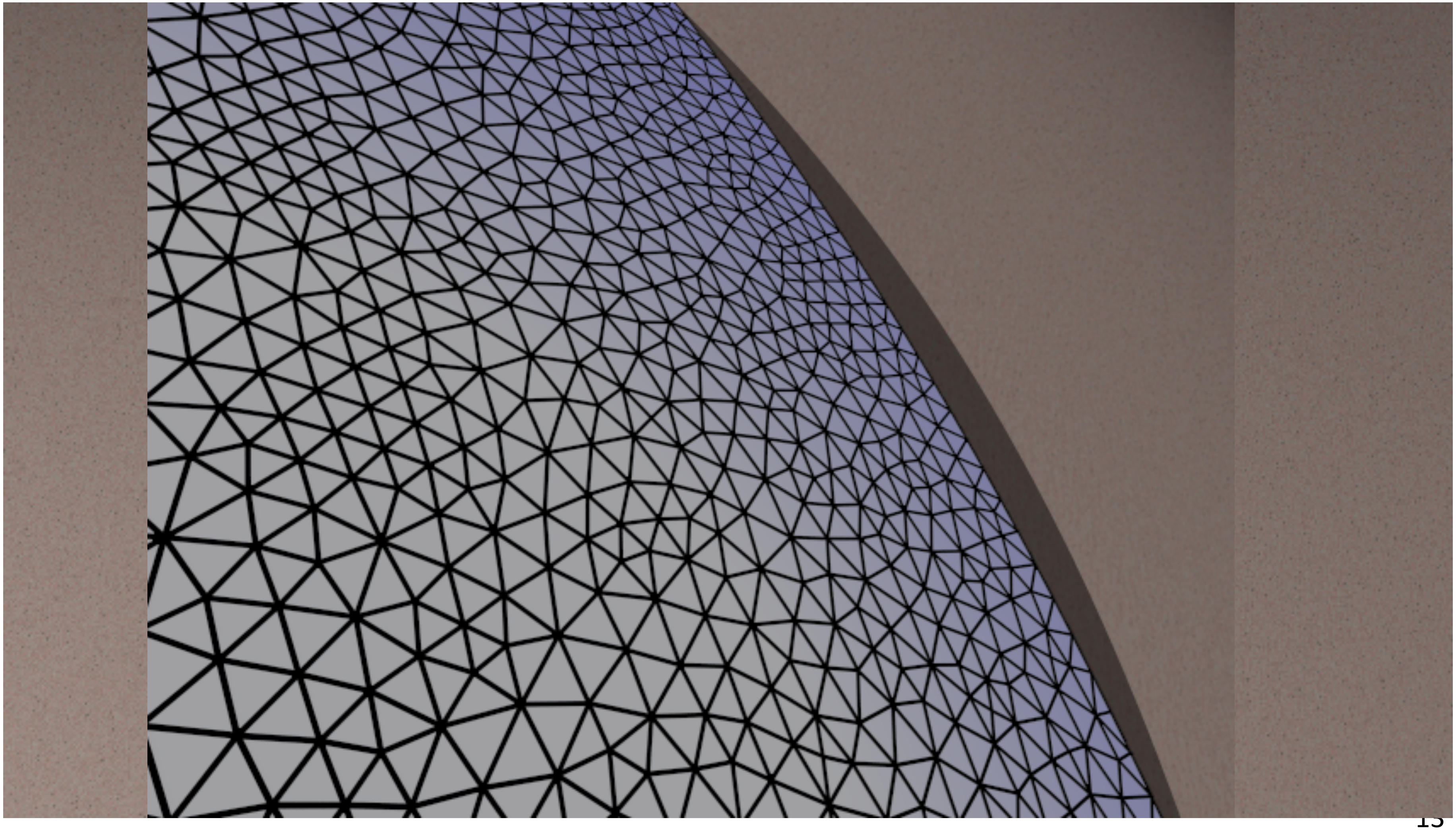
Recent Modifications for 3D

- This kind of bookkeeping becomes cumbersome, especially for multiple fracture surfaces that intersect in 3D
- Sierra now uses a submesh approach
- The bookkeeping has been greatly simplified, and contact surfaces are accurately represented

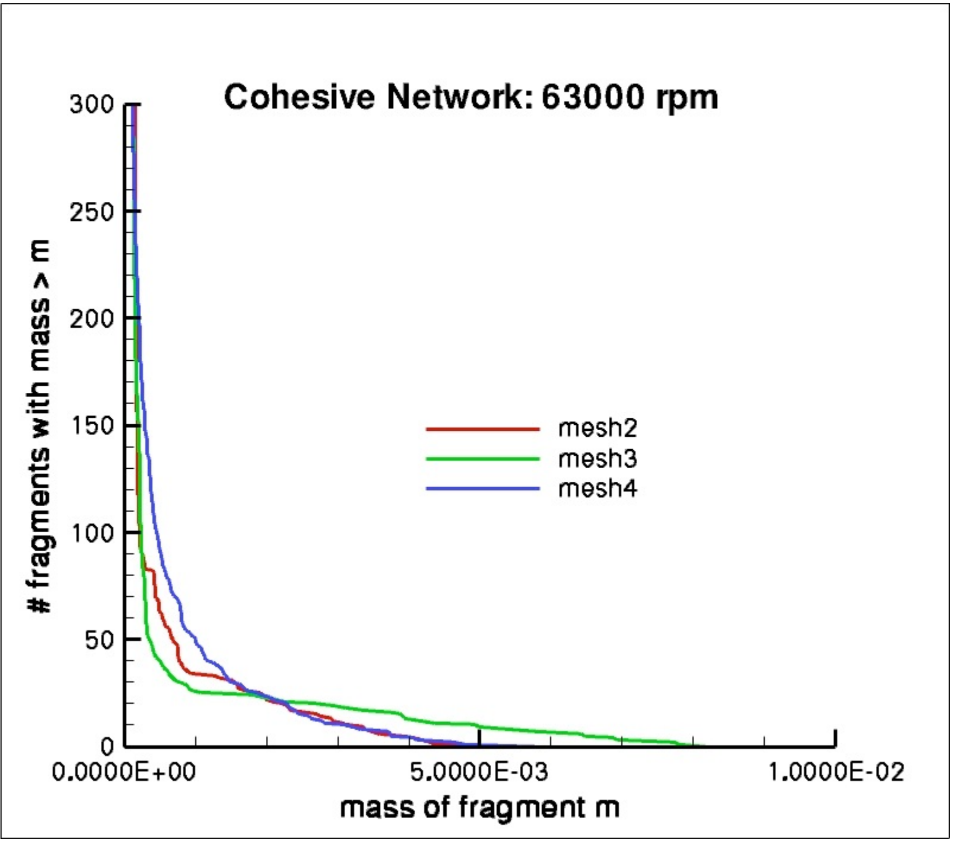


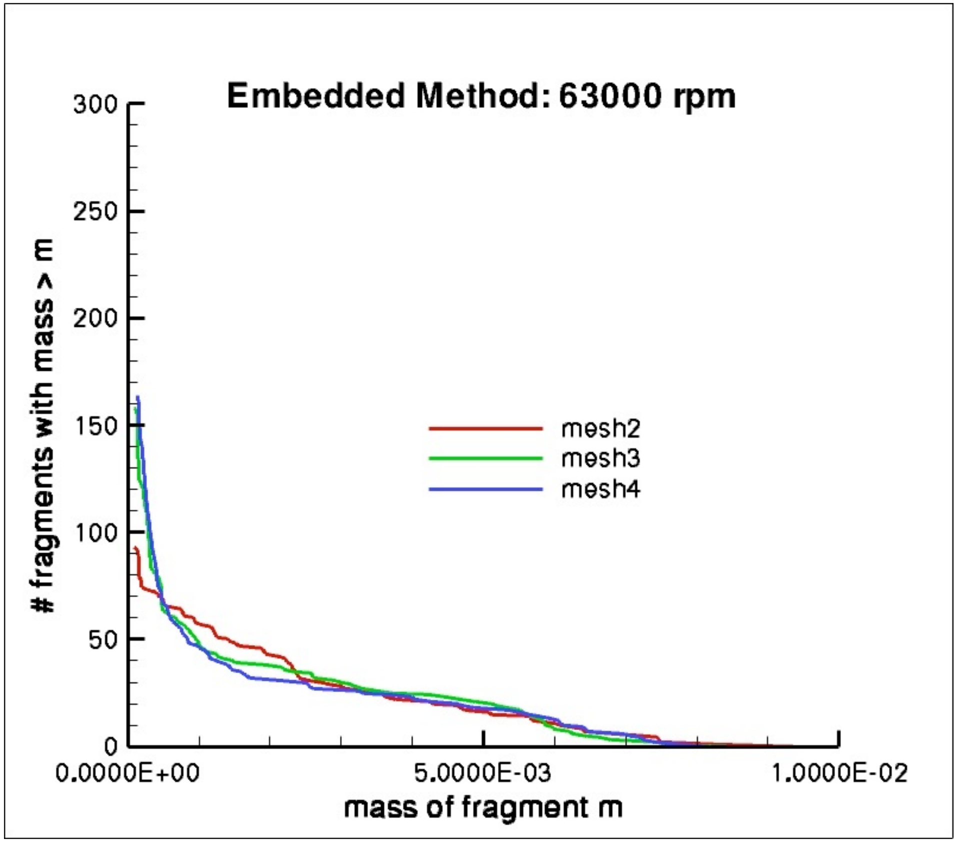
Ring Problem Revisited

- **Simulation over very coarse grid and branch events:**



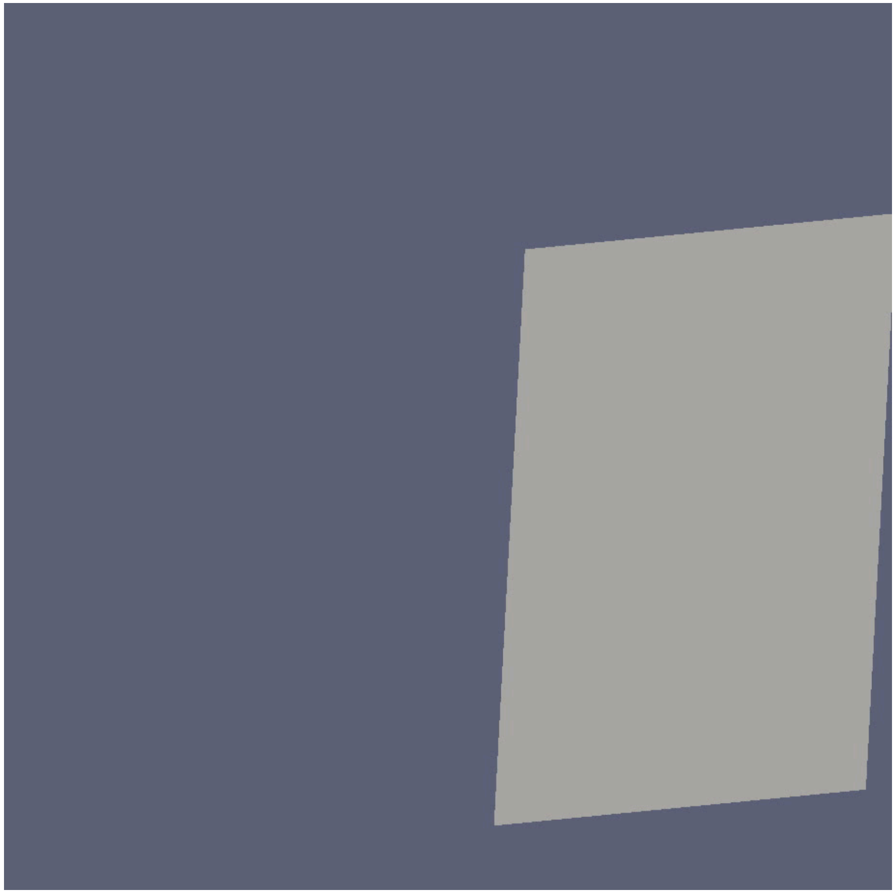
Comparison of Fragment Distributions





Issues with Embedded Approach

- To date, crack surfaces have been represented using piecewise-linear cuts
- Robust algorithms for evolving the geometry of such networks remain a challenge, especially in 3D
- We would like a method that can accurately model both the propagation of a single crack as well as a network of interacting cracks



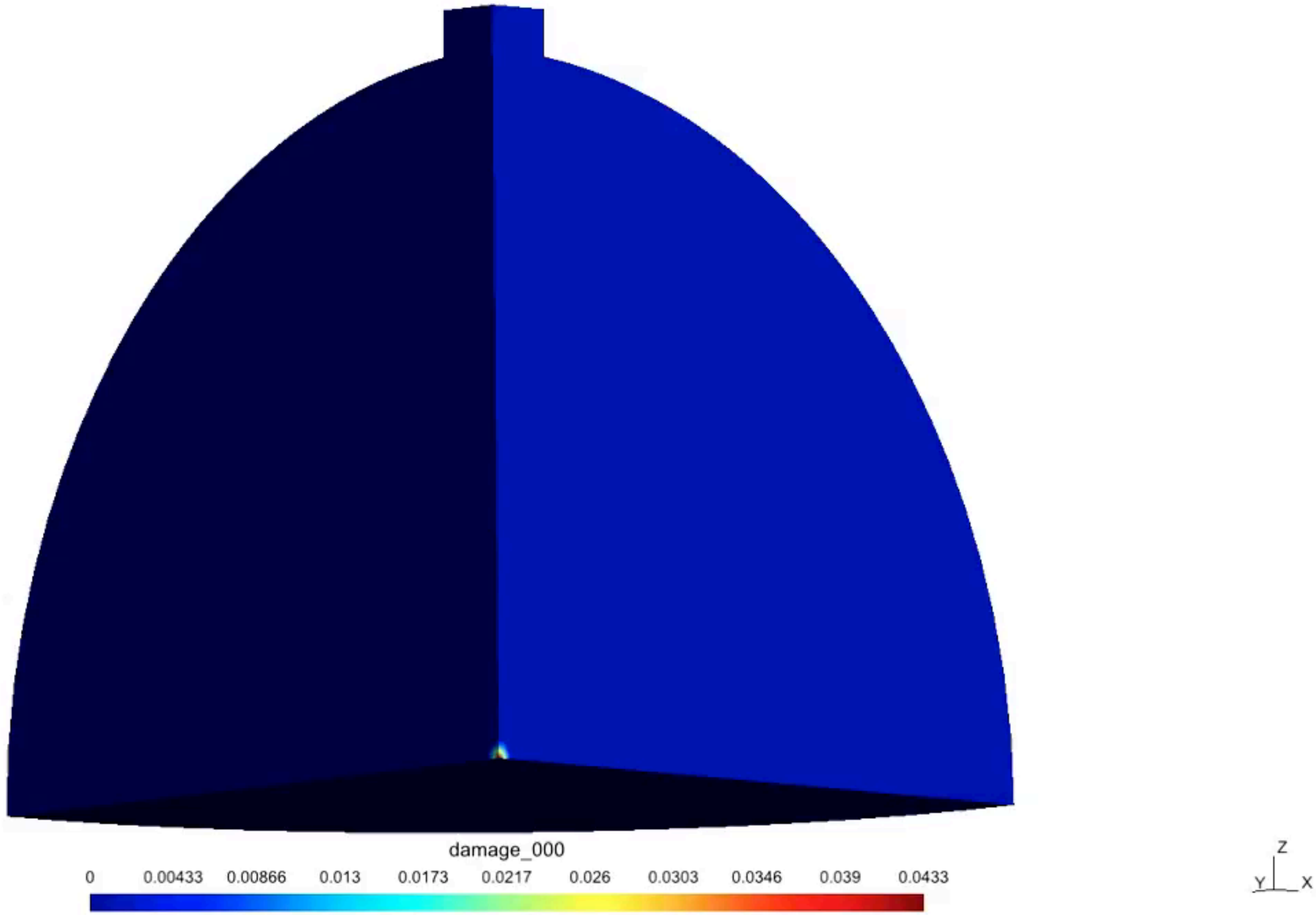
Gradient-Based Damage Models

- **The challenges associated with complex crack geometry in 3D have motivated recent efforts in what are essentially gradient-based damage models**
- **A simplistic approach - decay the stress through a scalar damage field D:**

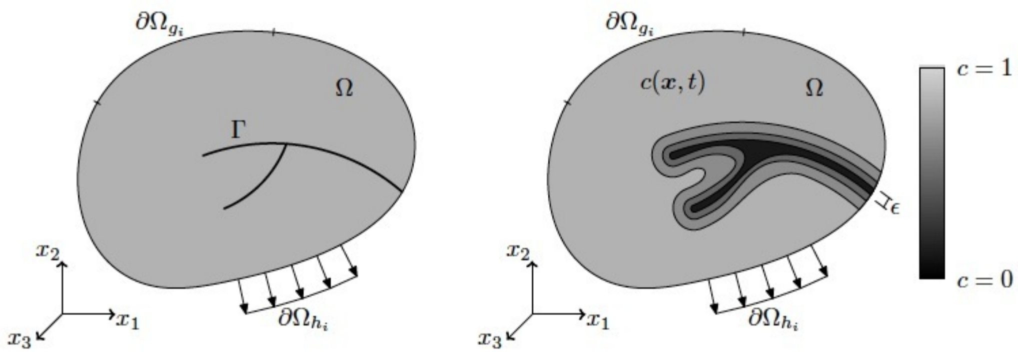
$$\boldsymbol{\sigma} = (1 - D)\mathrm{C}\epsilon \qquad 0 \le D \le 1$$

- **The issue: purely local approaches are not well-posed, and the damage will localize onto a smaller and smaller region as the mesh is refined.**
- **Phase-field methods for fracture (Karma, 2001) accomplish this by introducing a secondary equation for the damage field.**
- **We have looked at the Thick Level-Set (TLS) method (Moes et al. 2011) which introduces a gradient limiter.**

Damage vs. Fracture



Phase Field for Fracture Mechanics



- **Total potential energy**

$$\Psi_{pot}(\boldsymbol{u},\Gamma) = \int_\Omega \psi_e(\nabla^s \boldsymbol{u})\mathrm{d}\boldsymbol{x} + \int_\Gamma \mathcal{G}_c \mathrm{d}\boldsymbol{x}$$

- **Approximate the fracture energy by**

$$\int_\Gamma \mathcal{G}_c \mathrm{d}\boldsymbol{x} \approx \int_\Omega \mathcal{G}_c \left[\frac{(c-1)^2}{4\epsilon} + \epsilon \frac{\partial c}{\partial x_i}\frac{\partial c}{\partial x_i} \right] \mathrm{d}\boldsymbol{x}$$

Phase Field for Fracture Mechanics

- **Split elastic energy into tensile and compressive parts**

$$\psi_e(\varepsilon, c) \approx [(1-k)c^2 + k]\psi_e^+(\varepsilon) + \psi_e^-(\varepsilon)$$

$$\psi_e^+(\boldsymbol{\varepsilon}) = \frac{1}{2}\lambda\langle \mathrm{tr}\boldsymbol{\varepsilon}\rangle^2 + \mu \mathrm{tr}[(\boldsymbol{\varepsilon}^+)^2] \qquad \psi_e^-(\boldsymbol{\varepsilon}) = \frac{1}{2}\lambda(\mathrm{tr}\boldsymbol{\varepsilon} - \langle \mathrm{tr}\boldsymbol{\varepsilon}\rangle)^2 + \mu \mathrm{tr}[(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^+)^2]$$

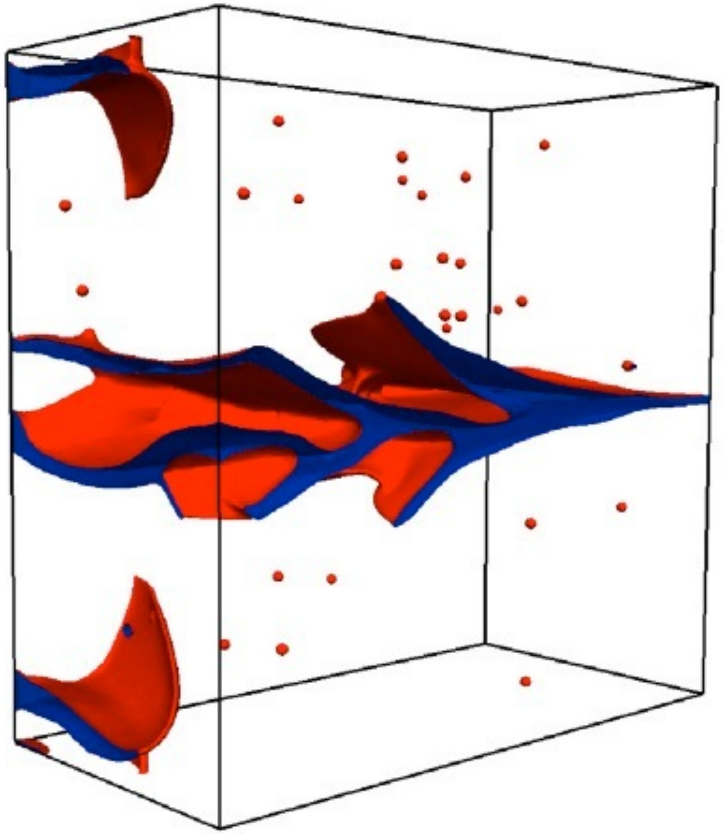
- **Strong form for dynamics Borden et al. 2012:**

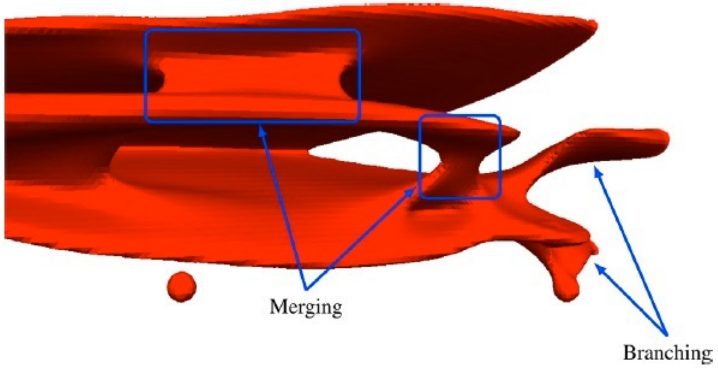
$$\frac{\partial \sigma_{ij}}{\partial x_j} = \rho \ddot{u}_i \qquad \text{on} \quad \Omega \times]0, T[$$

$$\left(\frac{4\epsilon(1-k)\psi_e^+}{\mathcal{G}_c} + 1\right) c - 4\epsilon^2 \frac{\partial^2 c}{\partial x_i^2} = 1 \qquad \text{on} \quad \Omega \times]0, T[$$

$$\sigma_{ij} = [(1-k)c^2 + k]\frac{\partial \psi_e^+}{\partial \varepsilon_{ij}} + \frac{\partial \psi_e^-}{\partial \varepsilon_{ij}}$$

3D Results





A Key to Fragmentation: Energy

- **Consider an elasto-damage model with softening, of the form (1D):**

$$\varphi(\epsilon, d) = \frac{1}{2}(1-d)E\epsilon^2 + Y_c(H(d) - d)$$

- **The energy dissipated over an extension of the damage zone is:**

$$\begin{aligned} \dot{e} &= \int_0^t \int_0^l \frac{1}{2}(\sigma\dot{\epsilon} - \dot{\sigma}\epsilon)\,\mathrm{d}x\,\mathrm{d}t = \int_0^t \int_0^l \frac{1}{2}E\epsilon^2\dot{d}\,\mathrm{d}x\,\mathrm{d}t = \\ &= \int_0^t \int_0^l (Y + Y_c(H'(d) - 1))\dot{d}\,\mathrm{d}x\,\mathrm{d}t = \int_0^t \int_0^l Y_c H'(d)\dot{d}\,\mathrm{d}x\,\mathrm{d}t \\ &= Y_c \int_0^l H(d)\,\mathrm{d}x \end{aligned}$$

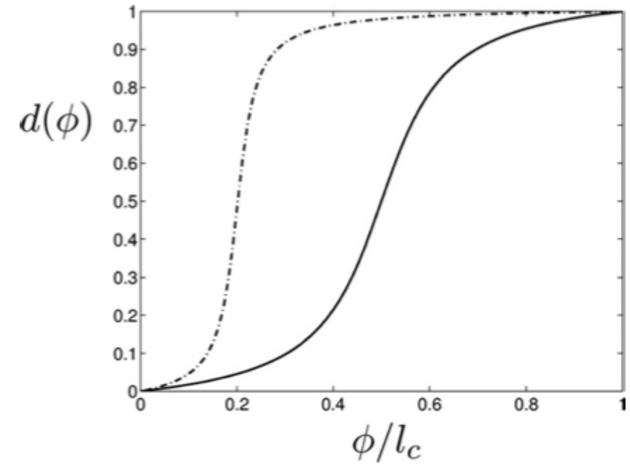
- **We have been able to reproduce theoretical estimates for fragment scaling with strain rates for TLS**

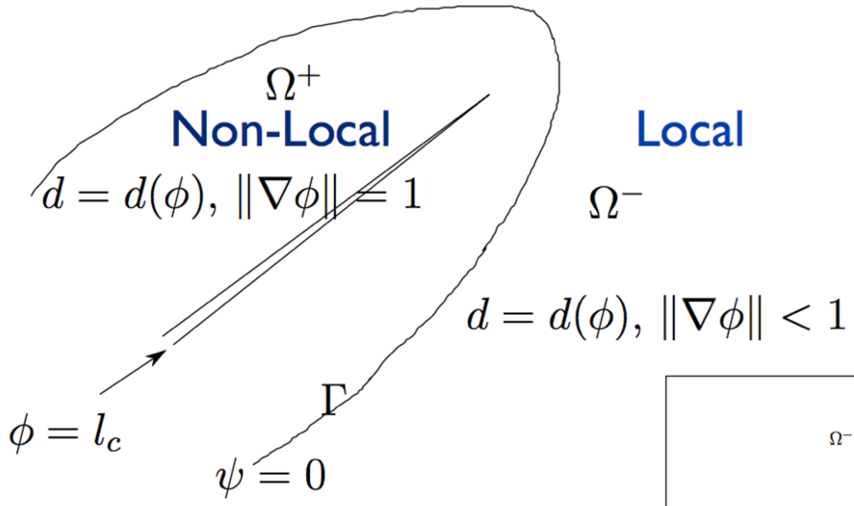
Summary and Future Directions

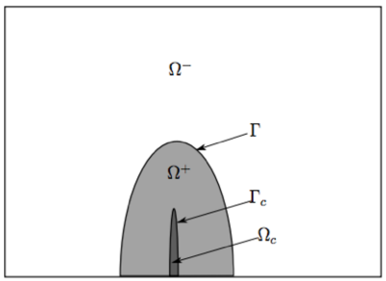
- Fragmentation problems involve a number of processes spanning spatial and temporal scales.
- These problems tend to be very stiff.
- While the embedded approach allows for an increase in accuracy, it is not a panacea on its own.
- Work in Sierra is ongoing to incorporate gradient-based damage models.
- The current plan is to couple these gradient-based methods with embedded approaches.

Thick-Level Set Approach

- **Introduce an ancillary relationship between the damage variable and a level-set function.**
- **Limit the gradient of the level-set in the non-local region:**

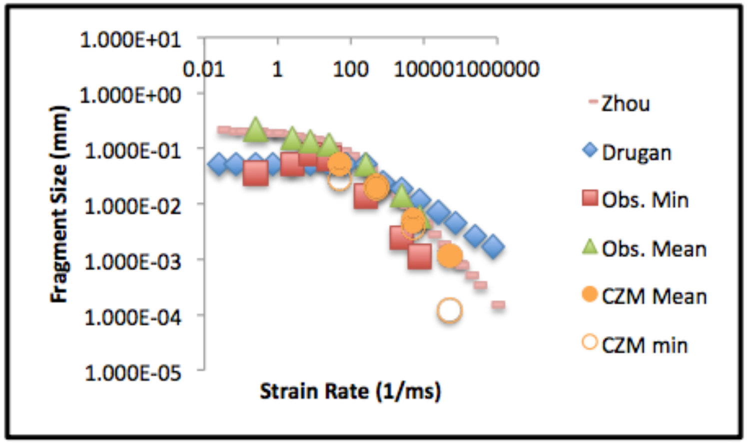


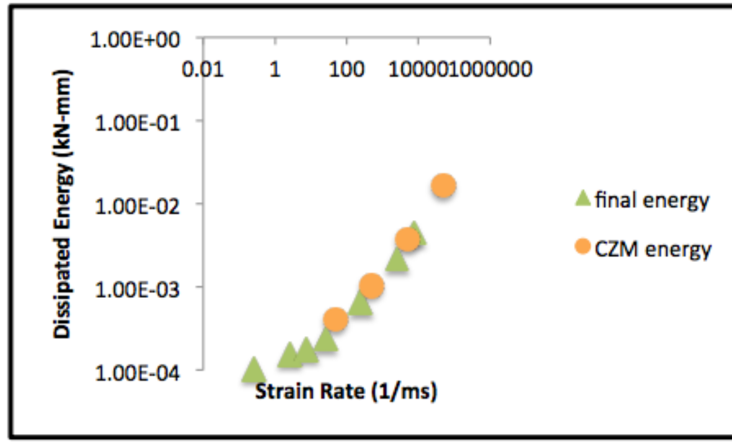




Results

- **Thick-level set results (1D) for fragment sizes and energy Stershic et al. (2015)**





- **Results were obtained by setting l_c to be half the smallest fragment size expected at the highest strain rate.**