SAND2009-3974C

An Overview of Large-Scale Computational Methods for Ballistic-Resistant Structure Design

Erik Strack
ALEGRA Code Development Team
Sandia National Laboratories

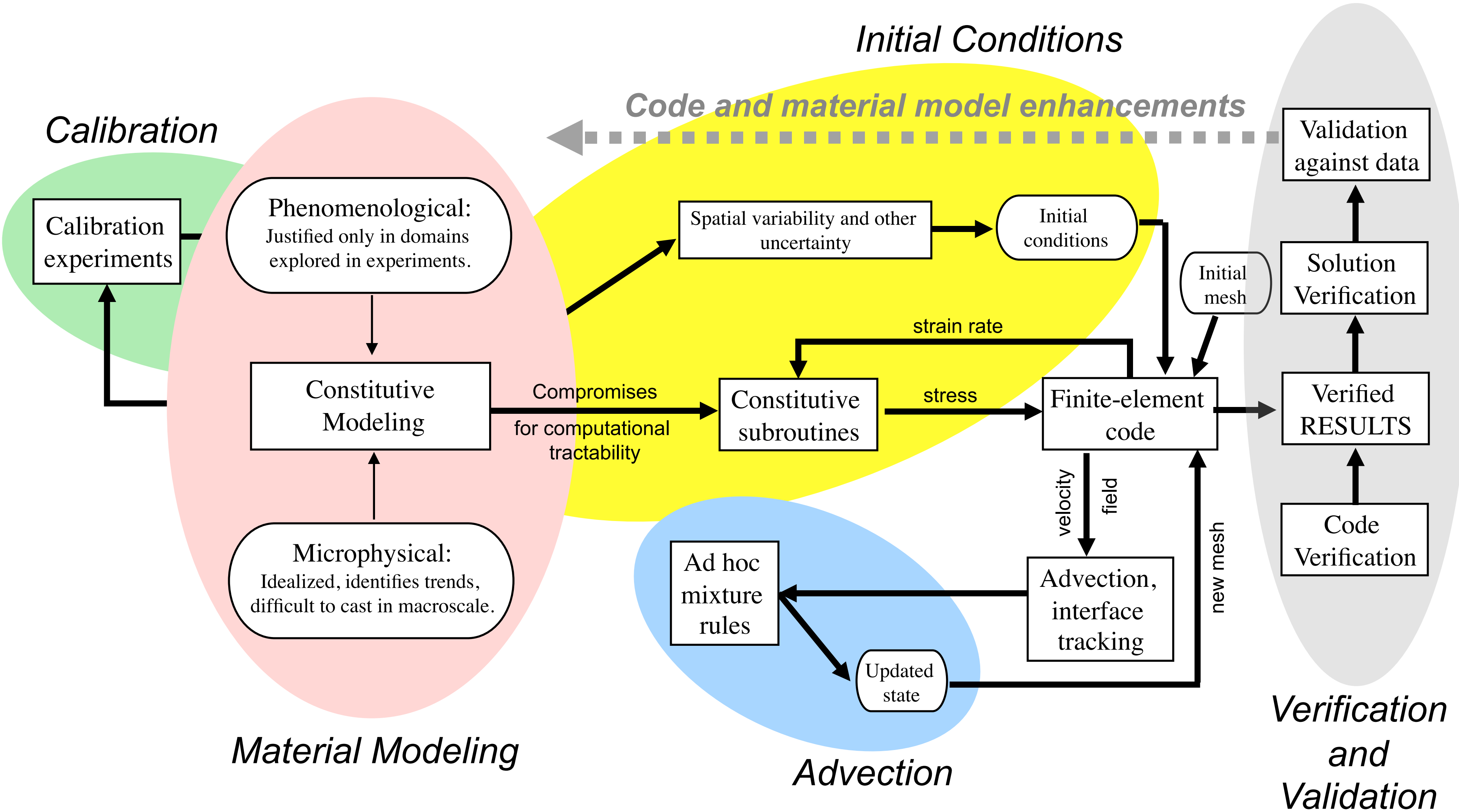
Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Presentation Contents

- Introduction – FEM methods
- Available computational methods
  - Lagrangian methods
  - Particle methods
  - Eulerian and ALE methods
- Outstanding issues
  - High-performance computing
  - Shock capturing
  - Verification and validation
  - Material modeling (EOS, complexity, fracture)
- Conclusion – the long road ahead

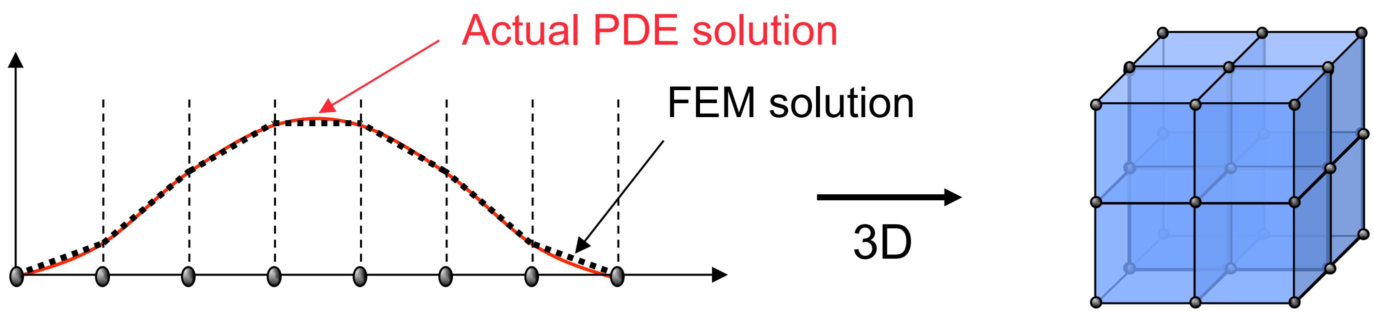
Sandia National Laboratories

Introduction: Finite-Element Modeling and Simulation



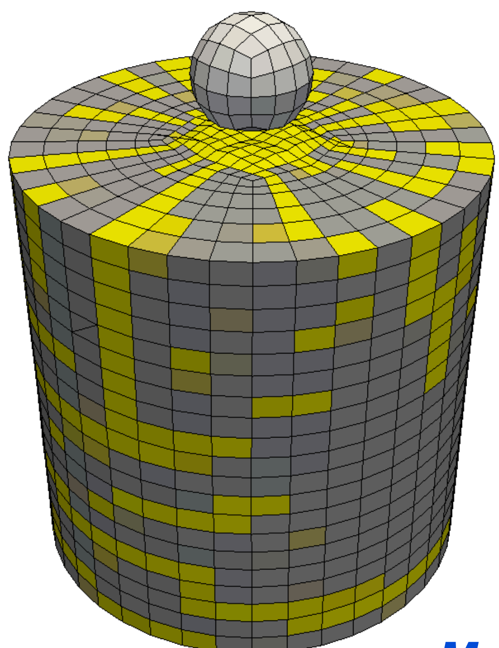
Sandia National Laboratories

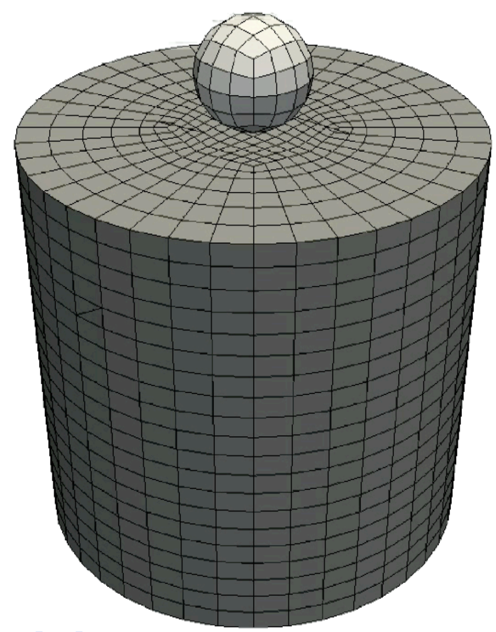
Lagrangian Methods



Quick review: Finite Elements are discrete volumes over which PDE's are solved.

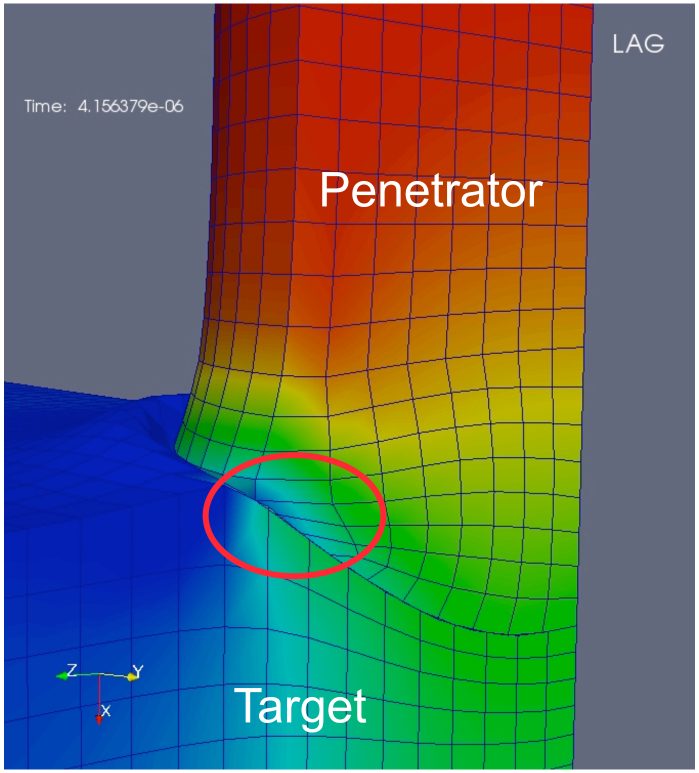
Convergence is crucial…



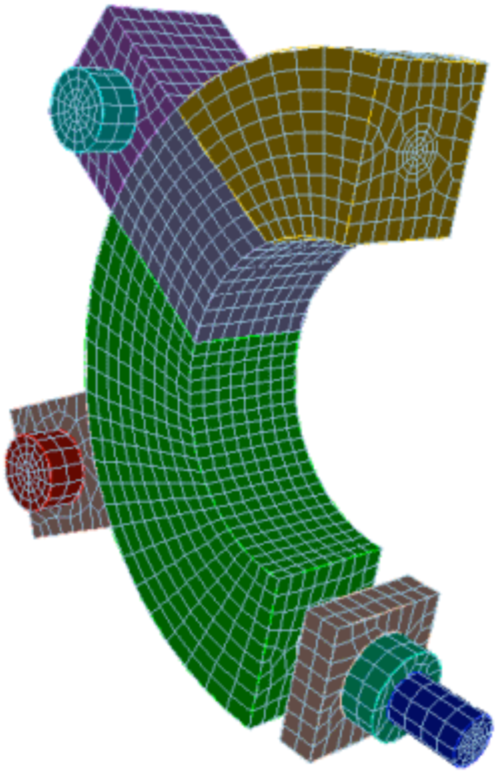


Mesh moves WITH material

Lagrangian Methods – Issues



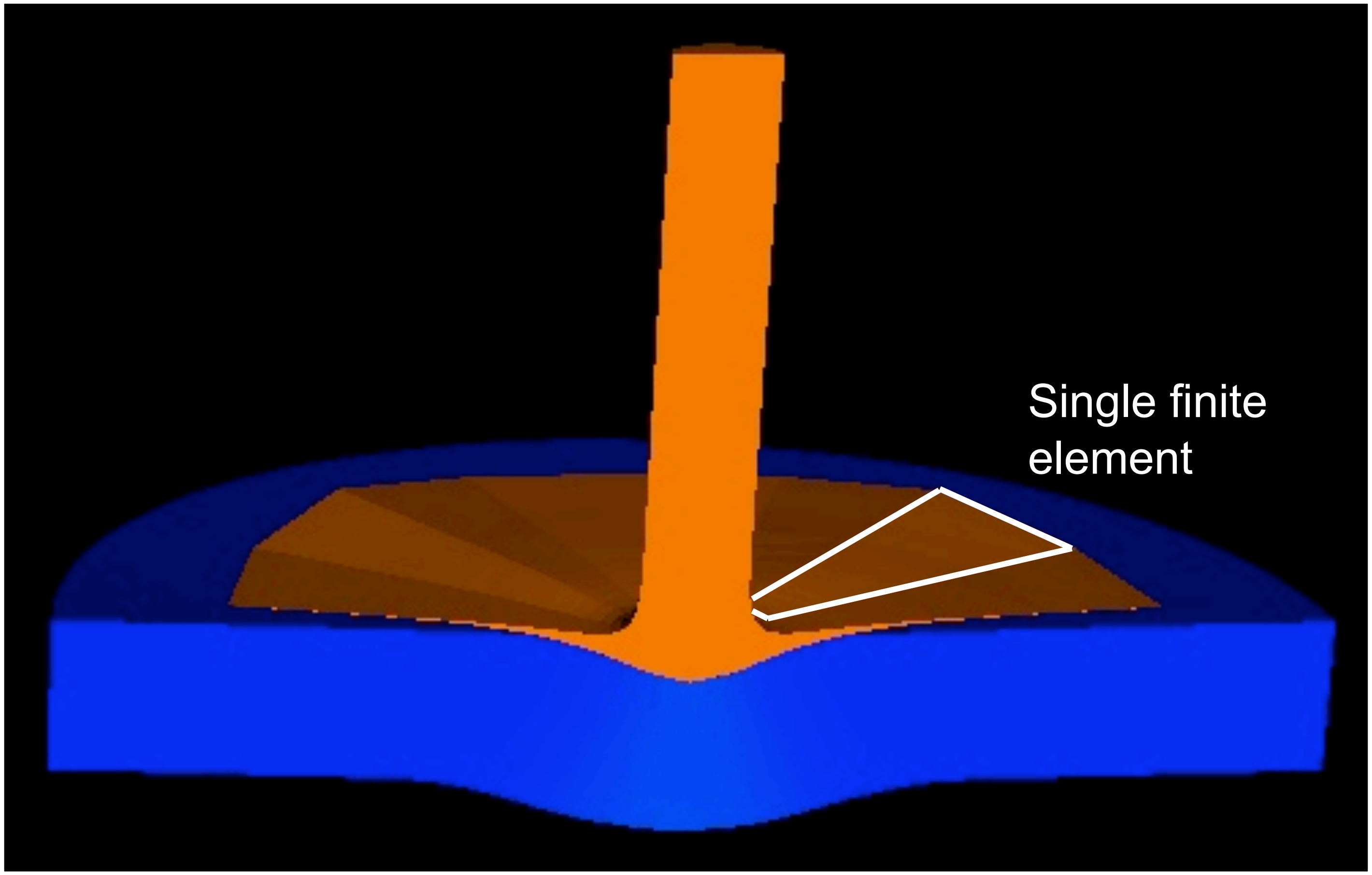
#1 Mesh tangling



#2 Mesh generation

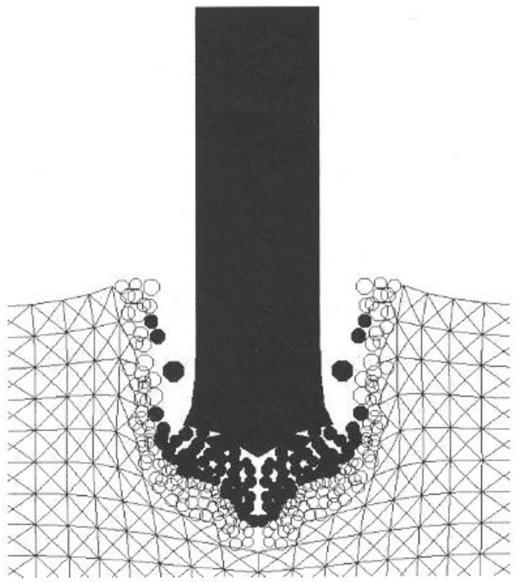
Sandia National Laboratories

Lagrangian Methods – Issues



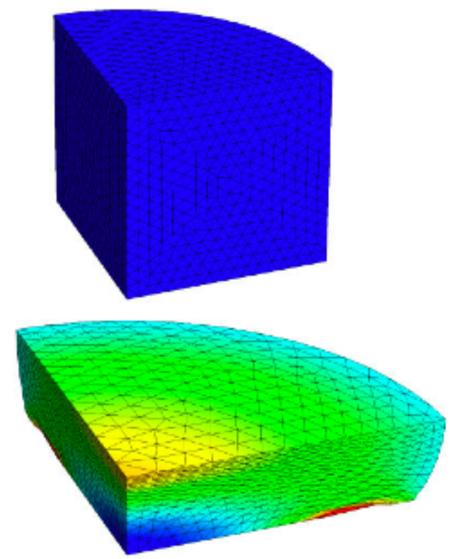
Element degeneration – up close

Lagrangian – Enhancements



Johnson & Holmquist

Convert to Particles

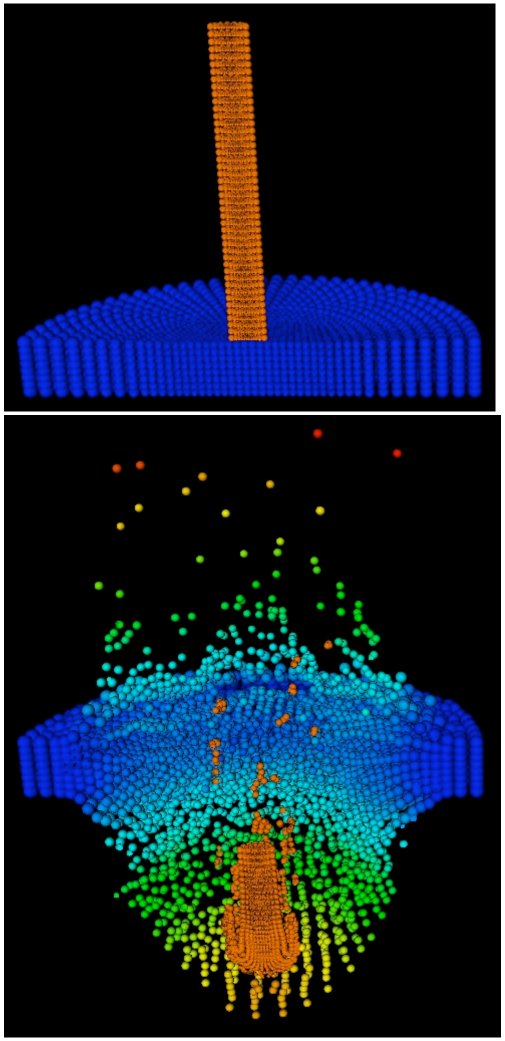


Puso and J. Solberg

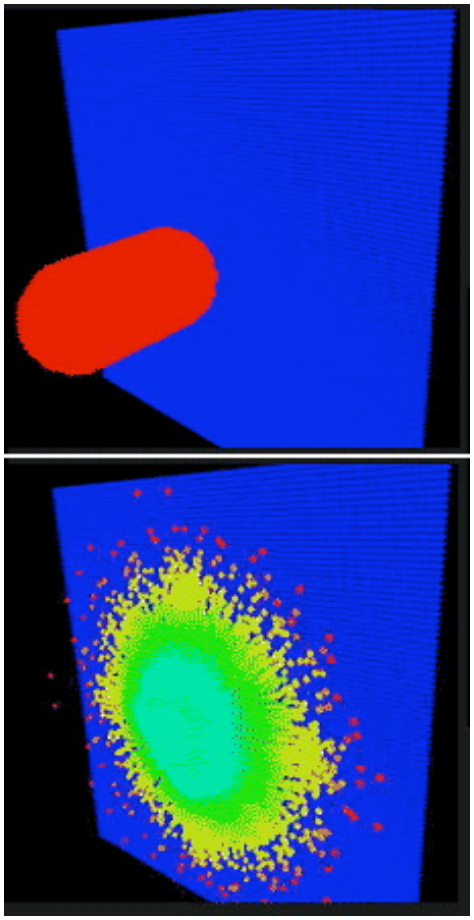
Nodal Tetrahedrons

Nodal tetrahedrons help with mesh generation

Particle Methods -- Continuous

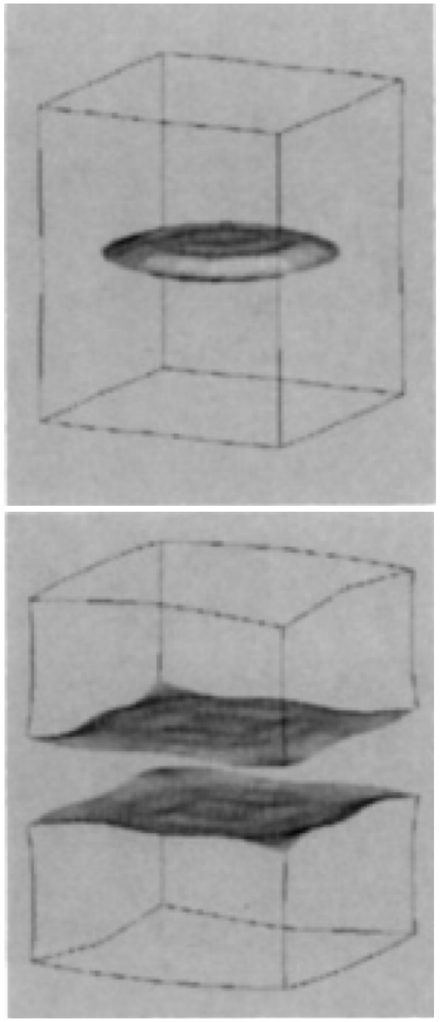


MPM



BAE Systems

SPH

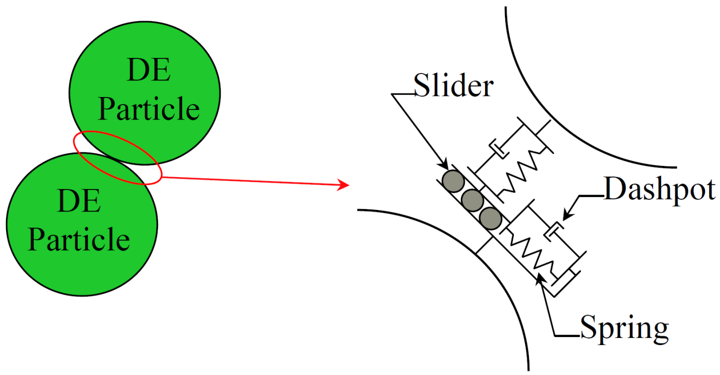


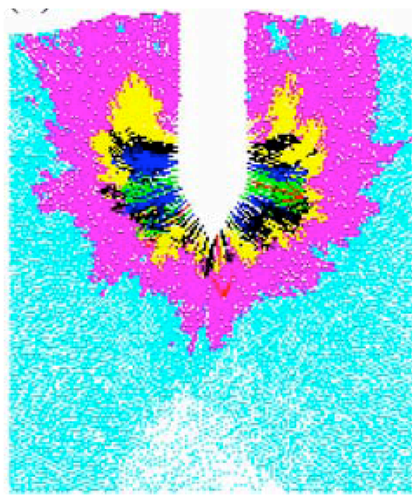
Krysl and Belytschko

EFG

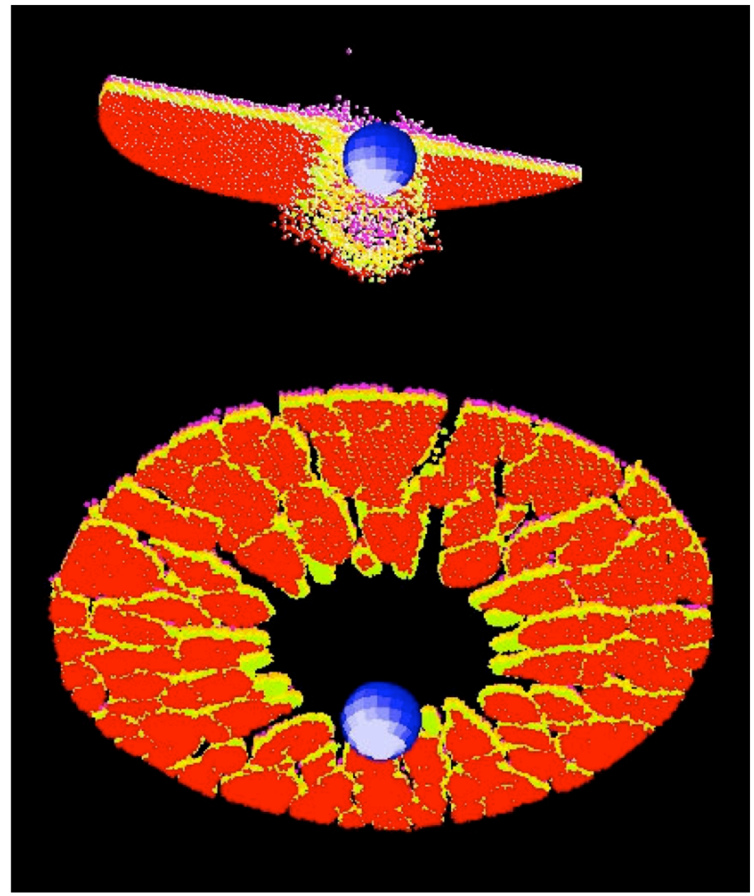
Sandia National Laboratories

Particle Methods -- Discontinuous





Bazantev et.al.



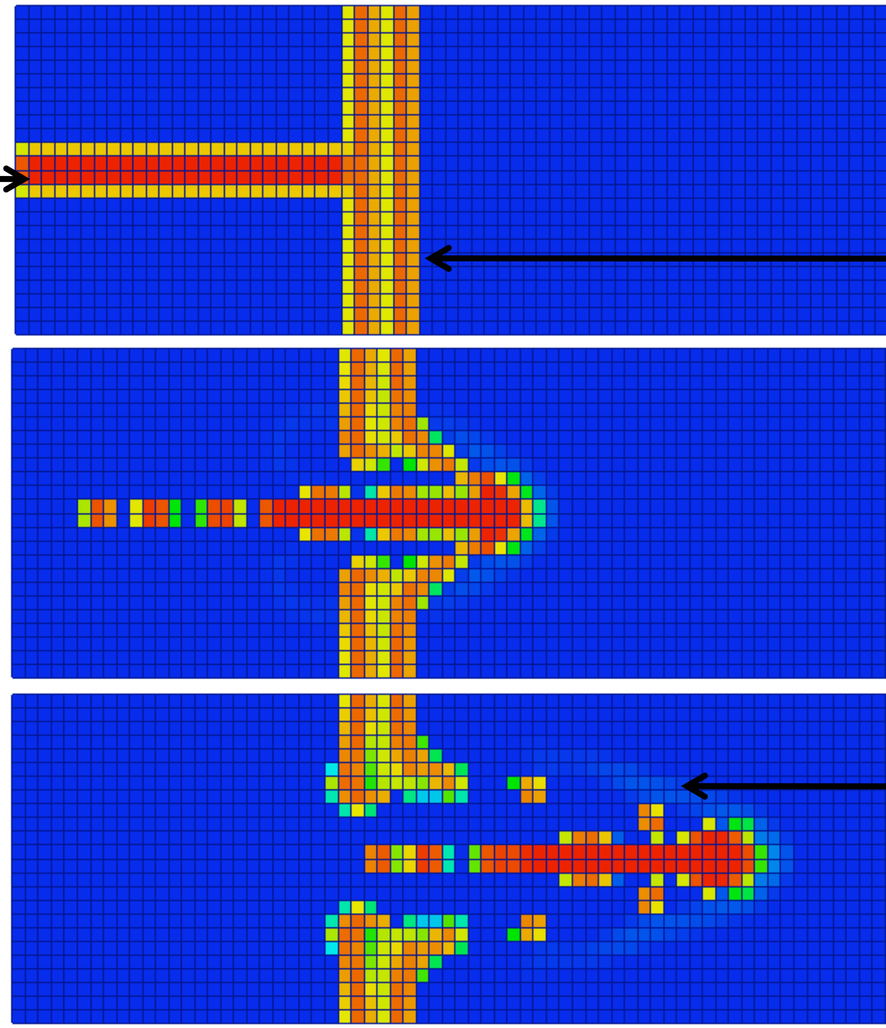
Silling et.al.

DEM

Peridynamics

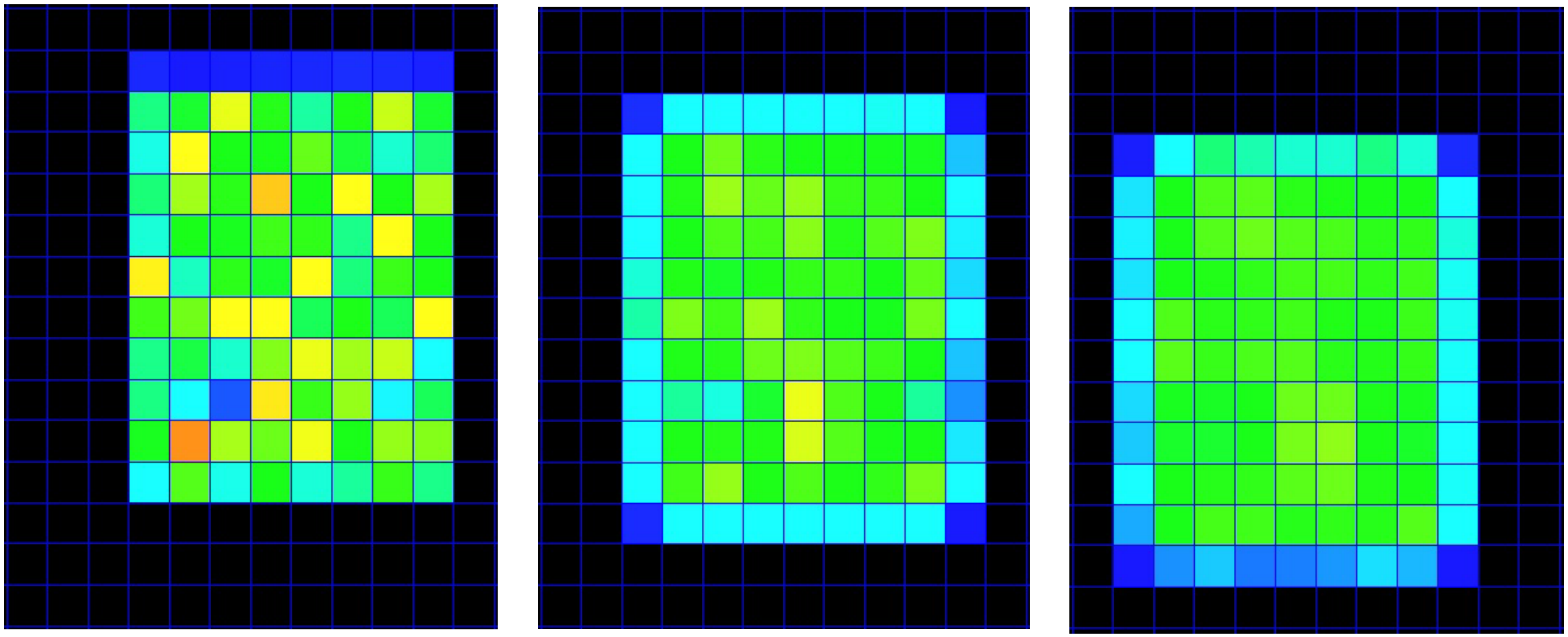
Sandia National Laboratories

Eulerian Methods



Material moves THROUGH (extremely coarse) mesh

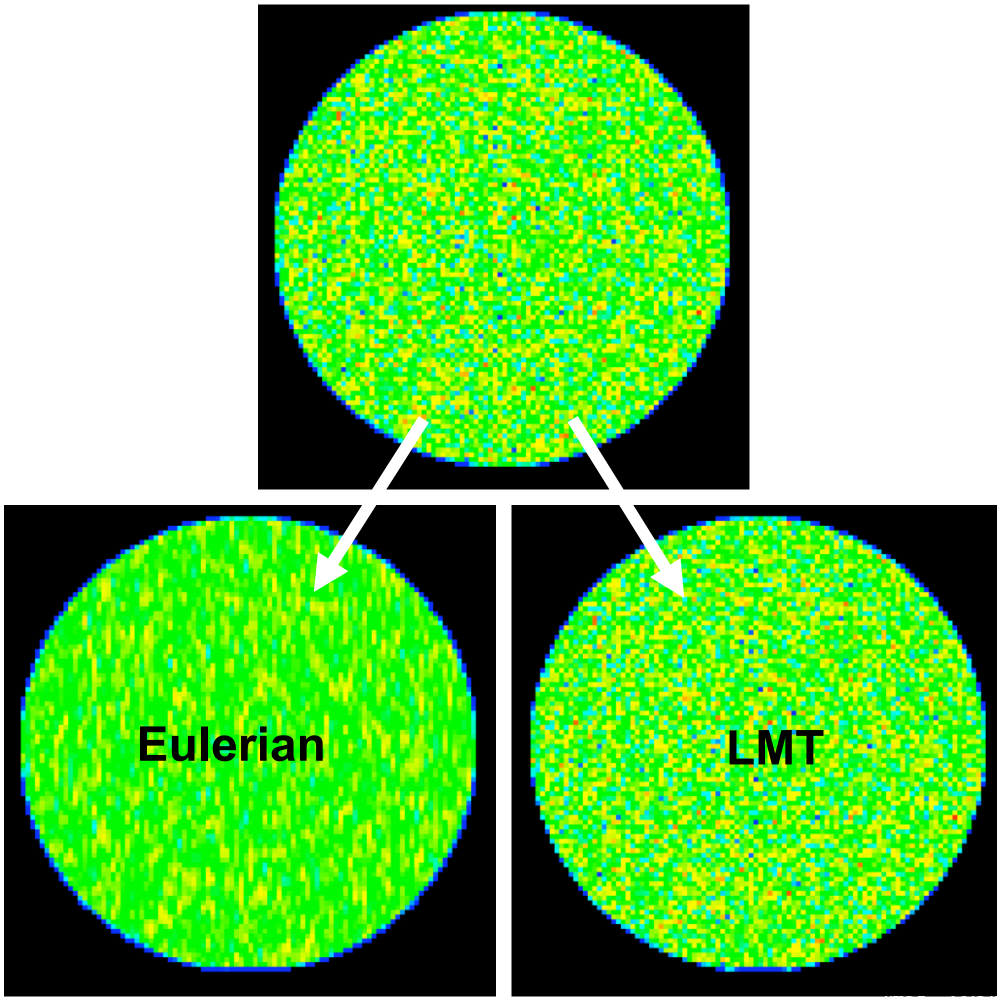
Eulerian Methods – Issue #1: Advection



Not so bad for continuous fields, bad for high-frequency or discontinuous fields (fracture)

Promising Solution : LMT

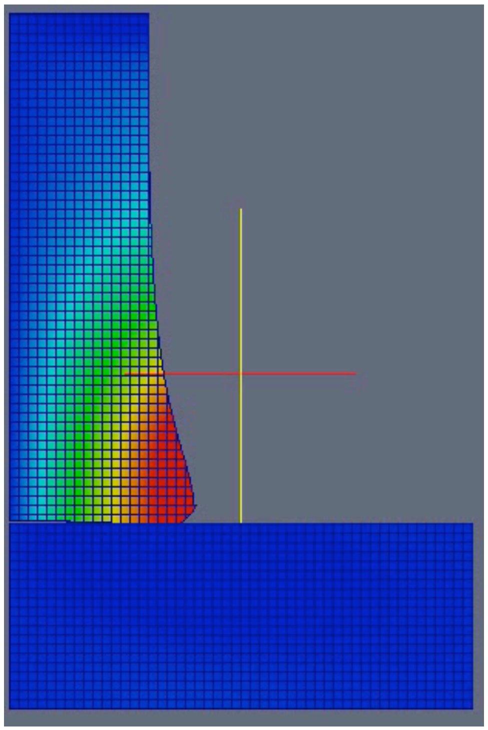
Initial State



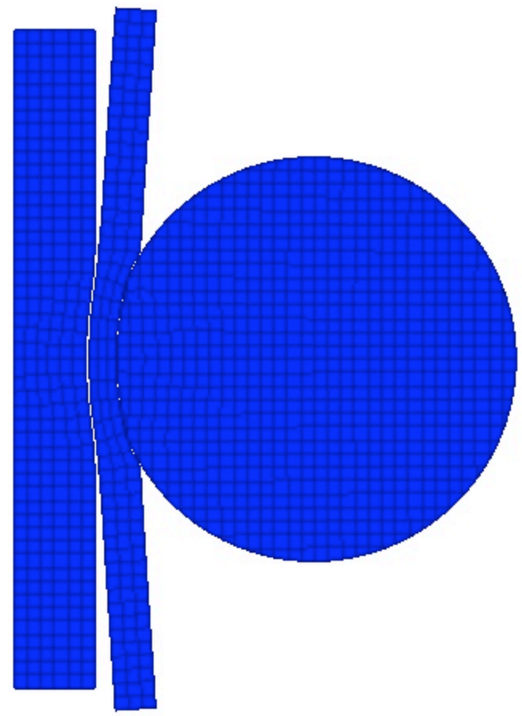
After Remap

Tracers are inserted in the mesh and moved with the material...

Eulerian Methods – Issue #2: Contact



Taylor Anvil Test

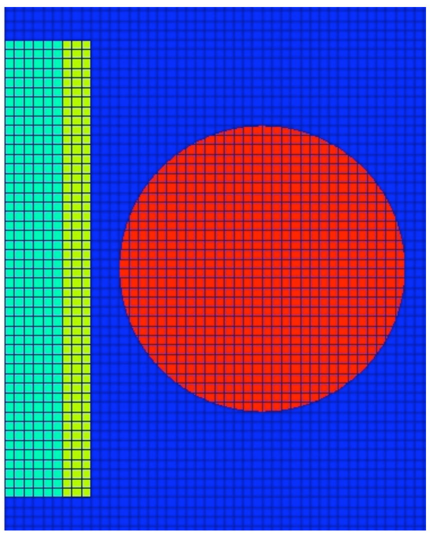


Lagrangian simulation of an impact

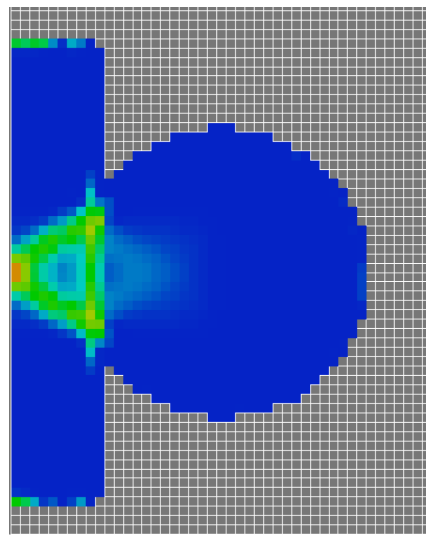
Friction can have a tremendous impact on predictions

Promising Solution: XFEM

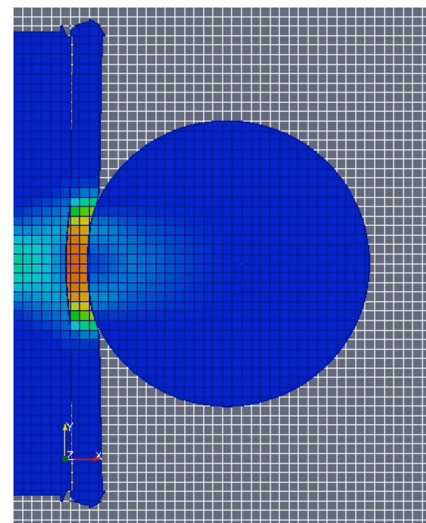
- X-FEM models intra-element contact as a true surface-phenomena
- Current state-of-the-art treatment is volumetric (no surfaces)
- X-FEM introduces (Lagrangian) surfaces within each Eulerian element
- Constitutive models for contact can be added (i.e. friction)



Initial mesh for both problems on right

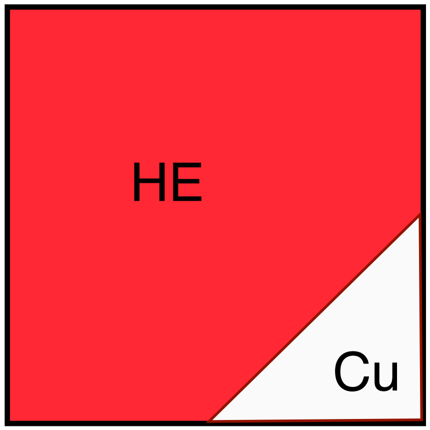


Standard Eulerian with Inter-material fracture

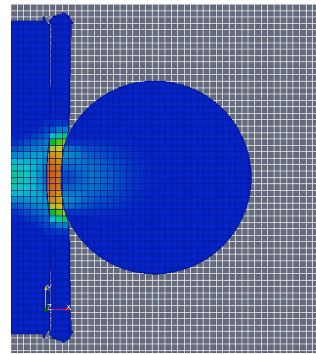


Eulerian X-FEM

Eulerian Methods – Issue #2: Mixing



HE and Cu share a common deformation rate.



XFEM (long-term)

Isentropic (short-term)

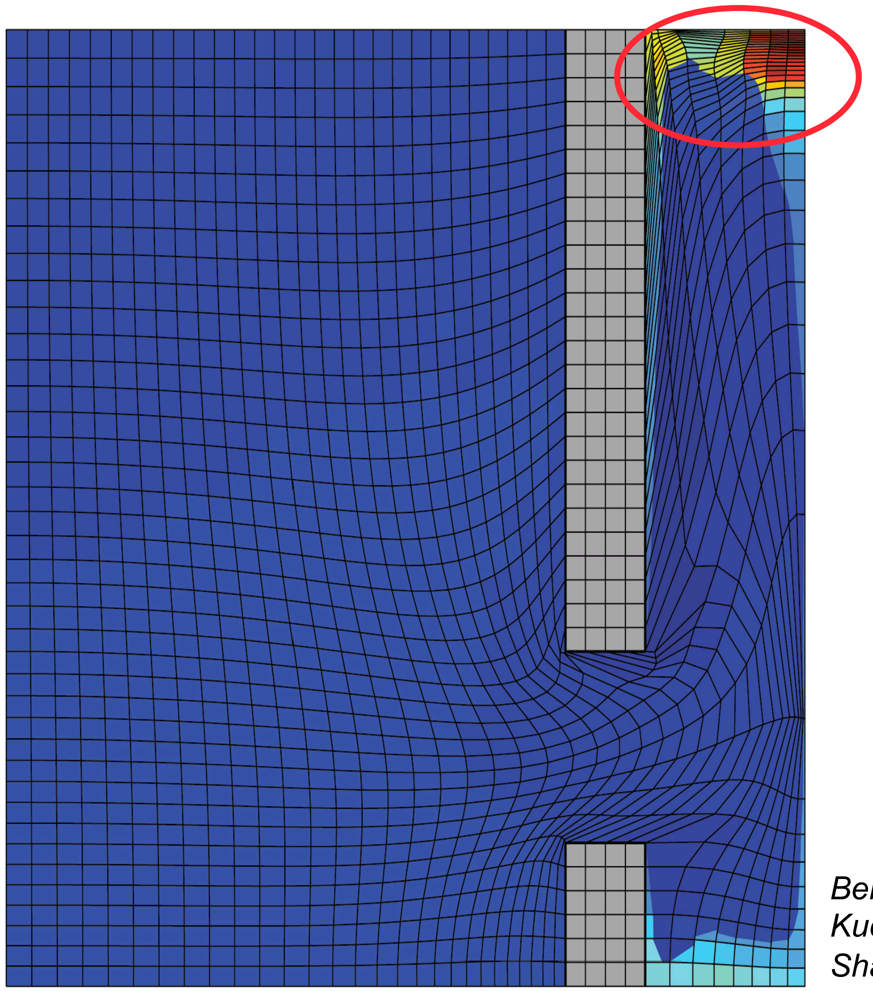
$$\frac{df_k}{dt} = f_k \left(\frac{B}{B_k} - 1 \right) \nabla \cdot u + \frac{f_k}{p} \frac{dp_k}{dt}$$

Implementations of mechanics-related mixed elements are generally ad-hoc

Single kinematic field drives bad states

Has a major impact on code robustness & accuracy

Arbitrary Lagrangian- Eulerian Methods



Issues still remain...

Berndt, Kucharik, Shashkov

Attempt to resolve contact and minimize advection effects

Drawback – complicated for users

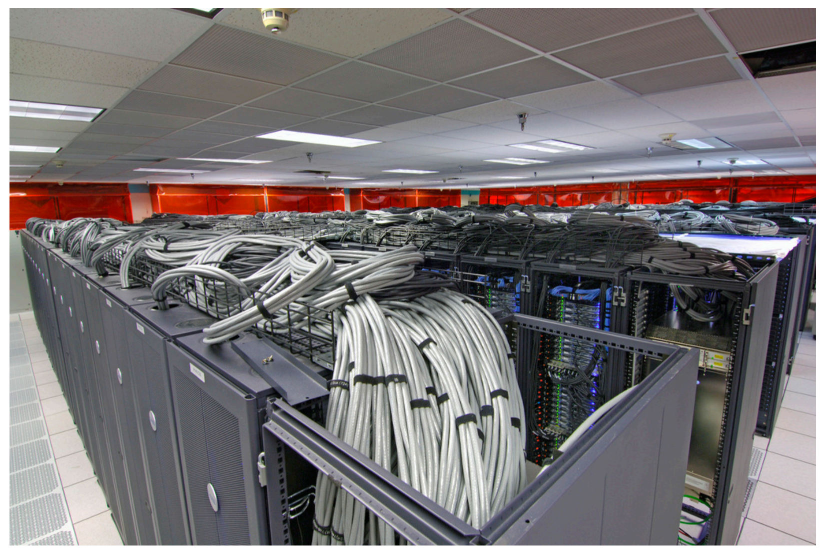
Presentation Contents

- Introduction – FEM methods
- Available computational methods
  - Lagrangian methods
  - Particle methods
  - Eulerian and ALE methods
- **Outstanding issues**
  - **High-performance computing**
  - **Shock capturing**
  - Verification and validation
  - Material modeling (EOS, complexity, fracture)
- Conclusion – the long road ahead

High Performance Computing Issues

- Keep algorithms running efficiently on next generation of processors
- Maintain massive code base

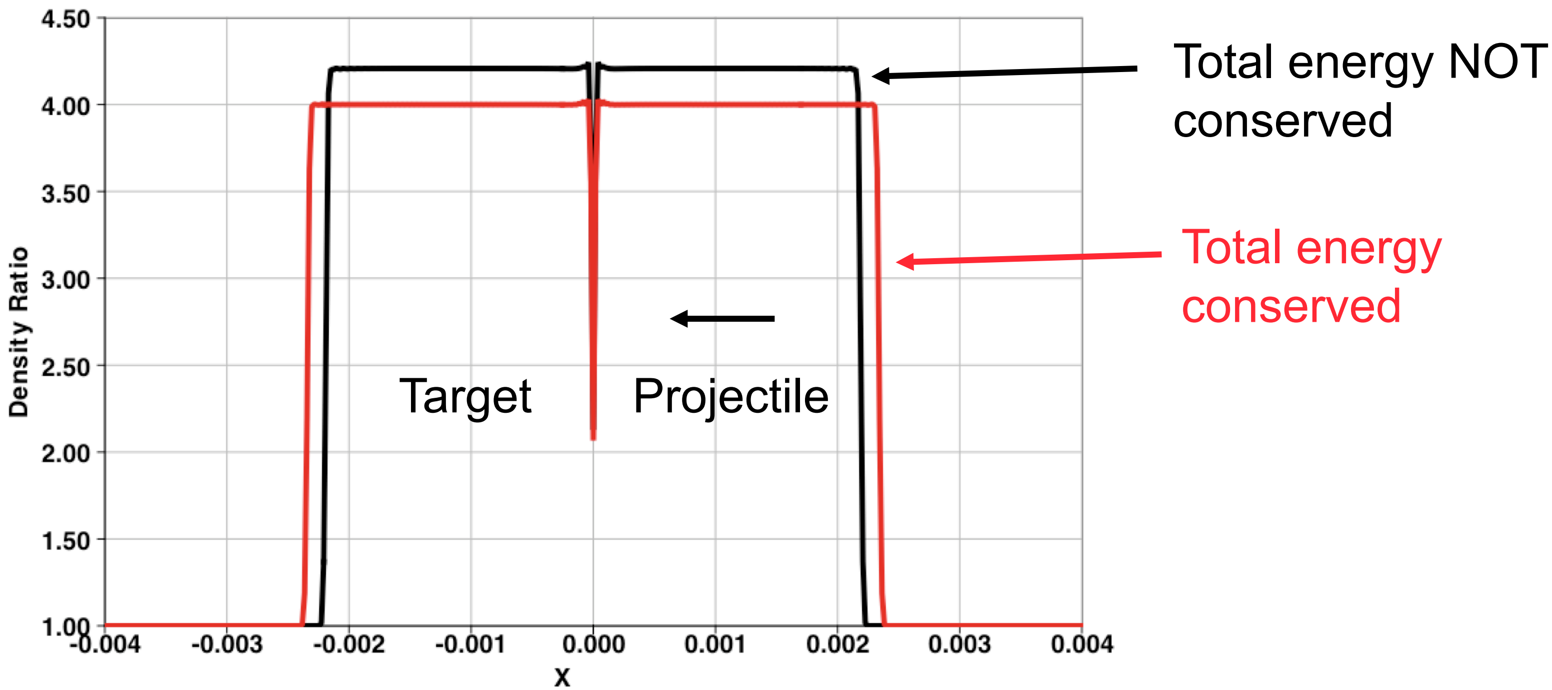
- Effectively use very large number of processors
- streamline massive communication (scalability)



Sandia National Laboratories

Algorithms – Shock Capturing

- Shock front needs to be spread over several cells
- Difficult to make algorithms robust and accurate
- Just one example of many algorithms that need work



Presentation Contents

- Introduction – FEM methods
- Available computational methods
  - Lagrangian methods
  - Particle methods
  - Eulerian and ALE methods
- **Outstanding issues**
  - High-performance computing
  - Shock capturing
  - **Verification and validation**
  - **Material modeling (EOS,** complexity, fracture**)**
- Conclusion – the long road ahead

Verification and validation are essential to the quality of simulation

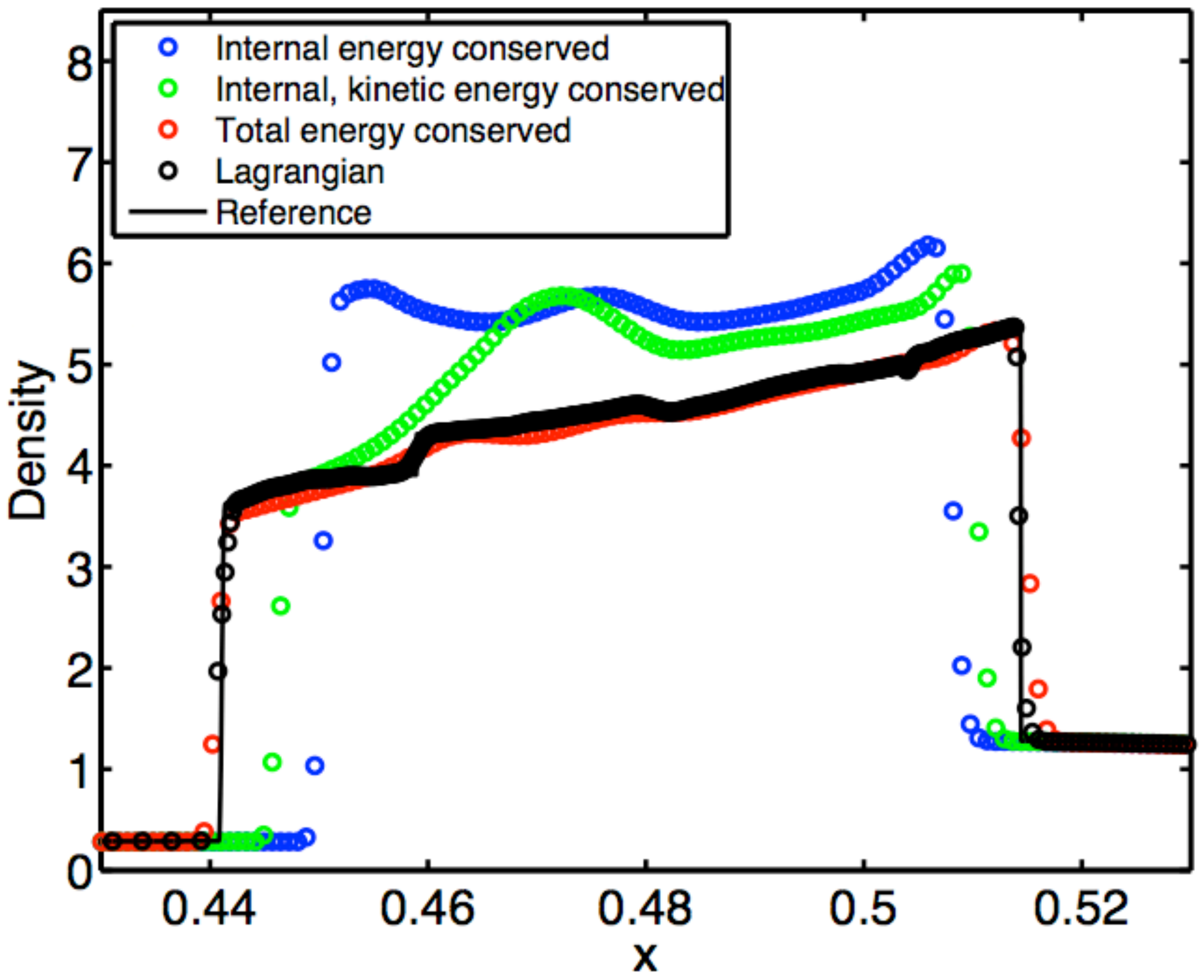
Complementary

- Verification ≈ **Solving the equations correctly**
  - **Mathematics/Computer Science issue**
  - **Applies to both codes and calculations**
- Validation ≈ **Solving the correct equations**
  - **Physics/Engineering (i.e., modeling) issue**
  - **Applies to both codes and calculations**
- Calibration ≈ **Adjusting ("tuning") parameters**
  - **Parameters chosen for a specific class of problems**
- Benchmarking ≈ **Comparing with other codes**
  - **"There is no democracy in physics."***

*L.Alvarez, in D. Greenberg, *The Politics of Pure Science*, U. Chicago Press, 1967.

Sandia National Laboratories

Verification – Impact

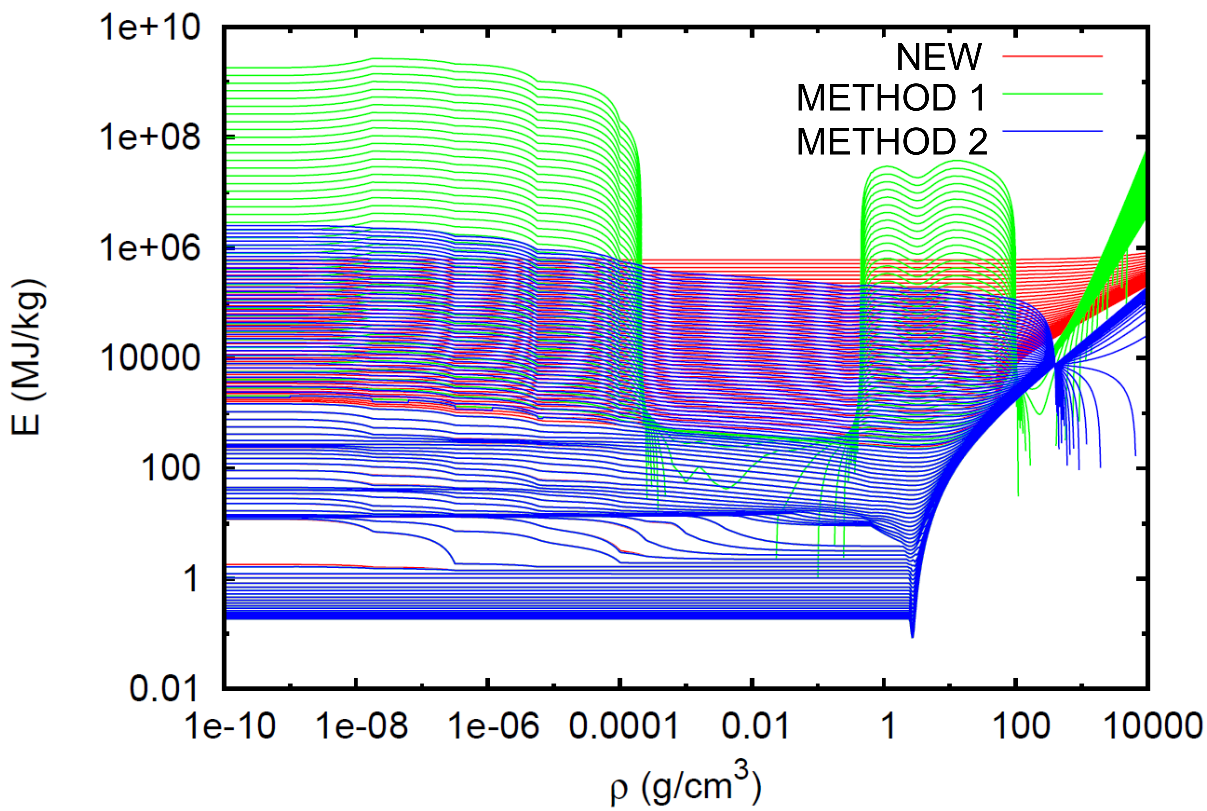


Numerical uncertainty plays an essential role in Uncertainty Quantification

1. Numerical simulations can be extremely useful.
2. Numerical errors in such simulations are unavoidable.
3. In many cases these numerical errors can dominate other forms of error.

- For the uncertainty to be quantified, the numerical uncertainty must be quantified...

Materials – Equations of State (EOS) Issues



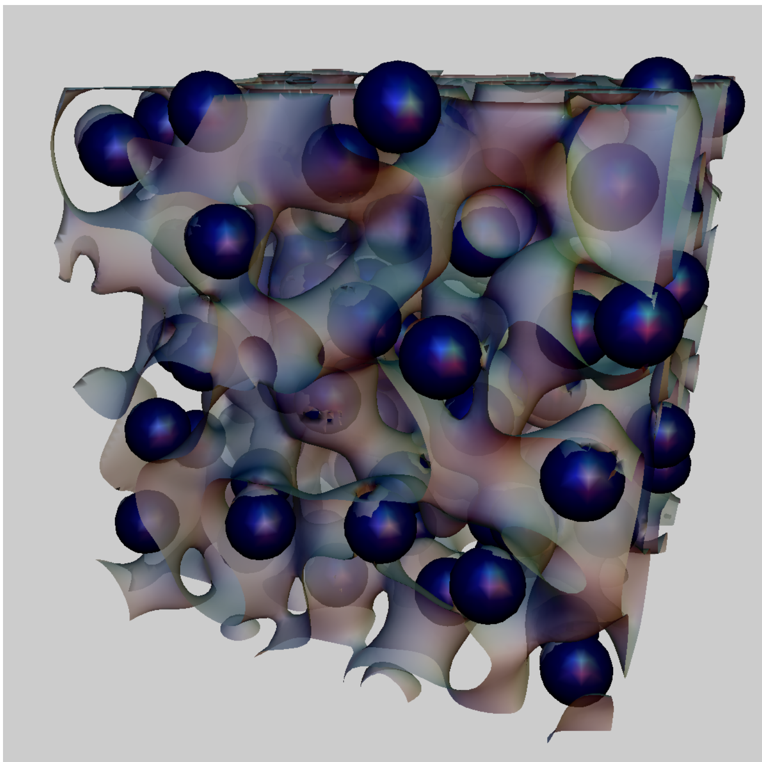
Very coarse tabulation

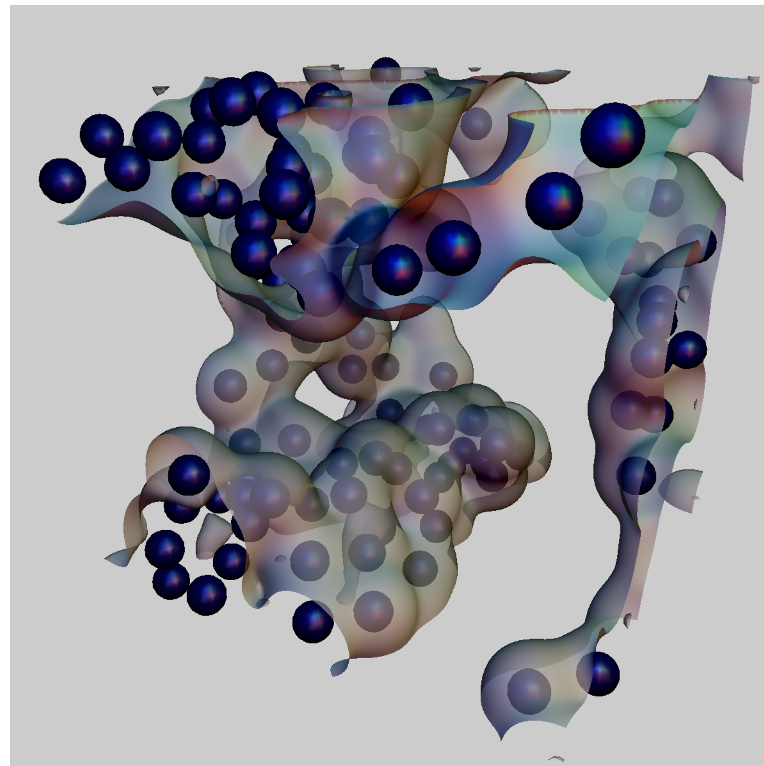
Existing models were designed for high pressures

Large number of EOS's needed

EOS Solutions

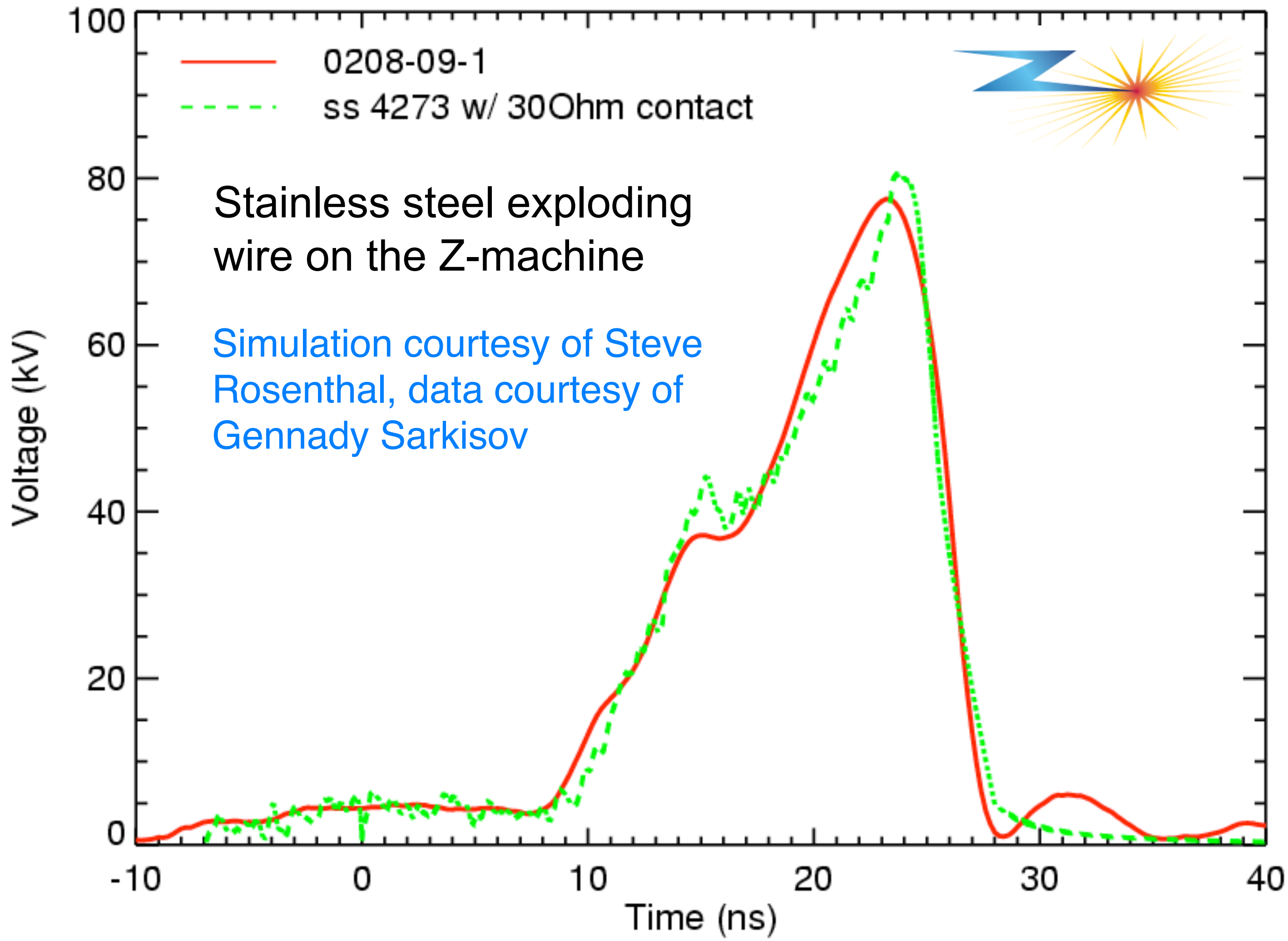
Density Functional Theory with Quantum Molecular Dynamics





Desjarlais et. al.

QMD Models Show Very Good Agreement



Sandia National Laboratories

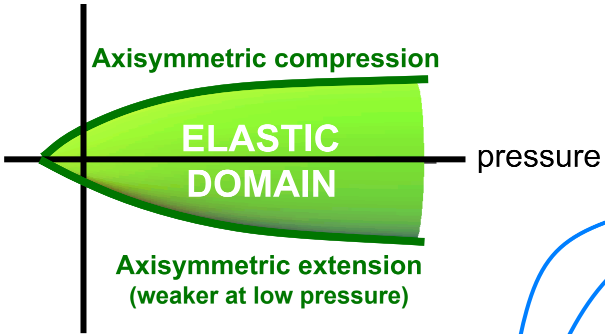
Presentation Contents

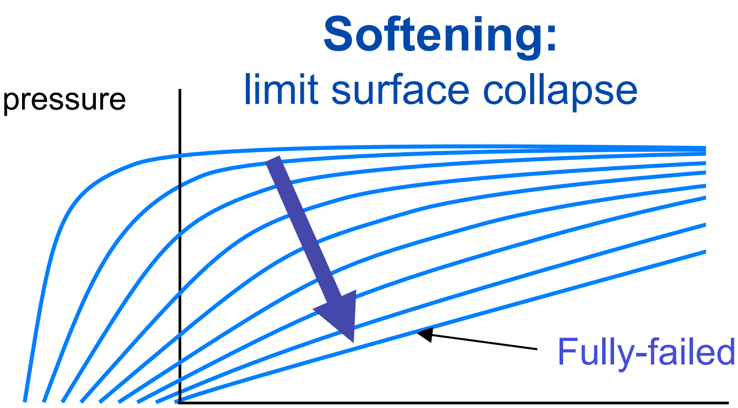
- Introduction – FEM methods
- Available computational methods
  - Lagrangian methods
  - Particle methods
  - Eulerian and ALE methods
- Outstanding issues
  - High-performance computing
  - Shock capturing
  - Verification and validation
  - **Material modeling (EOS, complexity, fracture)**
- Conclusion – the long road ahead

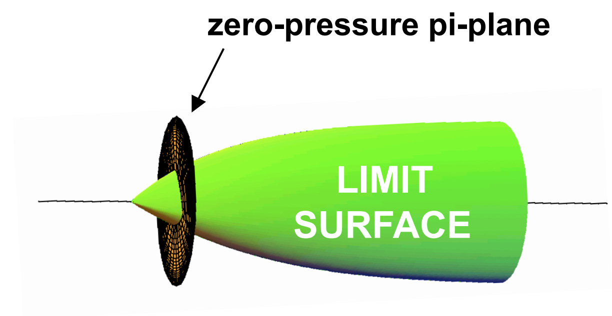
Complicated Material Models

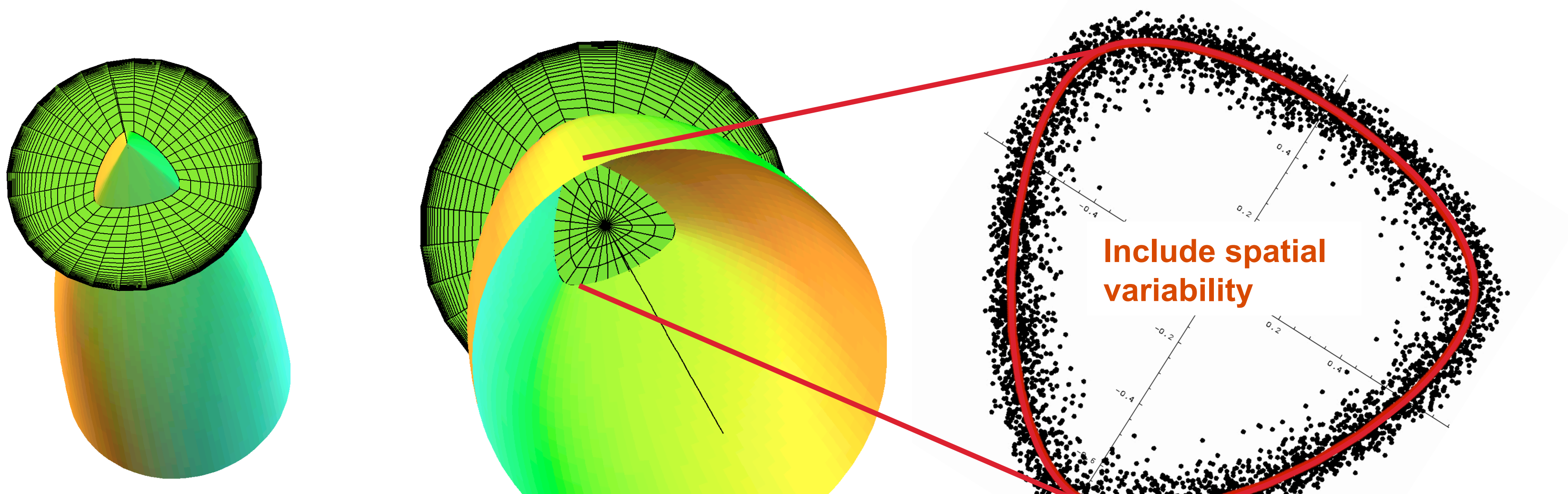
- Complicated models require complicated calibration procedures
- How do we incorporate material variability?
- What is the response outside of testing data?
- Can accurate meso-scale models be used to calibrate, and perhaps develop, continuum-scale models?

Brittle Constitutive Model



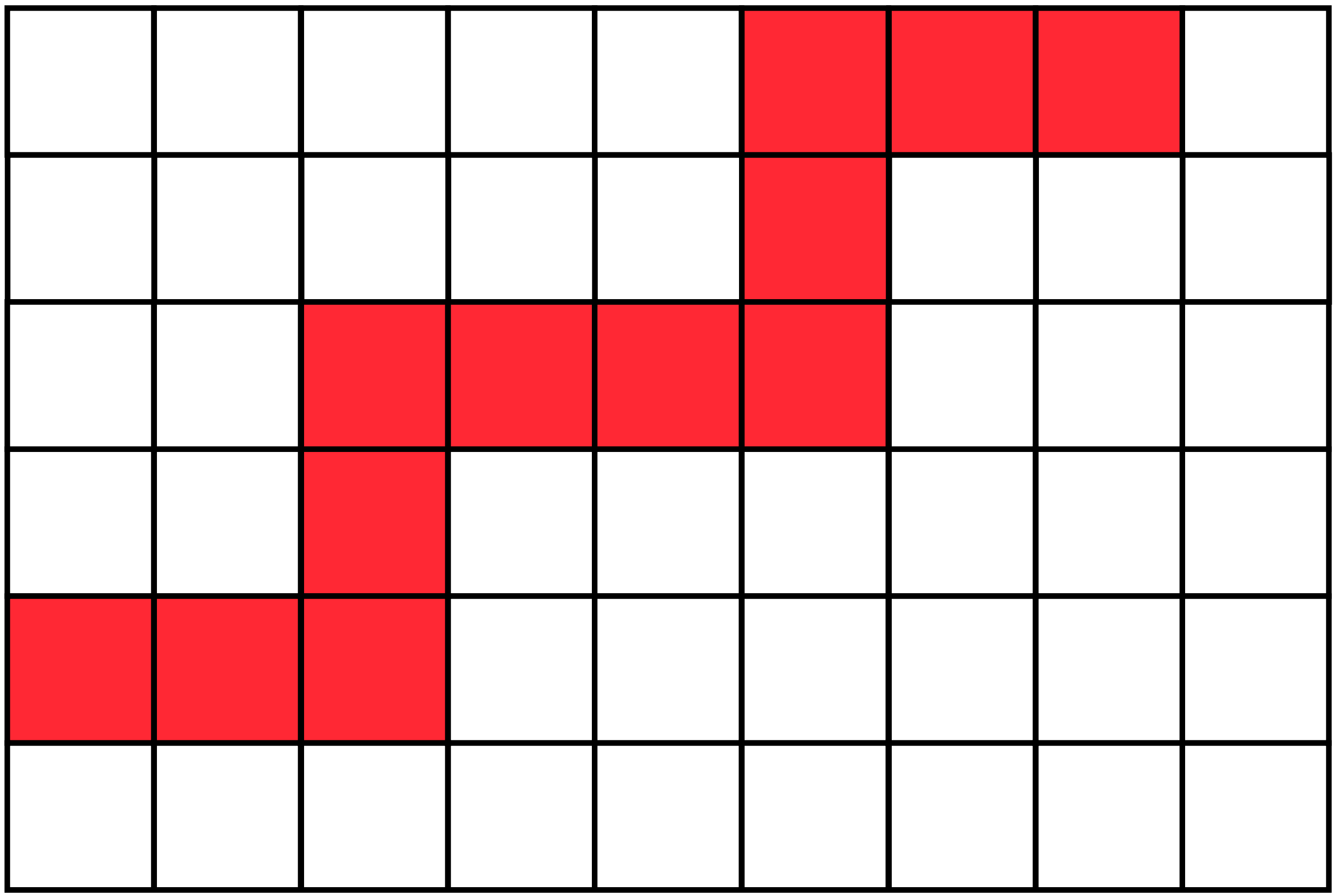






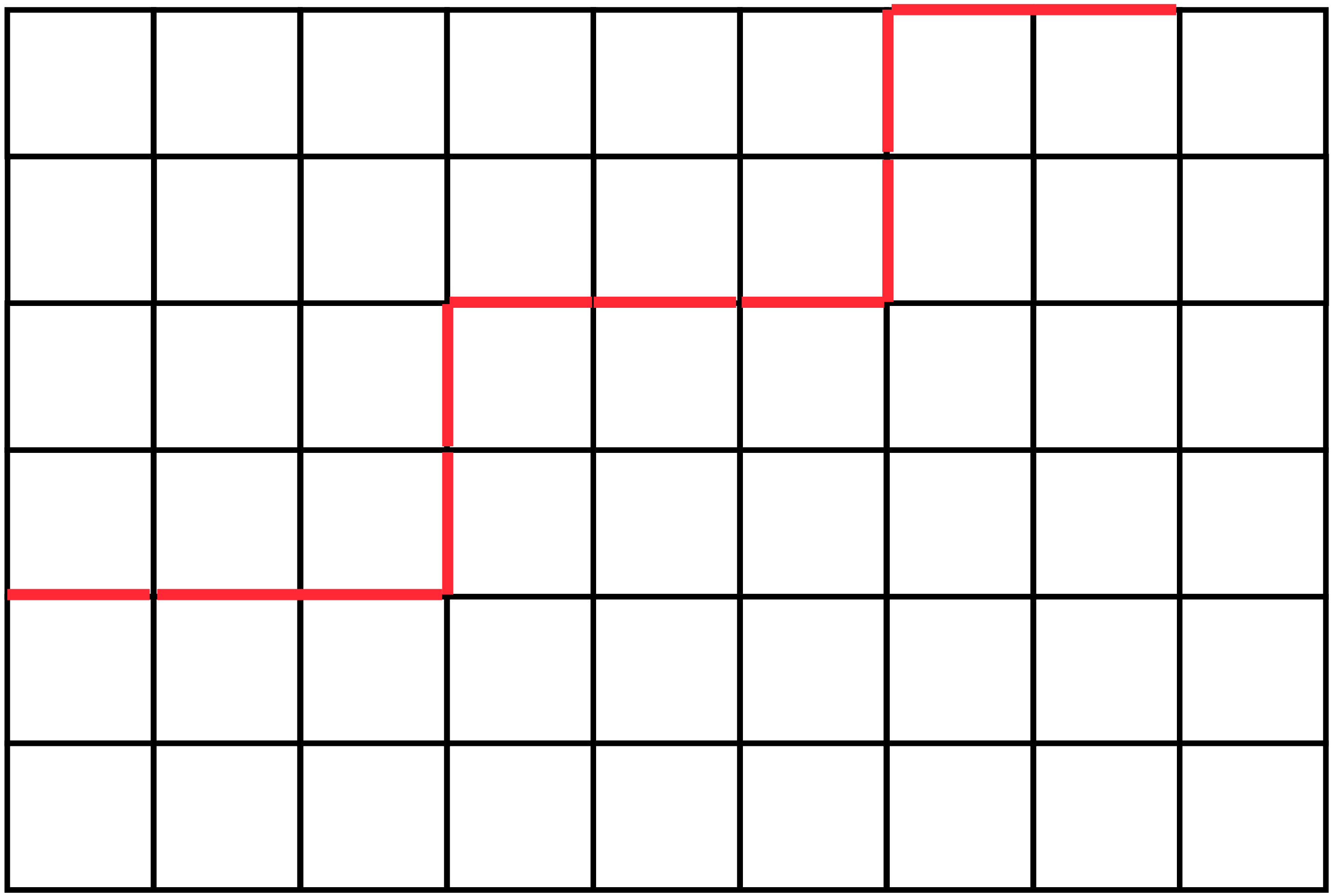
The model is essentially a *smooth* transition from a maximum principal stress (brittle) failure criterion at low pressure to non-softening plasticity at extremely high confinement.

Material Fracture – Issues



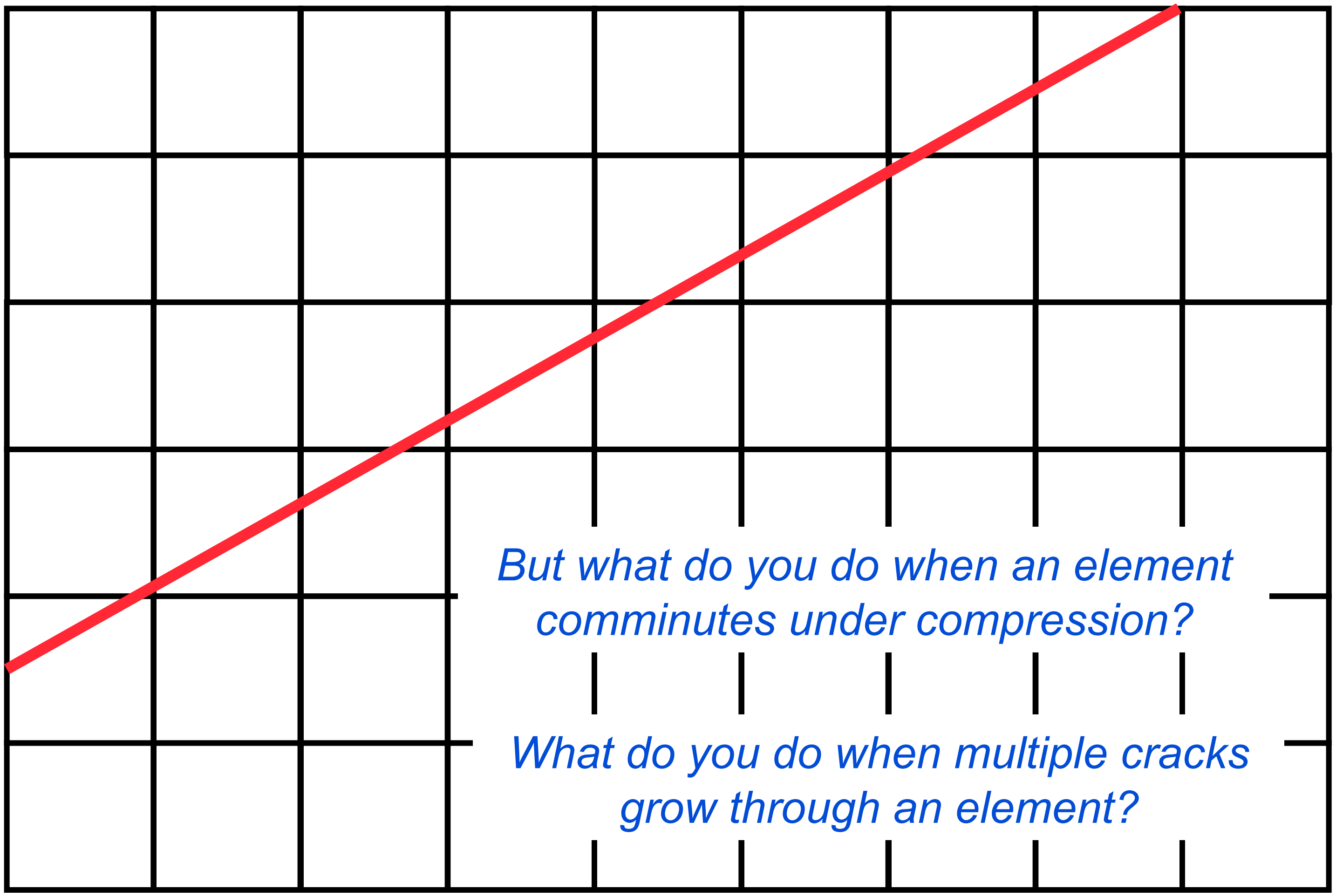
“Crack” pattern for a damage model must follow mesh

Material Fracture – Issues



Inserting “cracks” between elements isn’t much better

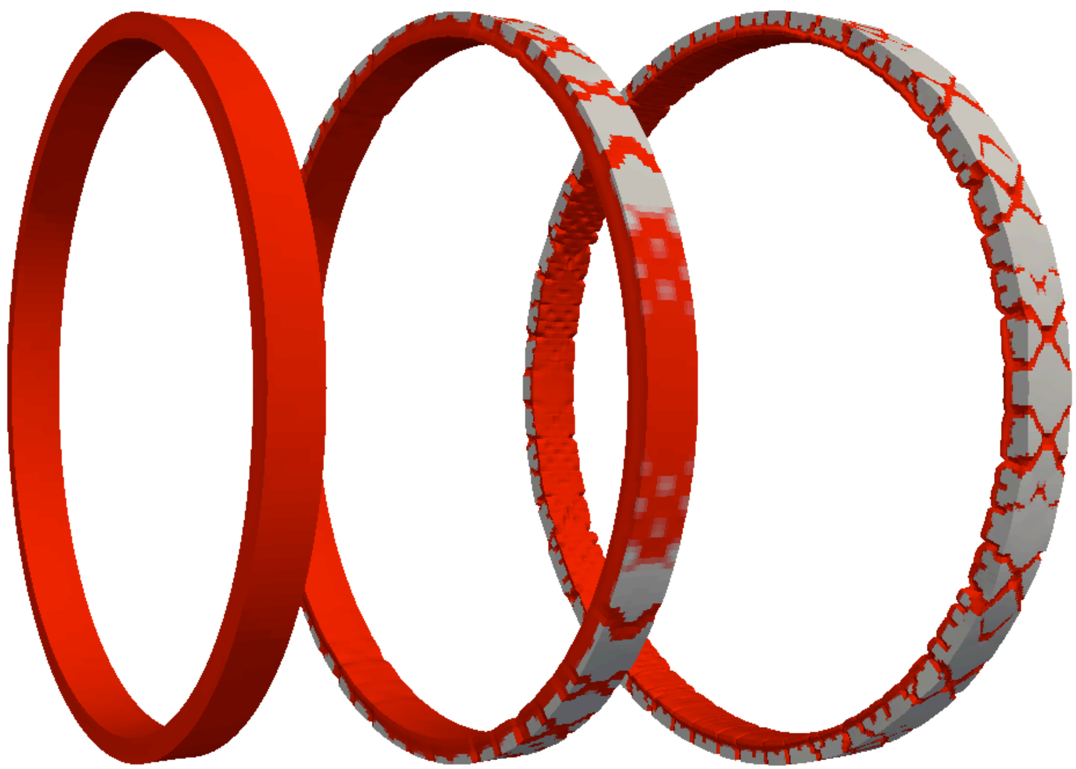
Material Fracture – Issues



Inserting cracks THROUGH elements is substantially better (XFEM)

Illustration – Severe Mesh Sensitivity using Homogeneous Properties

Mesh resolution study – refinement to the right



Johnson-Cook fracture model with homogeneous properties

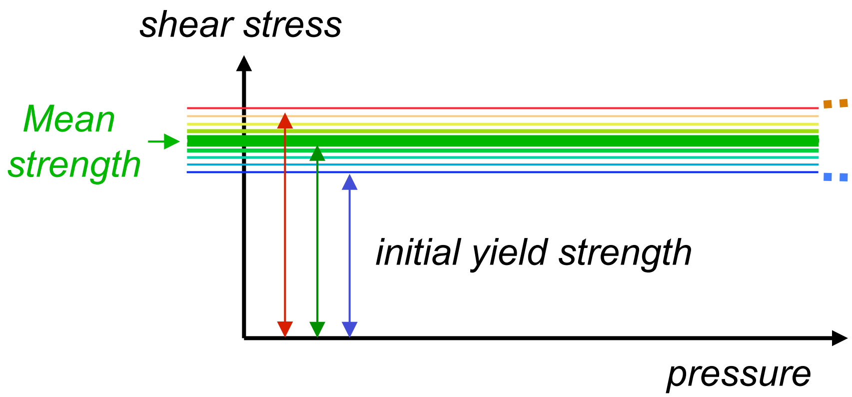
Goals and Constraints

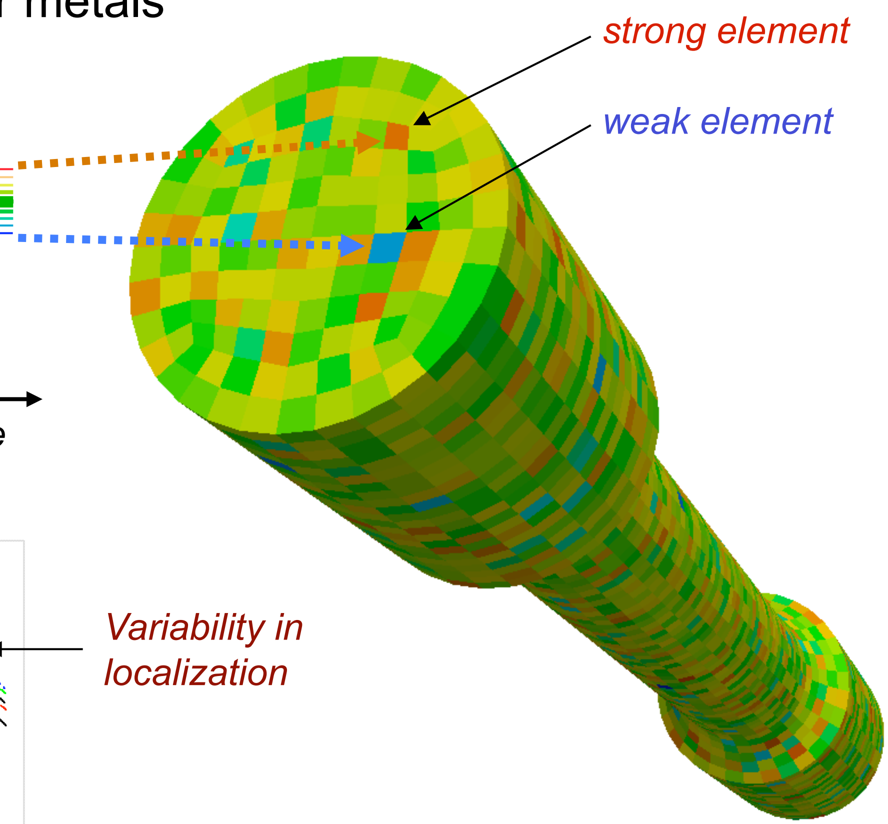
- **Capture the statistical variability of fragments measured in experiments**
- **Do this in a finite element framework in which *multiple full-size* components can be simulated**
  - **Will not attempt to model every single crack**
  - **Use a continuum (conventional) damage model as foundation**
- **Leverage decades of work on constitutive metal models**
- **Inspired by Rebecca Brannon (Utah/SNL), Rich Becker (LLNL), and Dennis Grady, Marlin Kipp, and Mel Baer (SNL)**

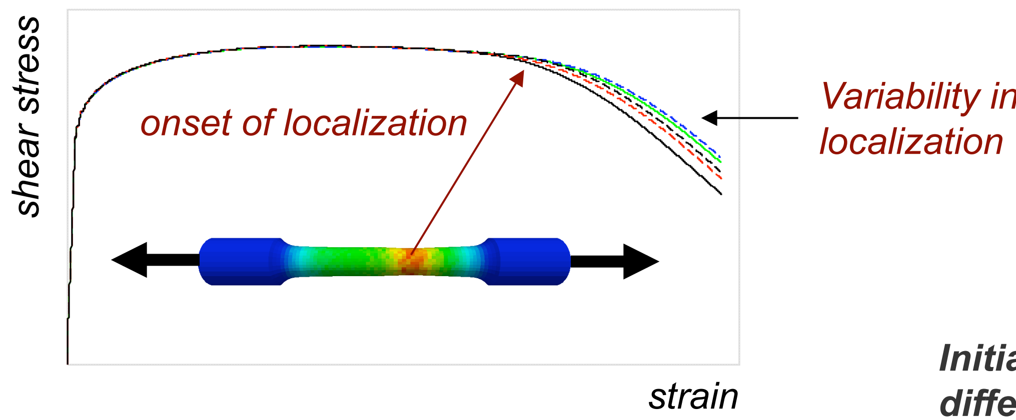
Spatially Variable Metal Model

Address Uncertainty at Finite Element Level

Spatially variable yield strength for metals







Onset of yield does not show variability – but onset of failure does

Initial state: each finite element has a different strength

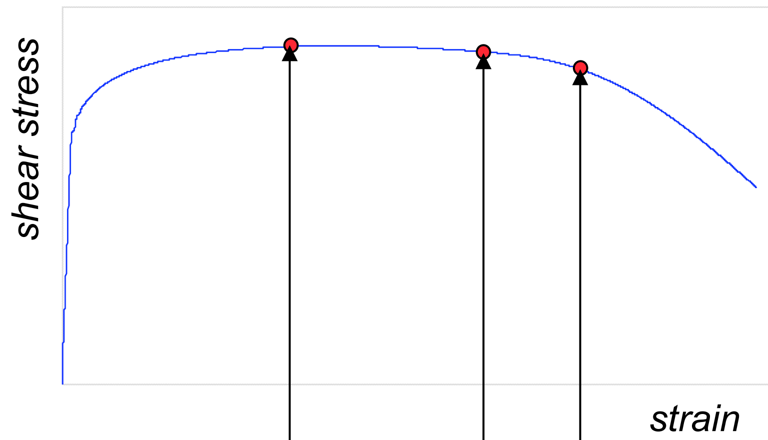
Inspiration: Meyer, Brannon, Becker, Grady, Kipp, Baer

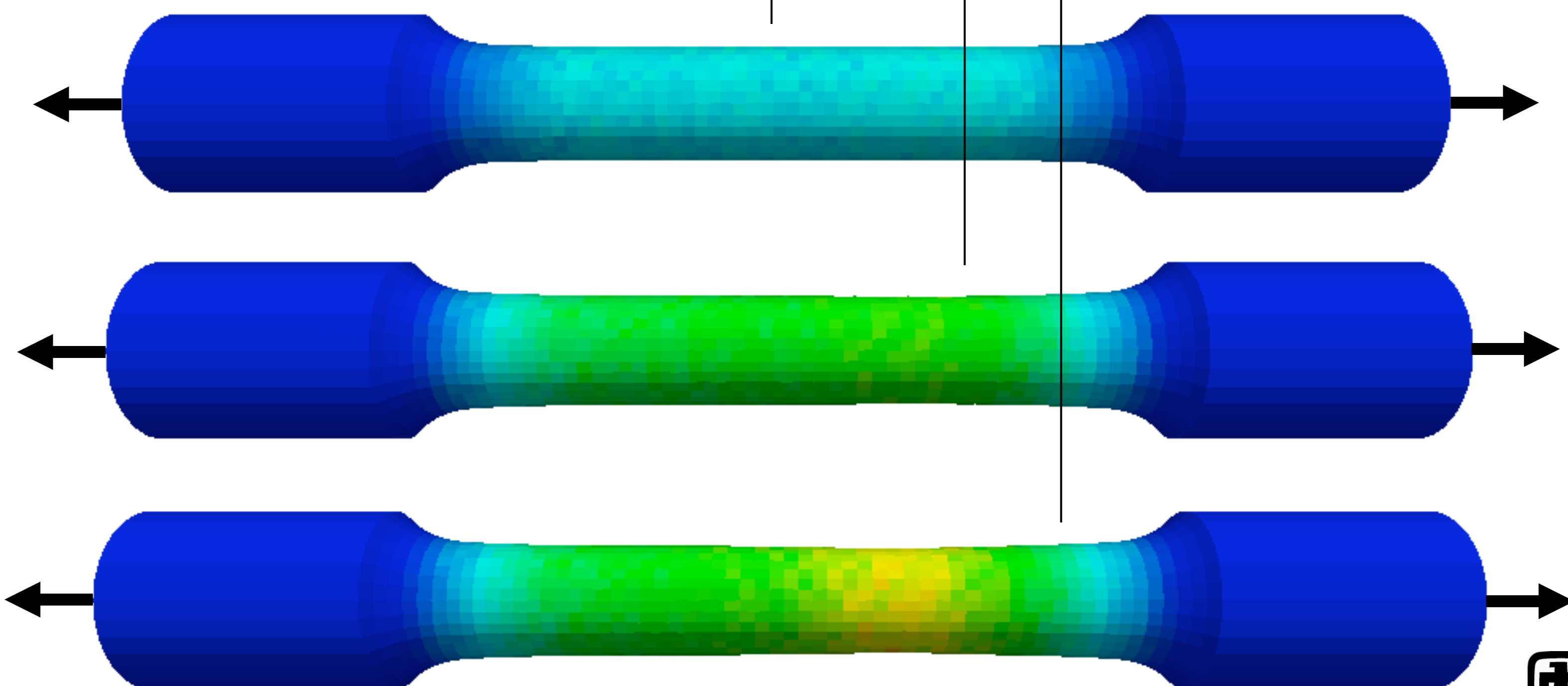
Sandia National Laboratories

Weaker Elements Redistribute Load with Stronger Elements – *Until Localization*

ASTM tension test results with spatial variability

Variability only plays a major role in localization

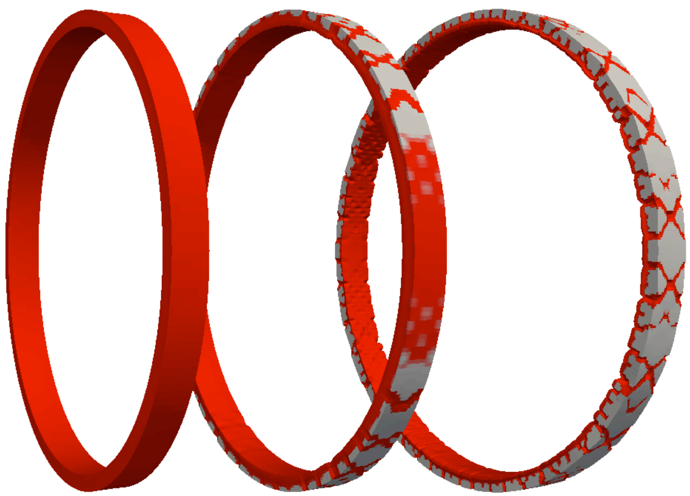




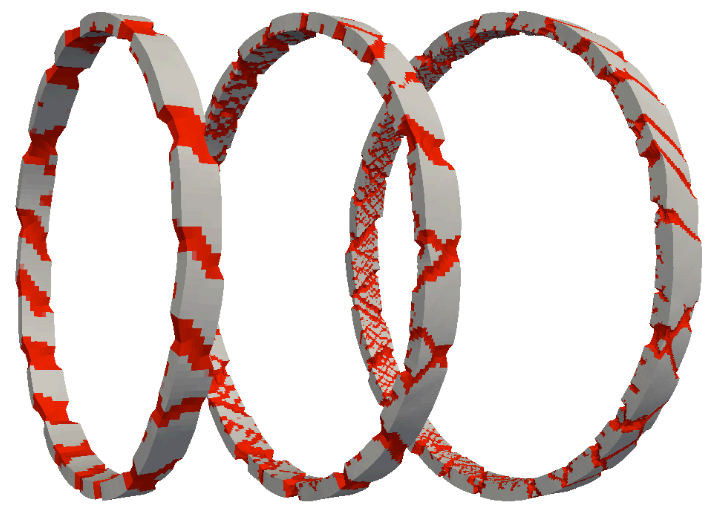
Sandia National Laboratories

Reduced Mesh Sensitivity using Spatially Variable Properties

Mesh resolution study – refinement to the right →



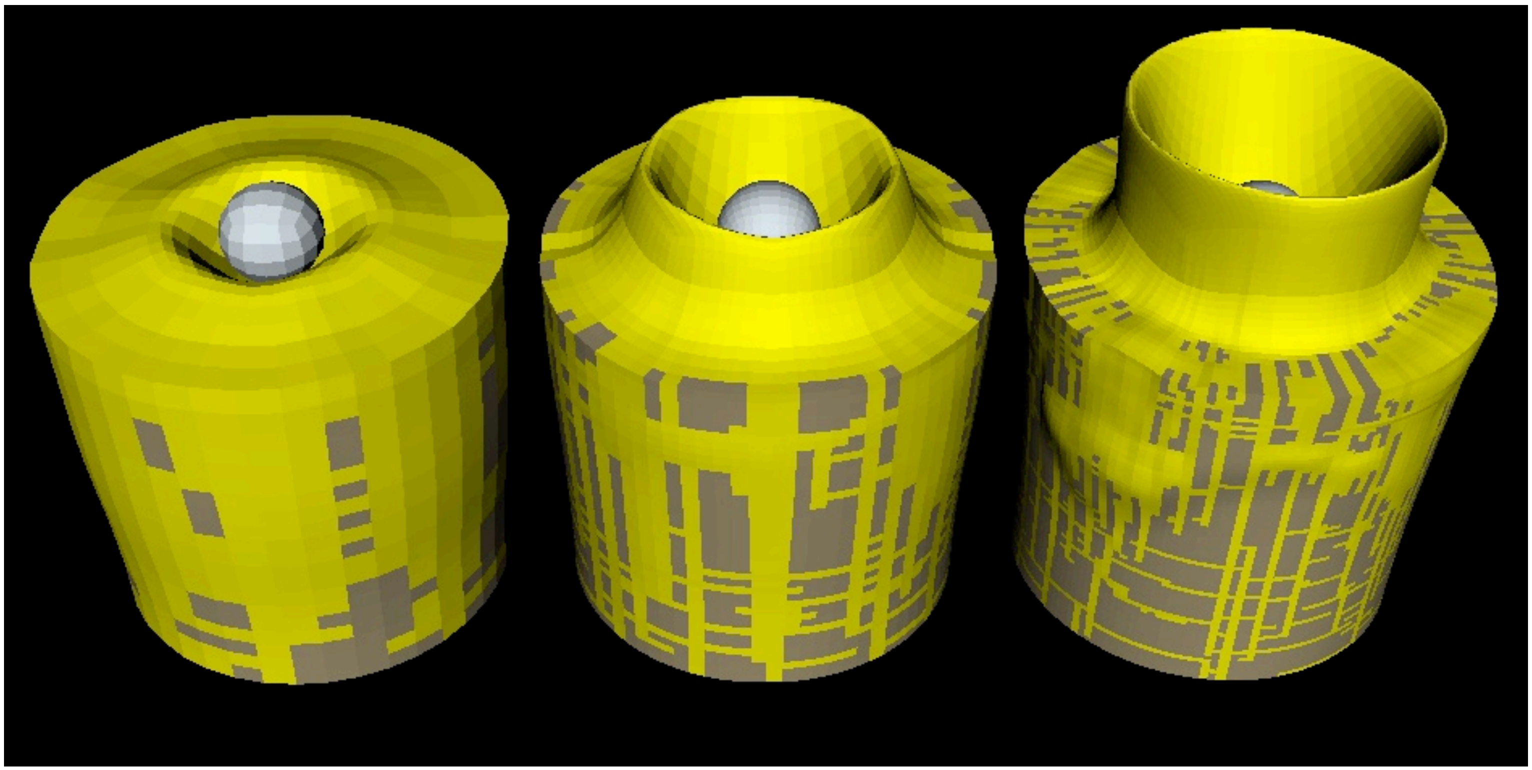
Homogeneous properties



spatially variable properties

Mesh Dependence for Ceramics

Mesh resolution study – refinement to the right →



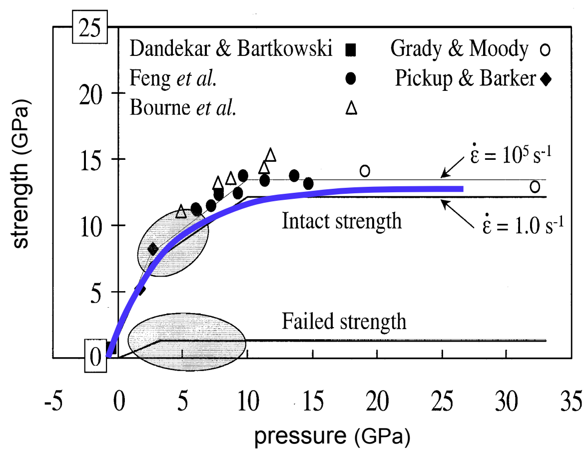
Conventional Damage Model without Spatial Variability

Brannon, Strack

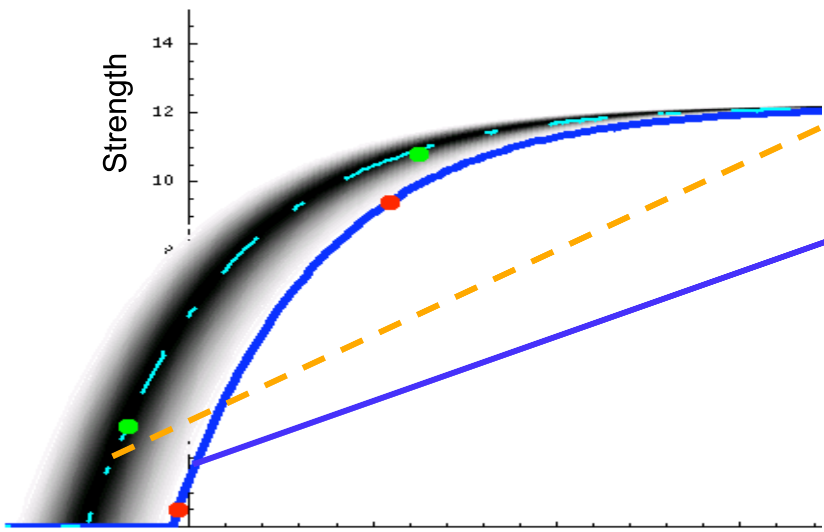
Spatially Variable Ceramic Model
Address Uncertainty at Finite Element Level

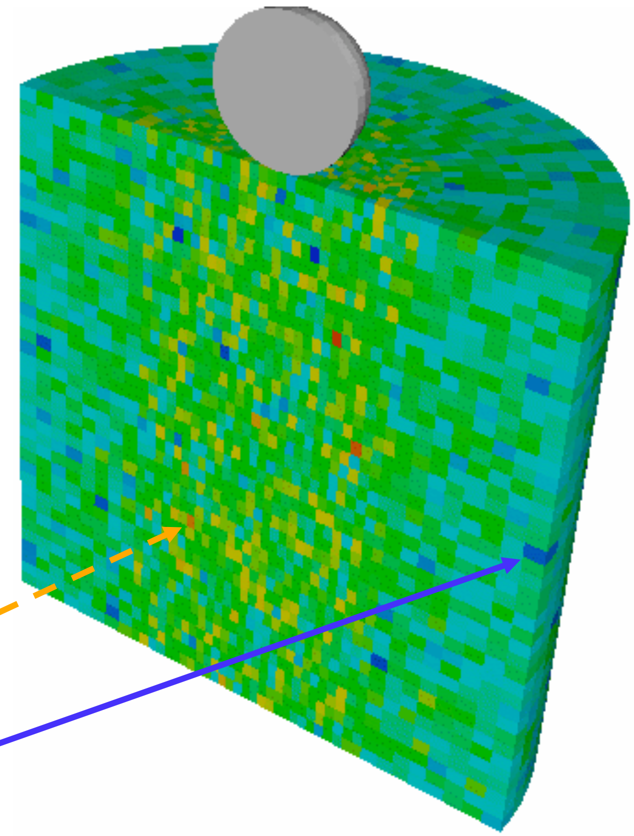
Conventional Strength Profile for Ceramics

(figure from Johnson & Holmquist)



Variable Strength Profile for Ceramics

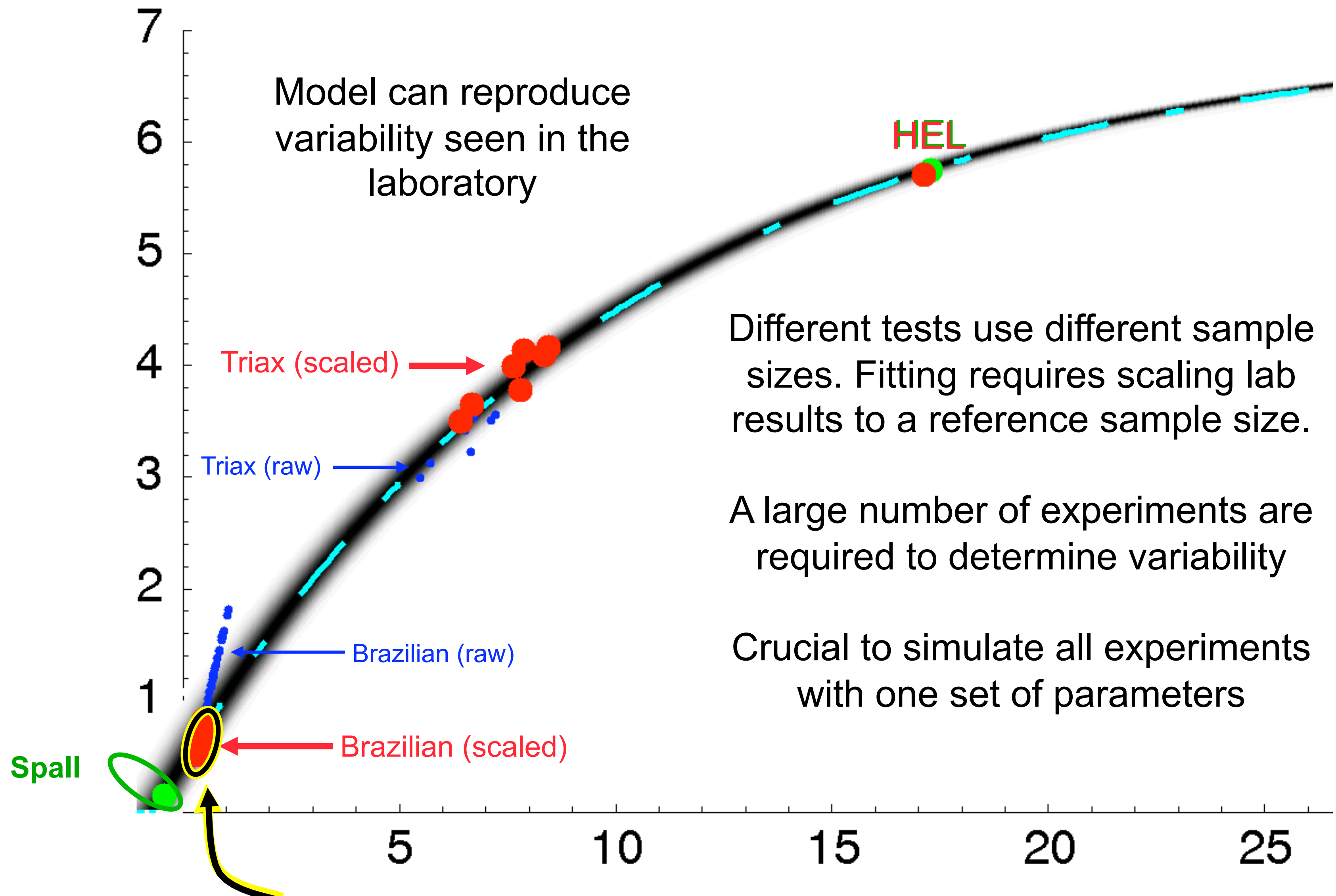




Initial state: small elements are stronger on average, but also more variable, as observed experimentally.

Inspiration: Meyer, Brannon, Becker, Grady, Kipp, Baer

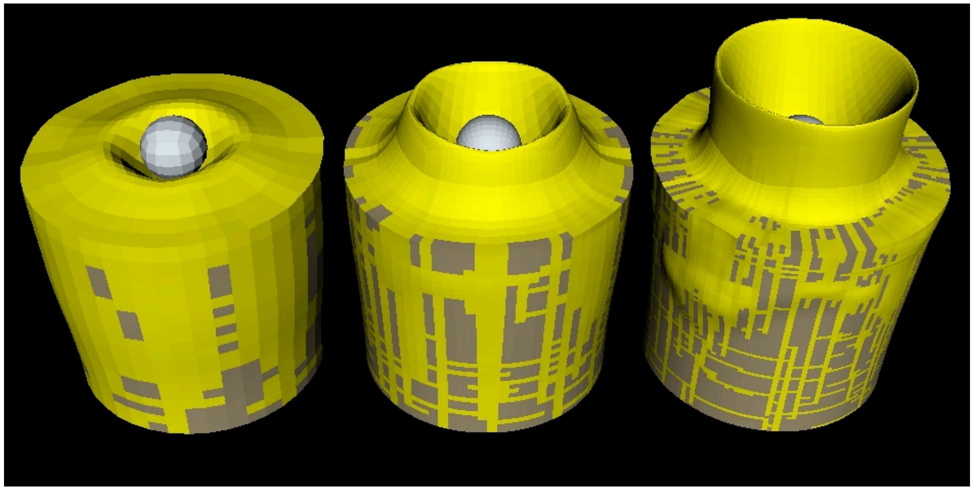
Comparison to Multiple Experiments



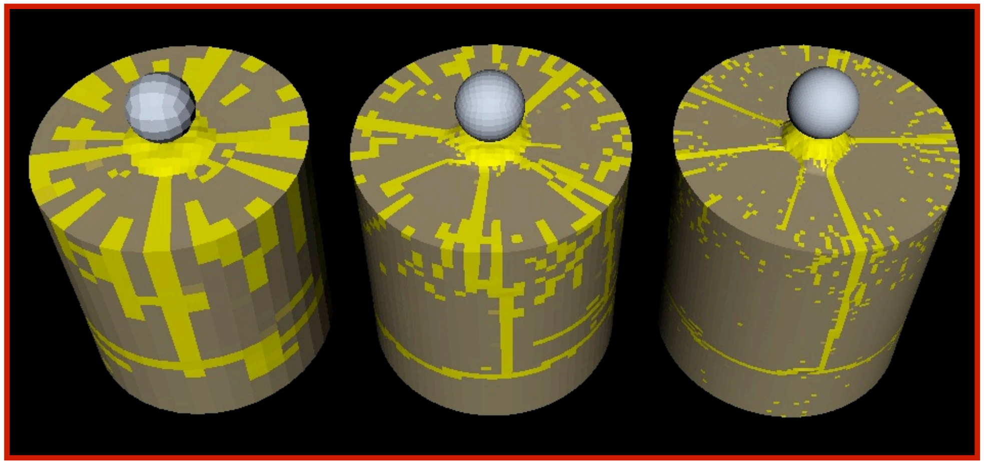
Reproduces the observed *distribution* of strength. Deterministic models use only a single point.

The Impact of Spatial Variability: With and Without Variability

Mesh resolution study – refinement to the right →

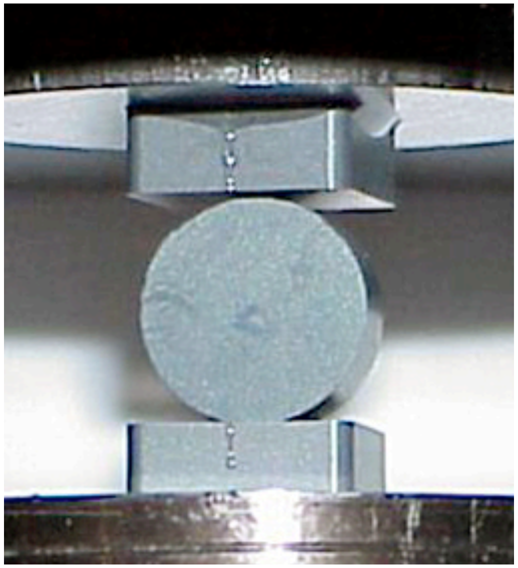


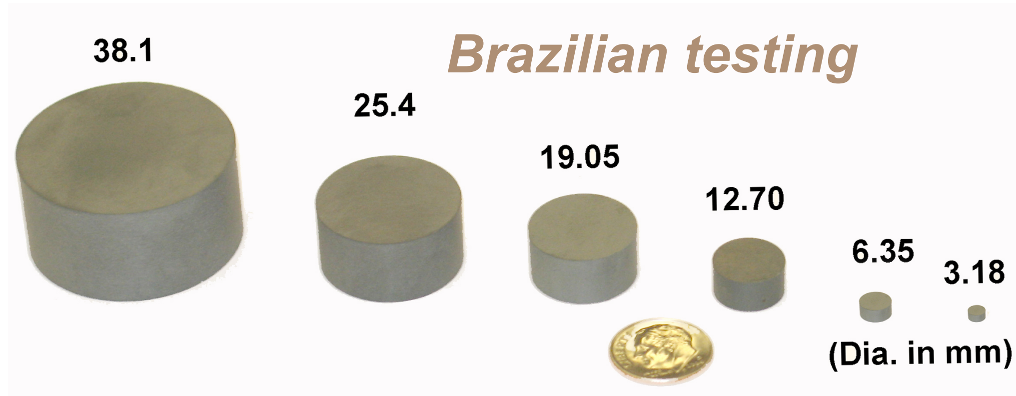
Conventional Damage Model without Spatial Variability

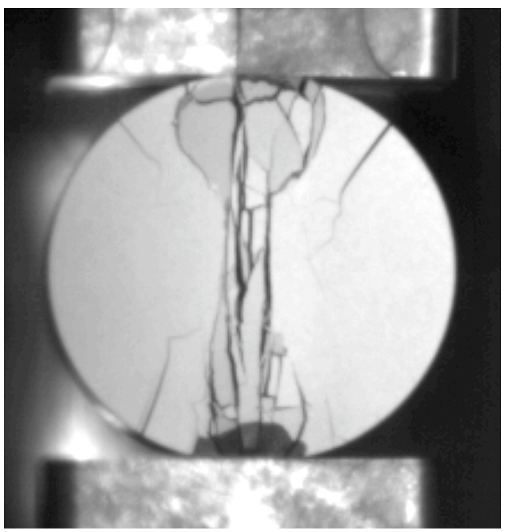


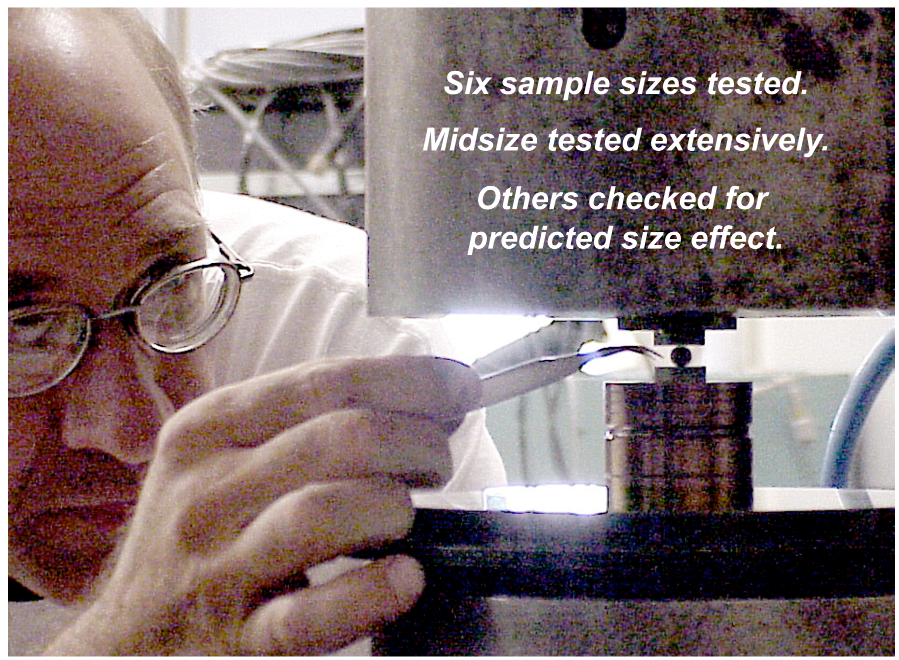
Reduced Mesh Dependence:
Same Model with Uncertainty, Size, and Rate Effects

Validation of the Size Effect

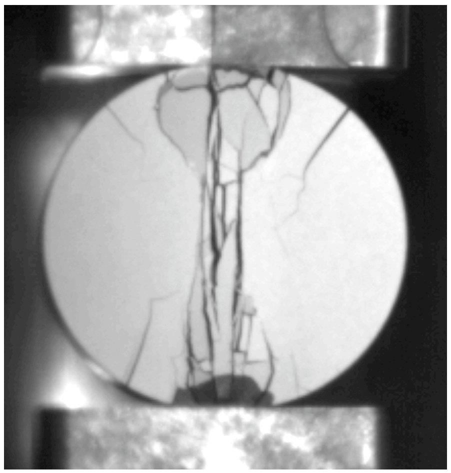




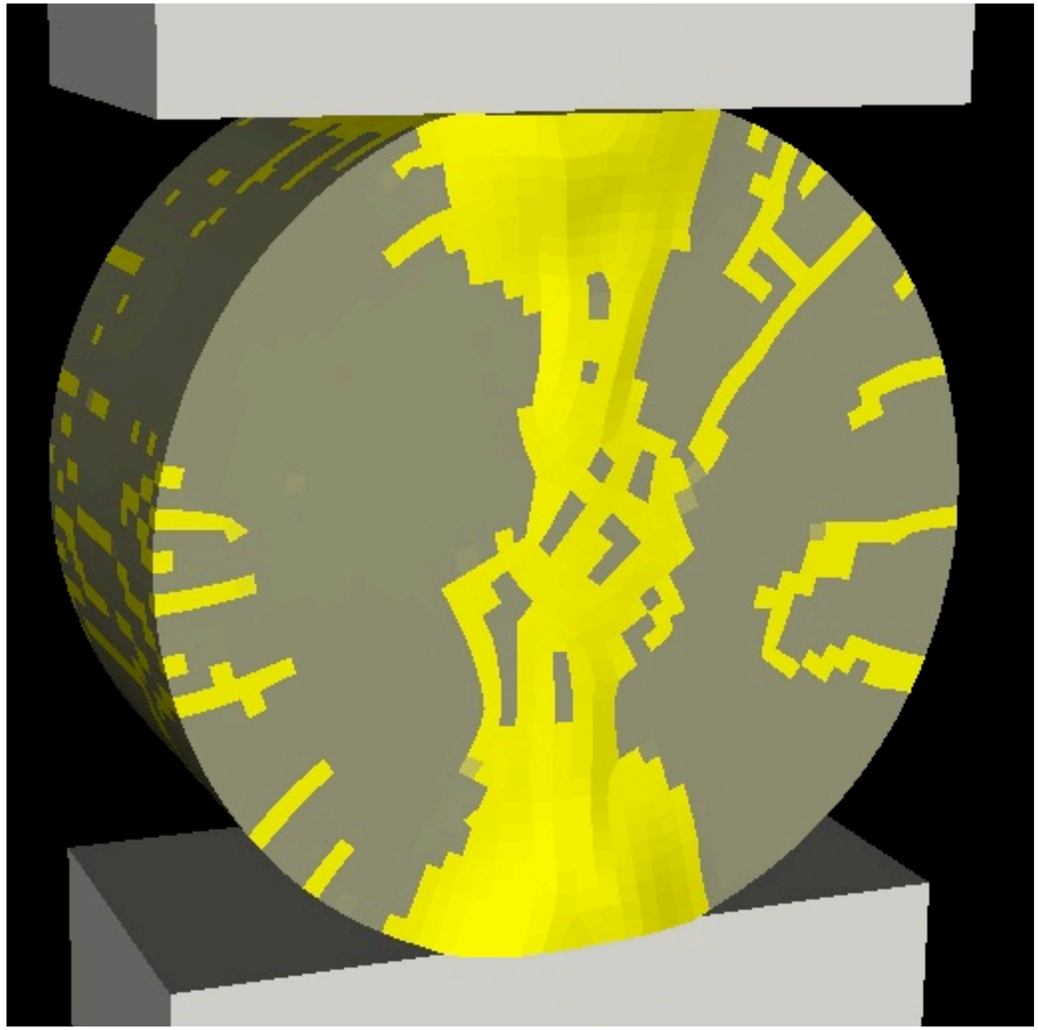




Brazilian Simulations

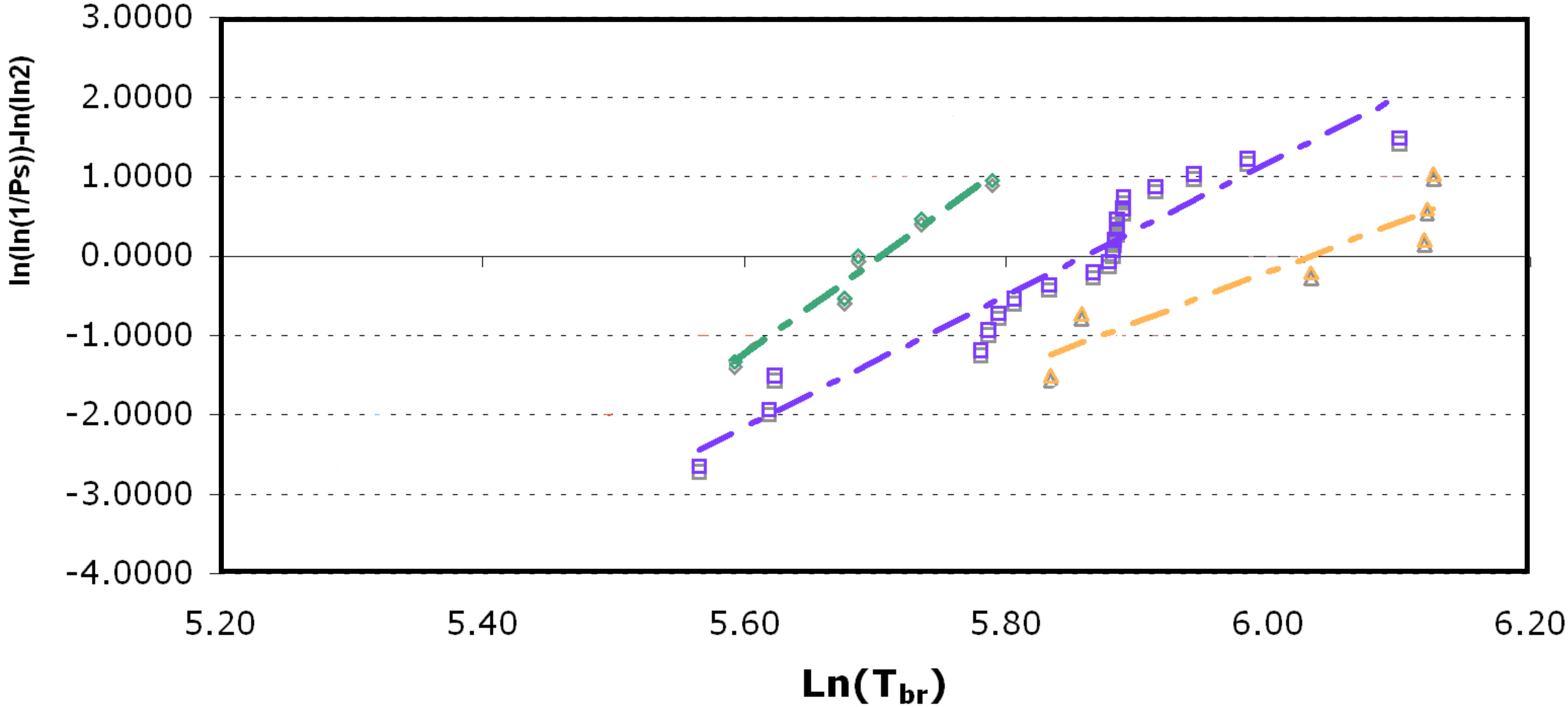


Crack pattern in experiment



Crack pattern in Simulation

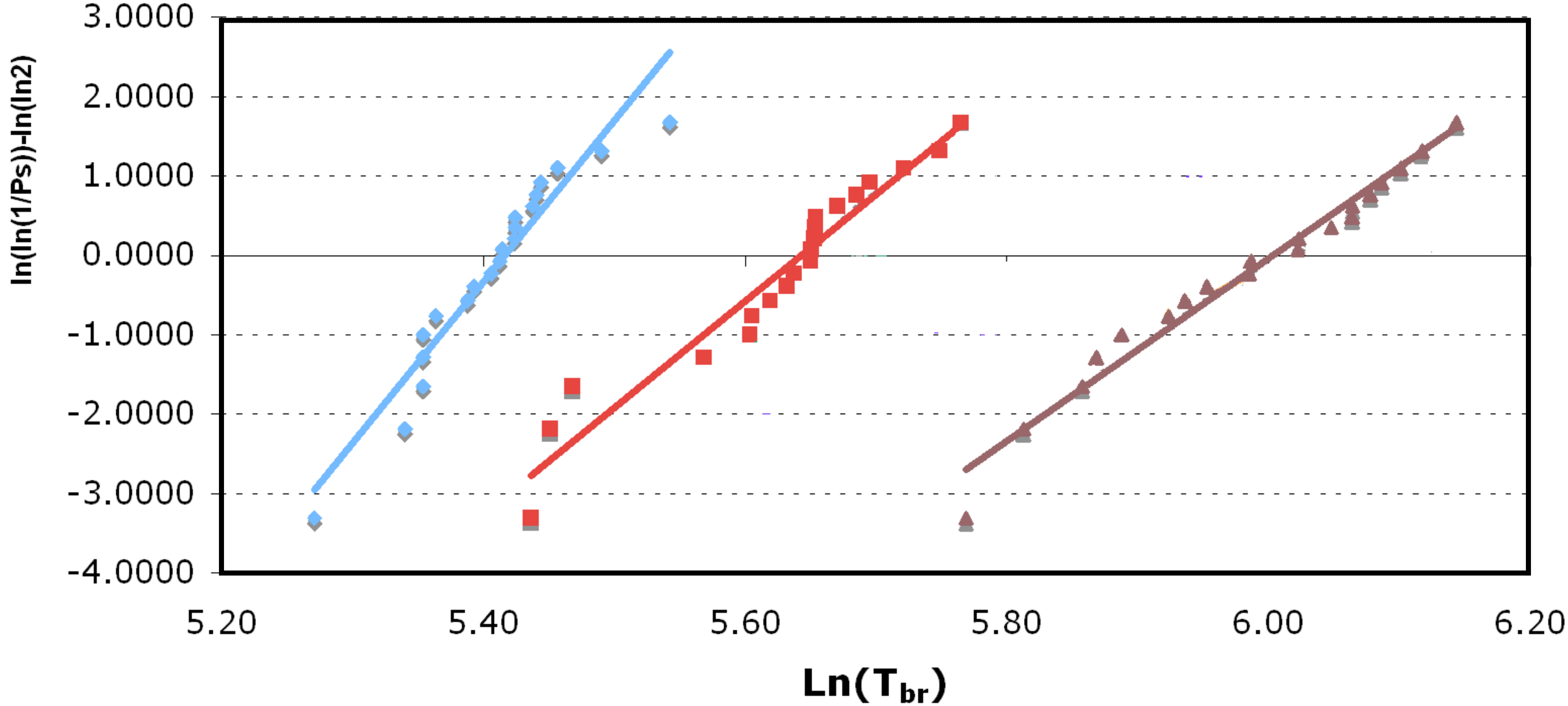
Brazilian Experimental Data



Experiments exhibit variability (Weibull modulus ~8)

Experiments exhibit size effect

Problem: Size effect Discrepancy in Simulated Brazilian Data



Statistics reasonable.
Correct trend of decreasing slope with decreasing sample size.
Quantitative comparison reveales remaining mesh dependency.

Presentation Contents

- Introduction – FEM methods
- Available computational methods
  - Lagrangian methods
  - Particle methods
  - Eulerian and ALE methods
- Outstanding issues
  - High-performance computing
  - Shock capturing
  - Verification and validation
  - Material modeling (EOS, complexity, fracture)
- **Conclusion – the long road ahead**

Conclusion

- Substantial improvements in existing methods are needed for truly predictive capabilities
- A predictive capability could be a *disruptive technology*
  - Rapid design and prototyping of *optimal* configurations
  - Rapid response to changing design requirements
  - Significant insight to physics
- Requires substantial "*glamorous*" work on:
  - Meso-scale modeling experimental techniques – *understanding the physics* of how materials fail
- Requires substantial "*non-glamorous*" work on continuum:
  - Physics algorithms and *empirical* models
  - Calibration – *running* mesoscale models
  - *Verification* and validation

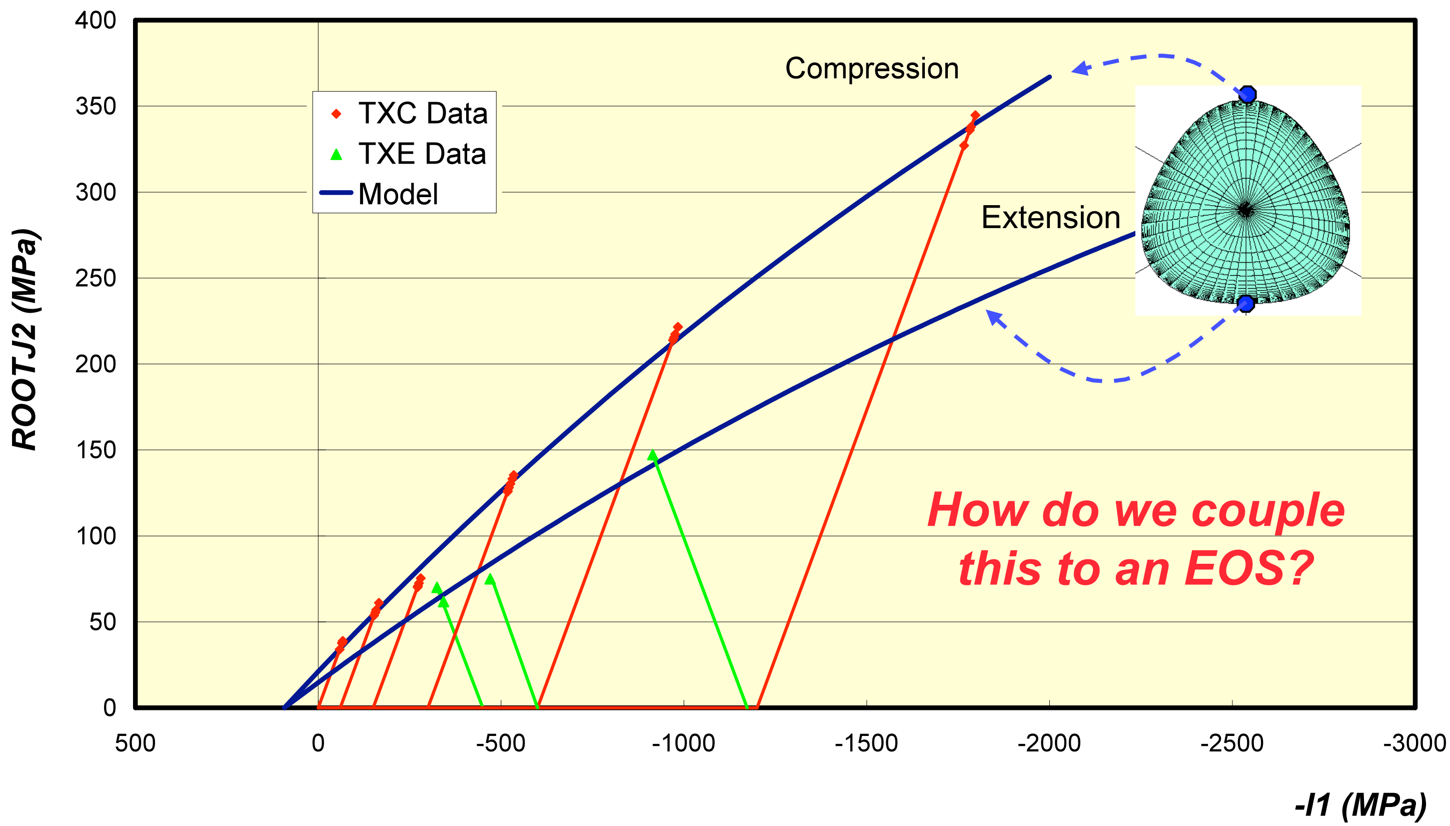
Sandia National Laboratories

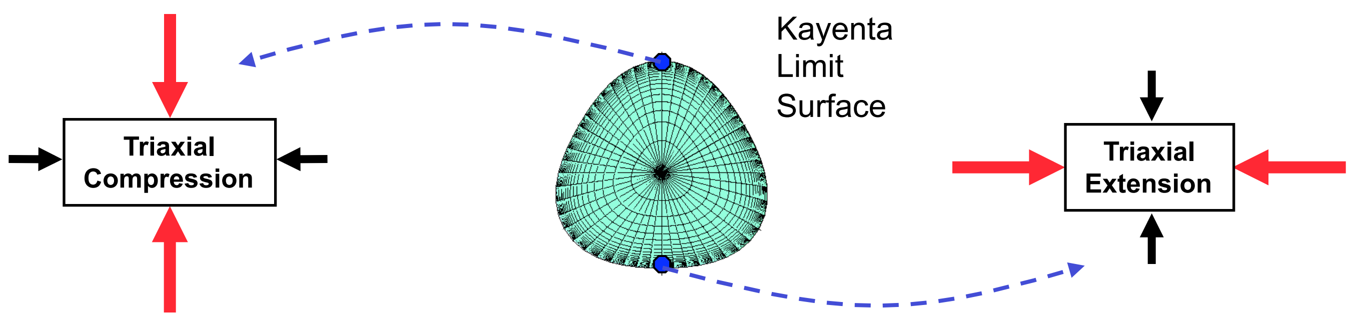
Some Thoughts on Future Directions

- Meso-scale models, and especially meso-scale simulation results from *validated* meso-scale simulations could provide *invaluable* information to continuum constitutive damage models
- The process of validating meso-scale models would encourage a tight integration with experimental researchers
- I believe experimental researchers should use the latest meso-scale models in their research
- I believe experimental researchers should to *also* use and *compare* their experiments to continuum constitutive models
  - Experimentalists will be able to highlight modeling issues better than design engineers
  - Models will help experimentalists determine the data that is necessary for further calibration and validation
- *Bottom line: I believe we need tightly integrated research spanning continuum model development, continuum model simulation, meso-scale model development, meso-scale simulation, design experiments, and research experiments for EACH material of interest*

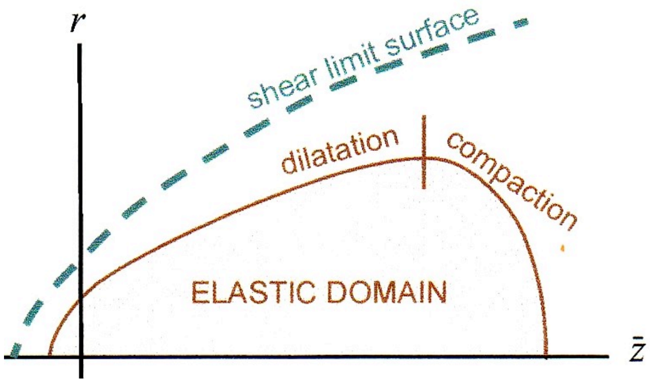
Backup Slides

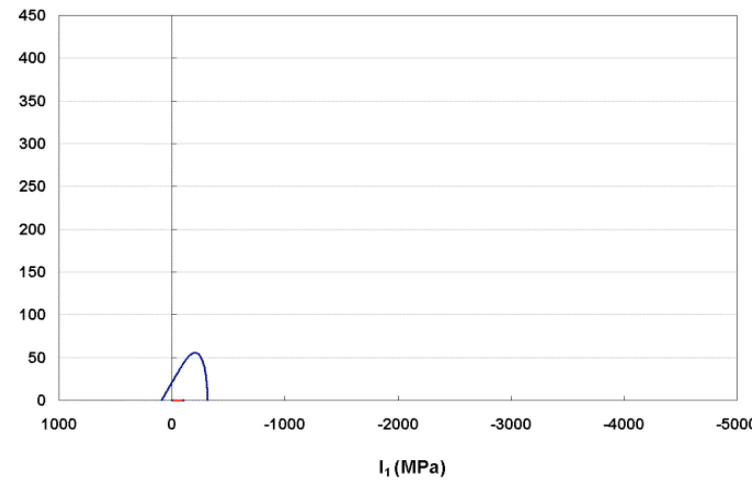
Third Invariant Dependence





Compaction and Dilatation





DiGiovanni et al,
2000