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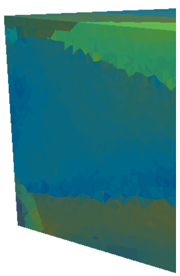

Multiscale Methods for Uncertainty Propagation for Polycrystalline Aluminum 6061-T6

US Congress on Computational Mechanics

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Problem Statement

We seek to:

- Develop an efficient algorithm for multiscale structural reliability prediction for applications where ductile crack nucleation is the mechanism of interest
- Stitch existing multiscale methods and constitutive models in a manner to make multiscale reliability calculations tractable

We will:

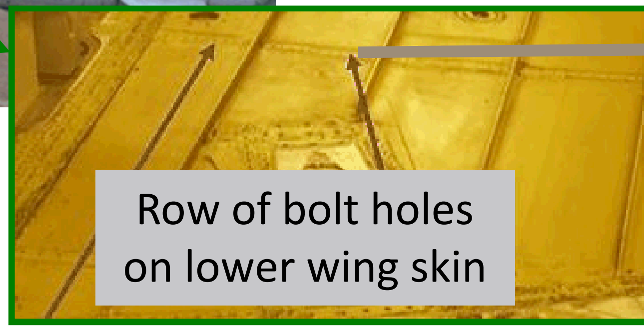
- Utilize Stochastic Reduced Order Models (SROMs) to efficiently transfer uncertainty across length scales
- In this presentation primarily focus on the implications of multiscale coupling on the propagation of meso-scale material uncertainty
- Additionally, discuss implications of the construction of the meso-scale finite element model

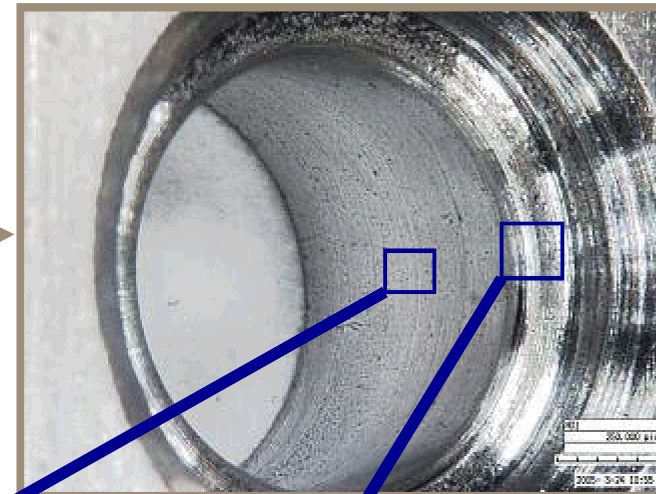
Outline

- Problem motivation
- Overall fracture prediction approach overview
- High fidelity framework and modeling details
- Modeling considerations studied here:
  - Multiscale coupling impacts
  - Meso-scale meshing (grain aligned element edges)
- Conclusions

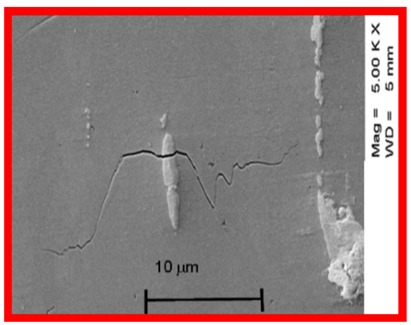
Why do multiscale? Because structural reliability is dependent on ***random*** microstructure (among other sources of randomness)

Engineering length scale (meters)

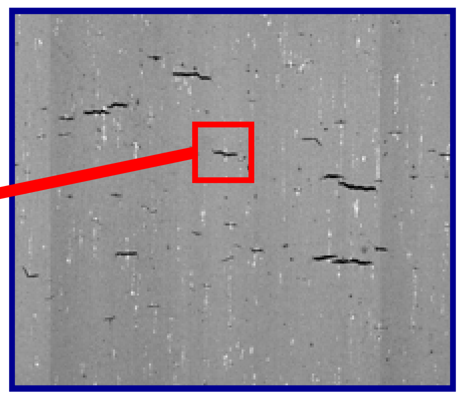




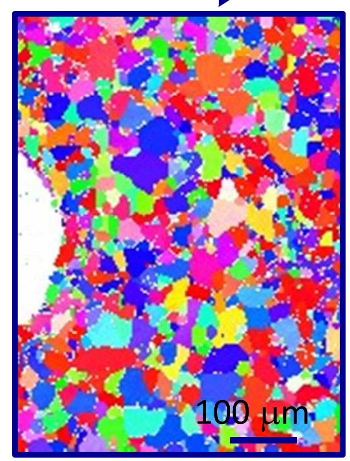
Structural feature (mm) – stress concentration or "hot-spot"



brittle particle



Microstructural length scale (µm)



EBSD data shows randomly oriented grains

randomly distributed brittle particles embedded in randomly oriented, anisotropic matrix

One multiscale calculation is necessary but not sufficient

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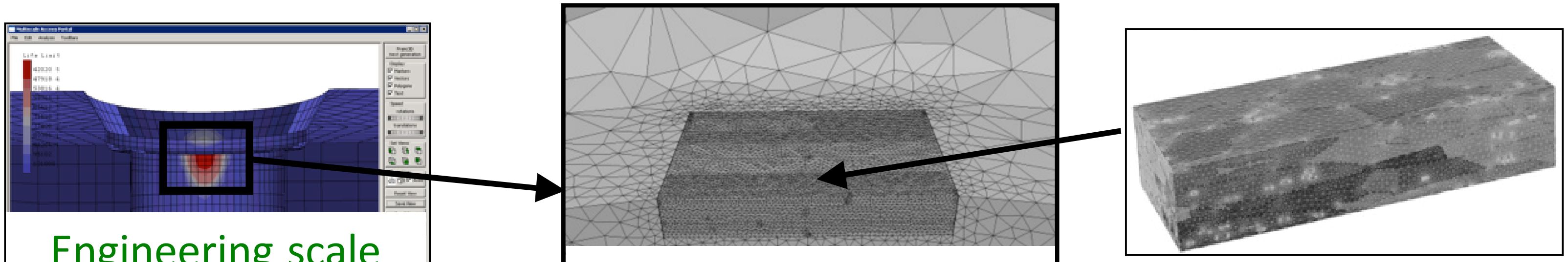


Engineering scale (millions of DOFs)

Multiscale calculation (XXLarge)

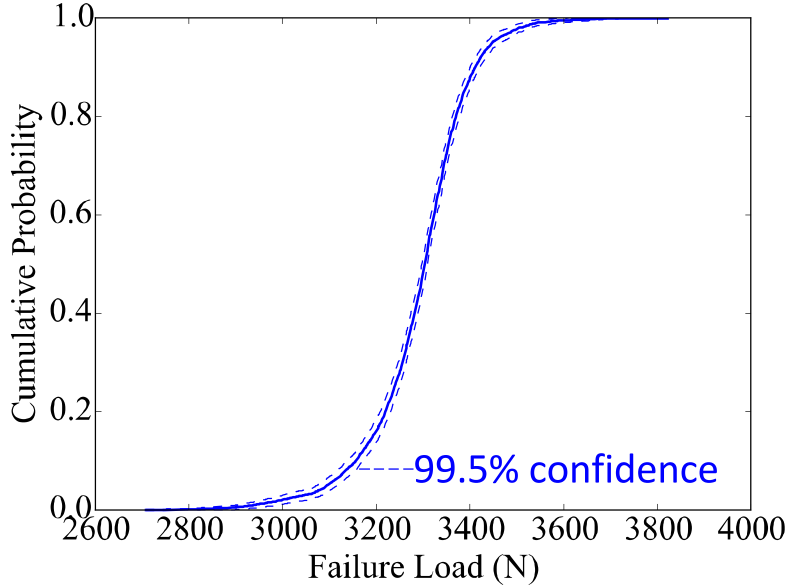
Microstucture scale (≥10s millions of DOFs)

Capturing the tail of the *cumulative* failure

requires many MC samples.

Our work aims to make this computationally tractable.

OUR CHALLENGE



High level goal: tractably propagate fine-scale uncertainty through multiscale calculations
Why does Sandia care? Fracture is local and random, *e.g.*, microstructure, and system/component reliability depends on phenomena occurring a various length scales.

Schematic of our novel hierarchical approach

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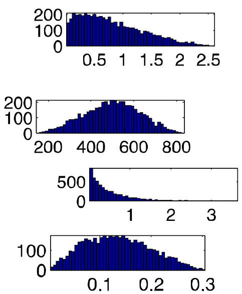
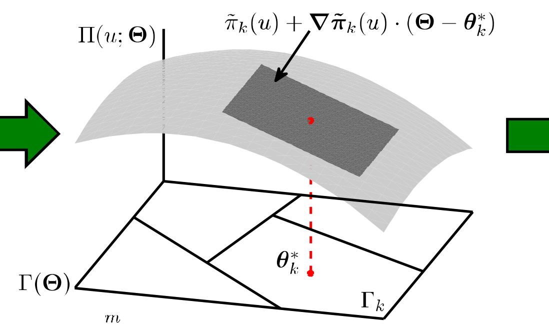
Low fidelity

uncertain data



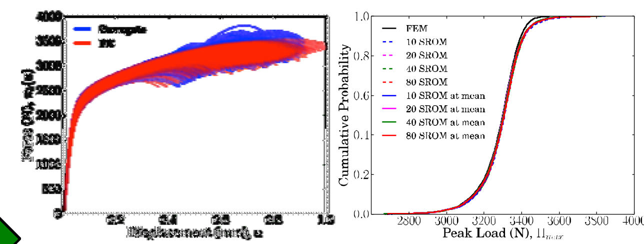
*SROM

MCS of engineering-scale response via SROM-surrogate

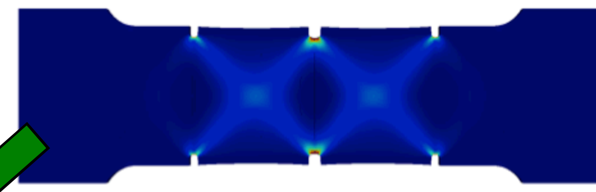


$$\tilde{\Pi}_L(u;\boldsymbol{\Theta}) = \sum_{k=1}^{m} 1(\boldsymbol{\Theta}\in\Gamma_k)\,[\tilde{\pi}_k(u) + \nabla\tilde{\pi}_k(u)\cdot(\boldsymbol{\Theta}-\boldsymbol{\theta}_k^*)]$$

Low-fidelity Probability of Failure



Hot-spot selection & prioritization



prior distribution

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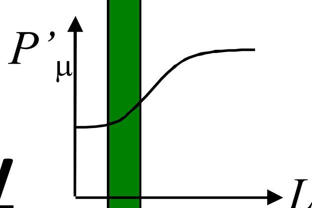
update

For hotspot i, iterate.
Repeat for all hotspots.

i++

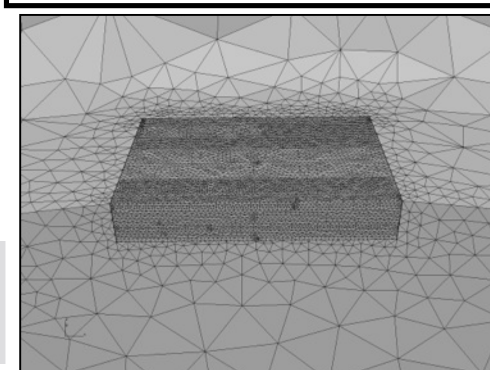
$$P_F(L) = \sum_{i}^{hotspots} P(L\,|\,a_i)P(a_i)$$

Higher fidelity

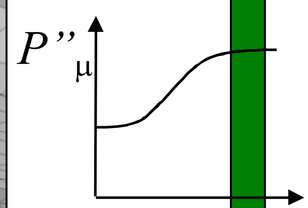


prior distribution of conditional failure

$P'_\mu(L\,|\,a_i)$

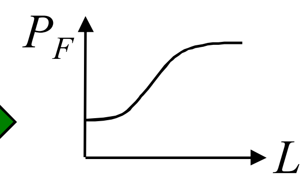


Multiscale calculation



posterior distribution of conditional failure

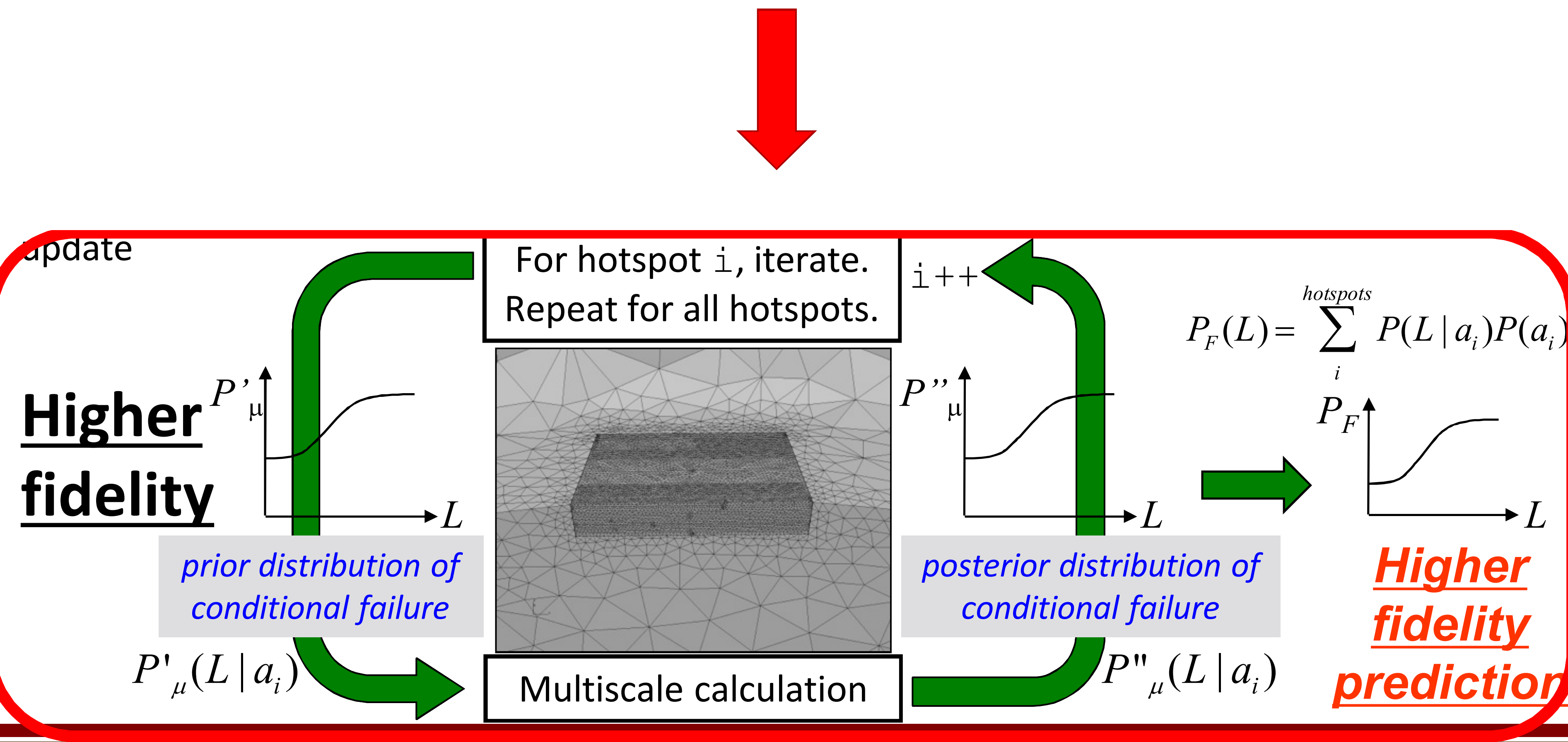
$P''_\mu(L\,|\,a_i)$



Higher fidelity prediction

Schematic of our novel hierarchical approach

This presentation's work focuses on this portion of the hierarchical approach



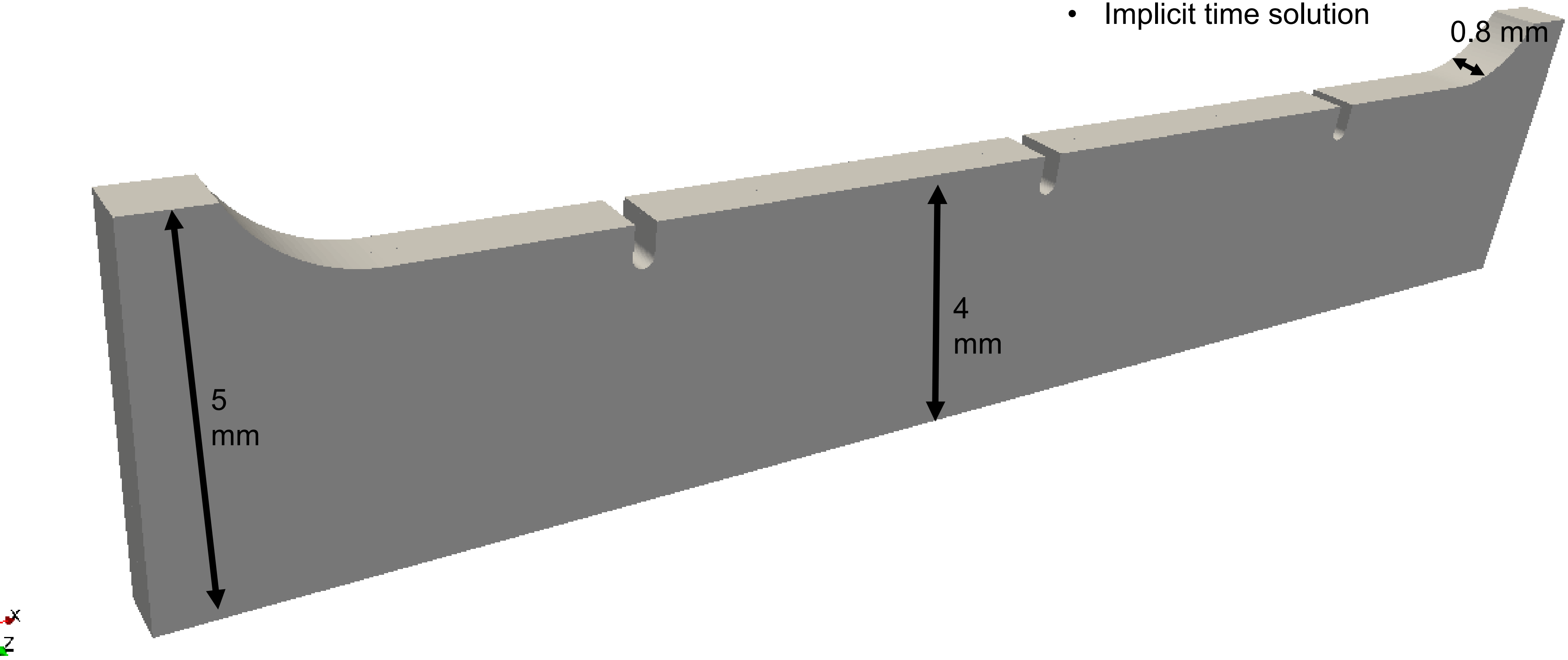
Engineering Scale Model

Material

- AL-6061
- Hill Plasticity

Model Details

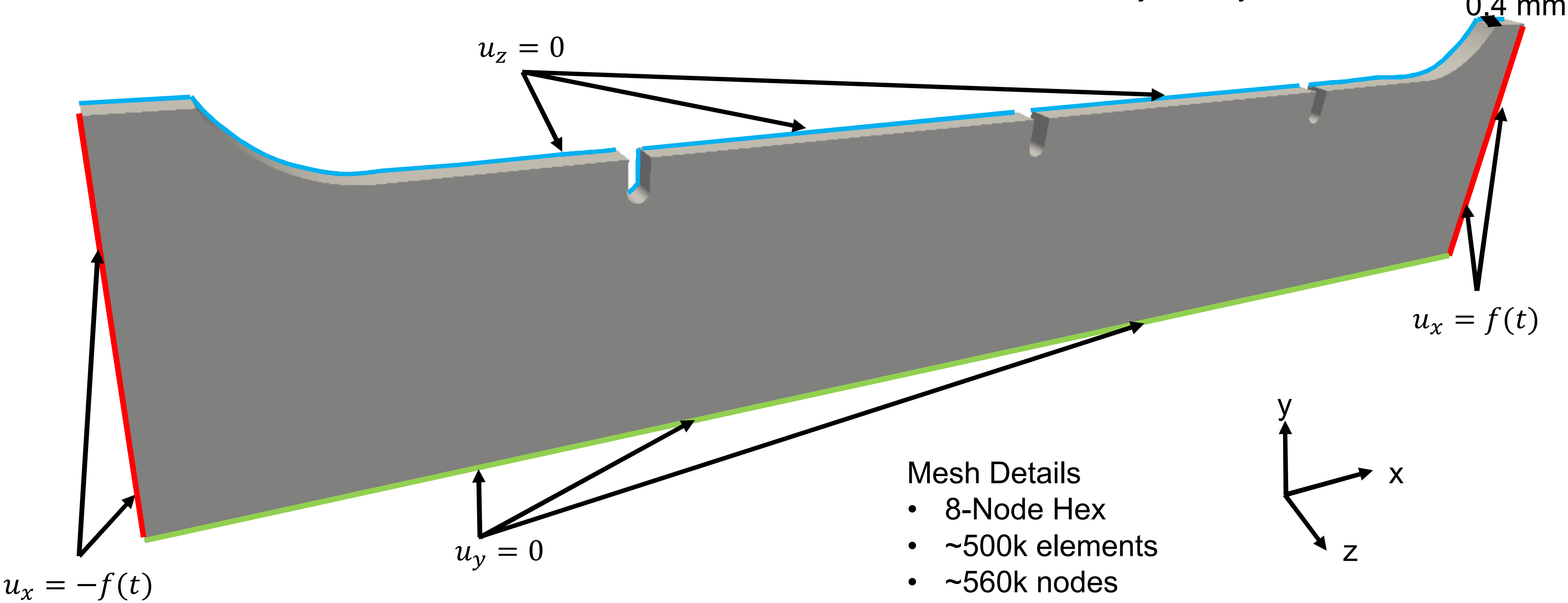
- Implicit time solution



Engineering Scale Model

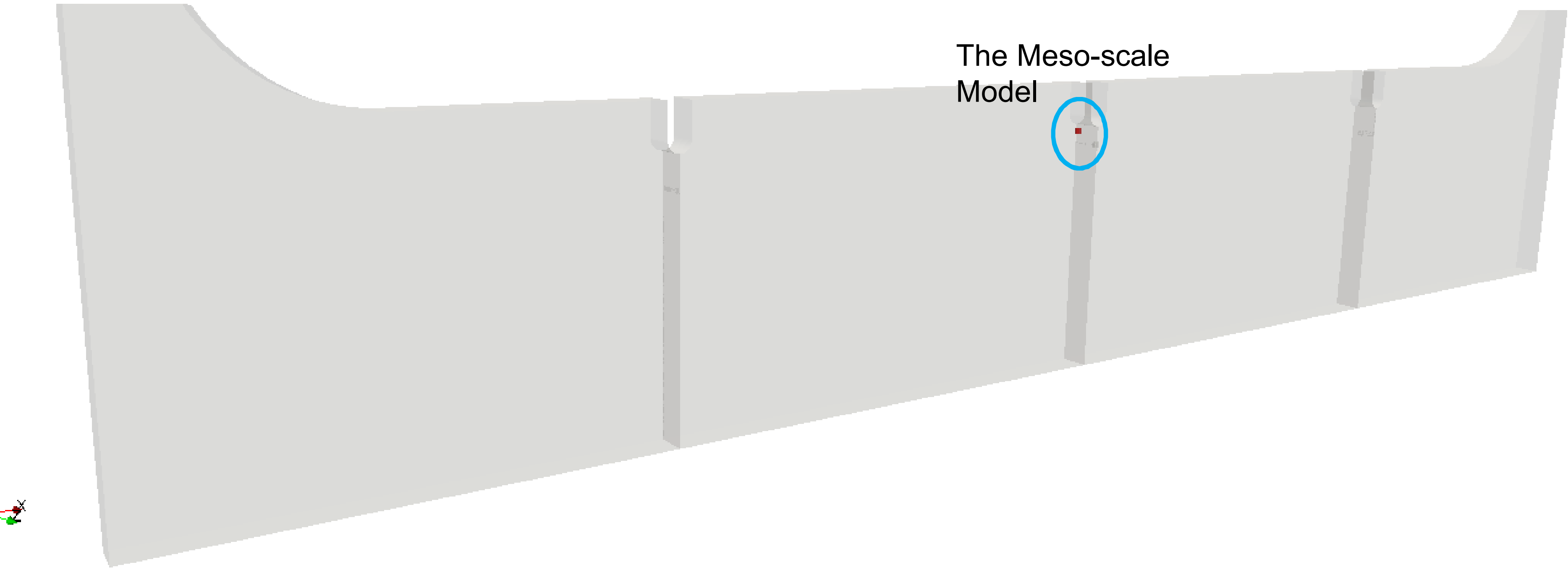
Material
- AL-6061
- Hill Plasticity

Model Details
- Implicit time solution
- Symmetry

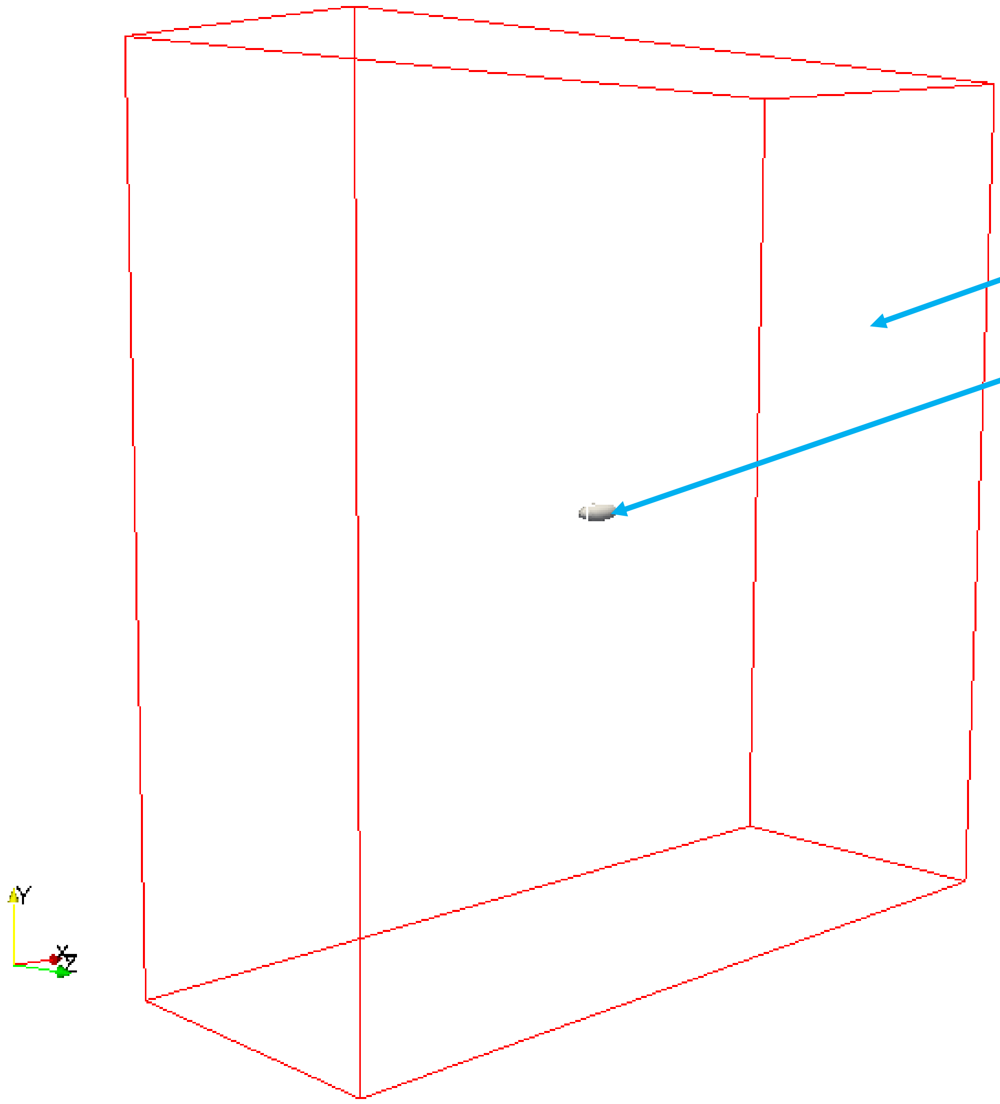


Mesh Details
- 8-Node Hex
- ~500k elements
- ~560k nodes

Switching Scales



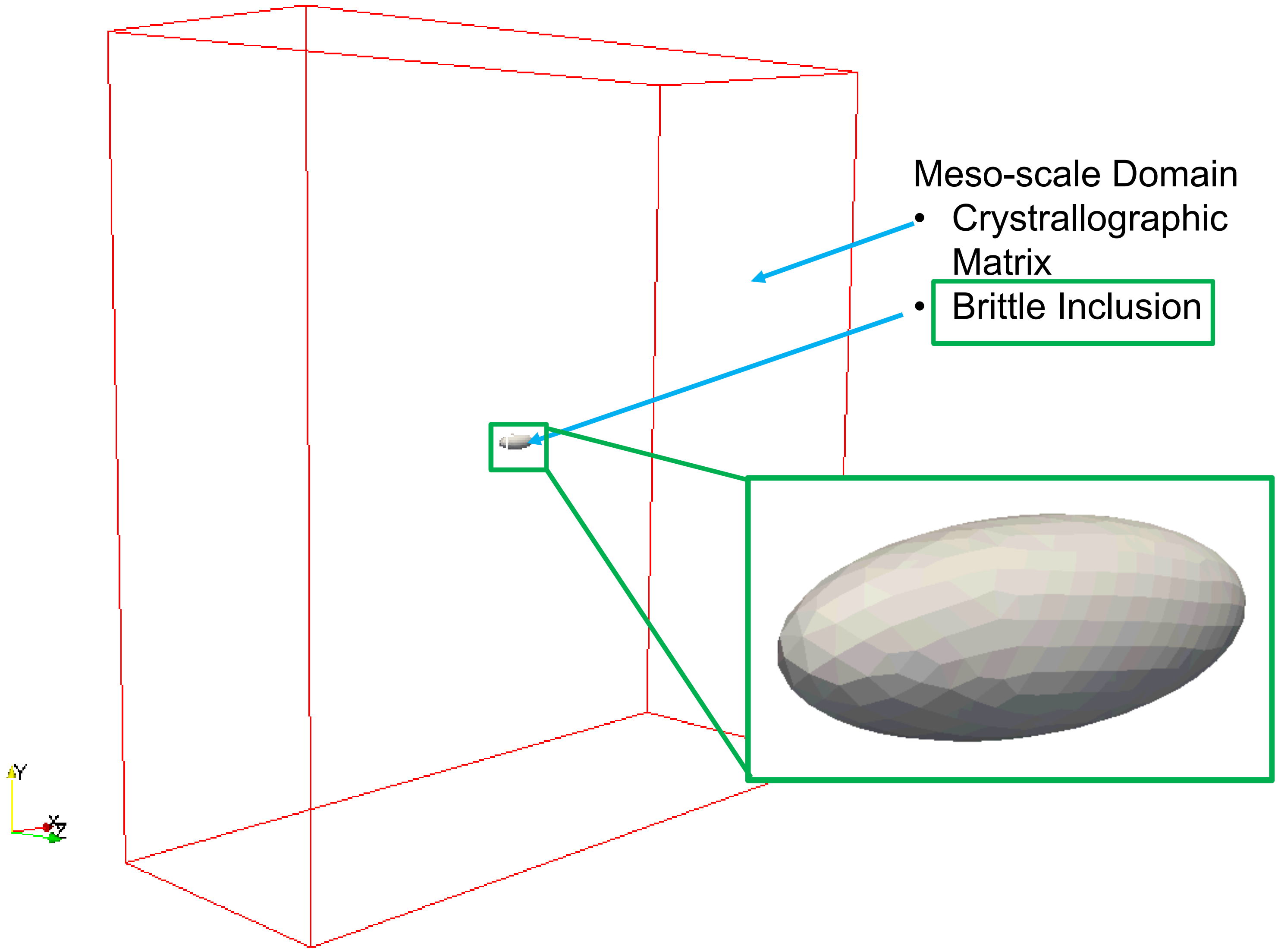
Meso-scale Model



Meso-scale Domain

- Crystrallographic Matrix
- Brittle Inclusion

Meso-scale Model

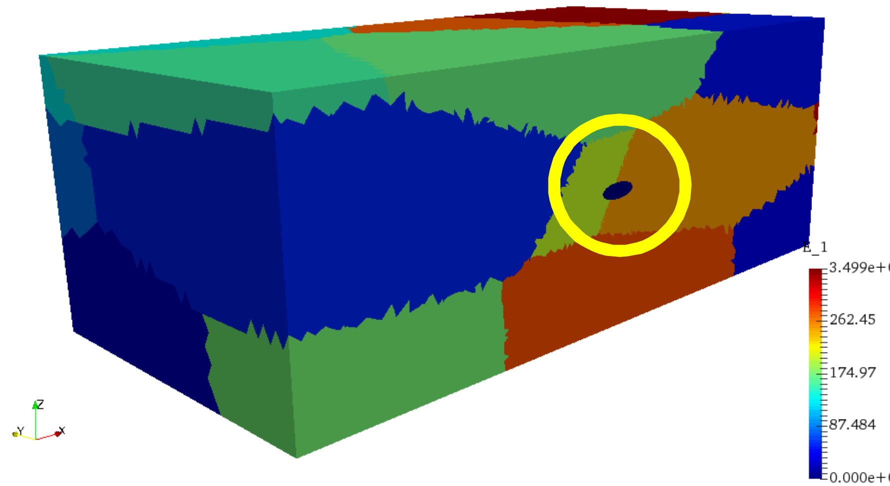


Meso-scale Domain

- Crystrallographic Matrix
- Brittle Inclusion

Brittle second phase – void nucleation

- Embed an ellipsoidal particle, 5 x 1.8 μm
- Coherent mesh at particle/matrix interface
- 1 morphology (grain geometry) w/ ~27 grains
- 10 statistical samples of grain orientations
- Grain orientation statistics to match measured experimental data
- Assumed elastic mechanical properties for particle (pure iron)
  - E = 211 GPa, $\nu = 0.29$
  - Strength 540 MPa
- Assumed perfect and rigid particle/matrix interface bond



Cross-section through major-axis of ellipsoid

Multiscale model considerations

Wish to study the impact of:

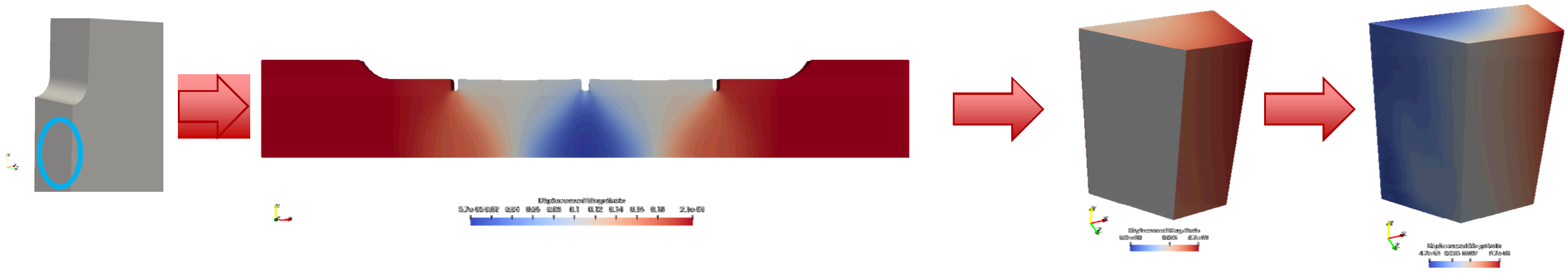
- Multiscale coupling
- Meso-scale model meshing with respect to grains

On the propagation of uncertainty in grain material orientation with respect to:

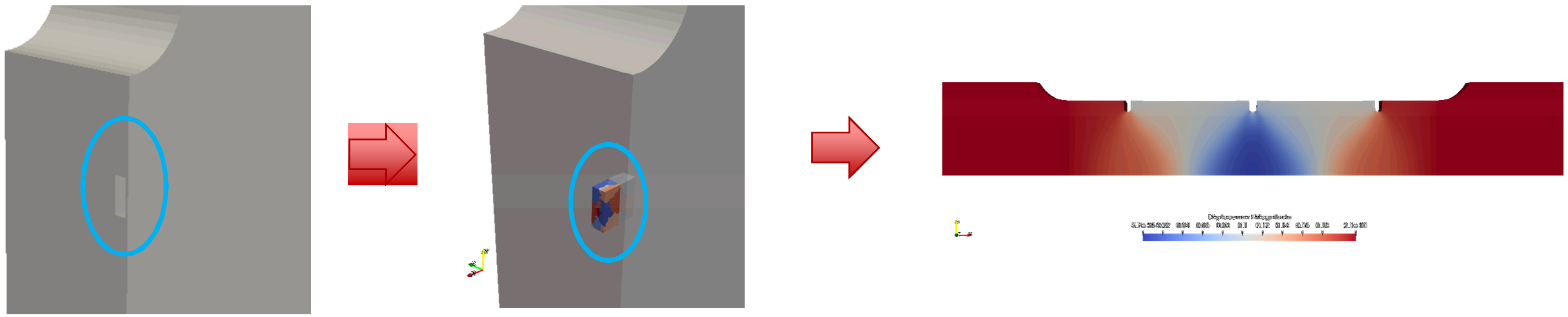
- Brittle inclusion average stress
- Brittle inclusion maximum stress

Coupling approaches

Submodeling (one-way coupling)



MPC Coupling, Concurrent multiscale modeling (two-way coupling)



Coupling approaches

Submodeling (one-way coupling)

- No homogenization
- Map computed displacements from engineering scale model as Dirichlet boundary conditions on the extents of the meso-scale model

MPC Coupling, Concurrent multiscale modeling (two-way coupling)

- No homogenization
- Directly embed meso-scale model into location of interest

Coupling approaches

Submodeling (one-way coupling)

Moderately Expensive:
Compute once for each unique engineering scale model

Moderately Expensive:
Compute for each UQ random sample

MPC Coupling, Concurrent multiscale modeling (two-way coupling)

Very Expensive:
Compute for each UQ random sample

Watch mean, first-principal stress in the particle

Assuming elastic and brittle, monitor the mean first-principal stress in the particle.

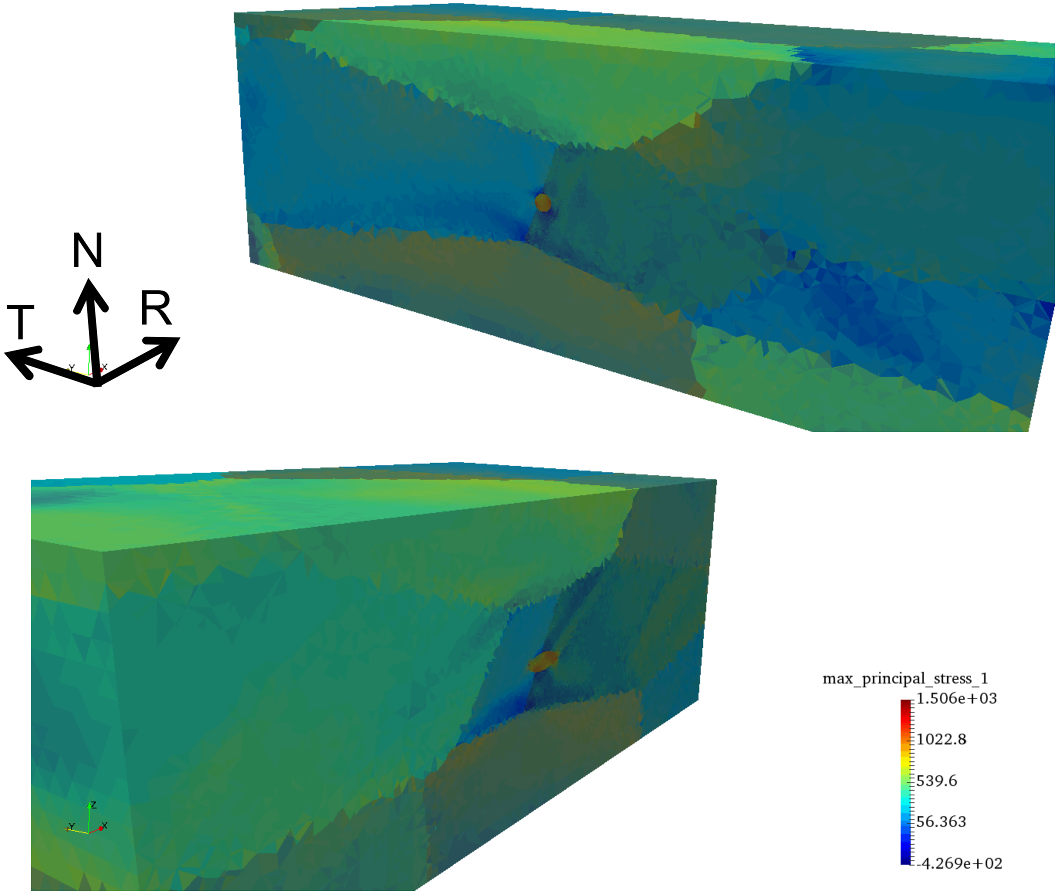
$$Pr(\bar{\epsilon}_{RVE} \in S)$$

$$S = \{\bar{\epsilon}_{RVE} \in \mathbb{R} : g(\bar{\epsilon}_{RVE}) \leq 0\}$$

$$g(\bar{\epsilon}_{RVE}) = \bar{\sigma}_{p,cr} - \bar{\sigma}_p(\bar{\epsilon}_{RVE})$$

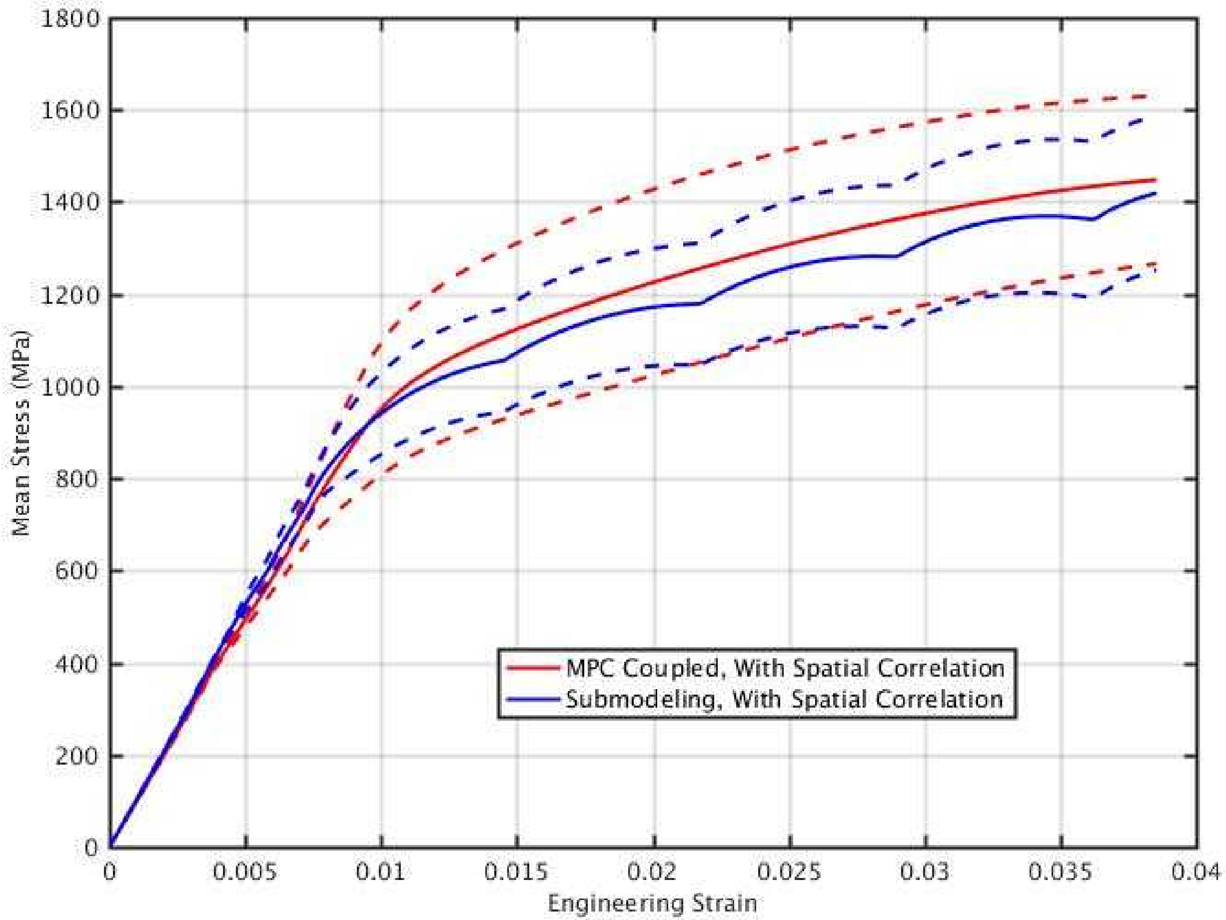
$$\bar{\sigma}_{p,cr} = 540 \text{ MPa}$$

Maximum principal stress contour plot for s123 (showing two cross-sections)



Coupling Comparison

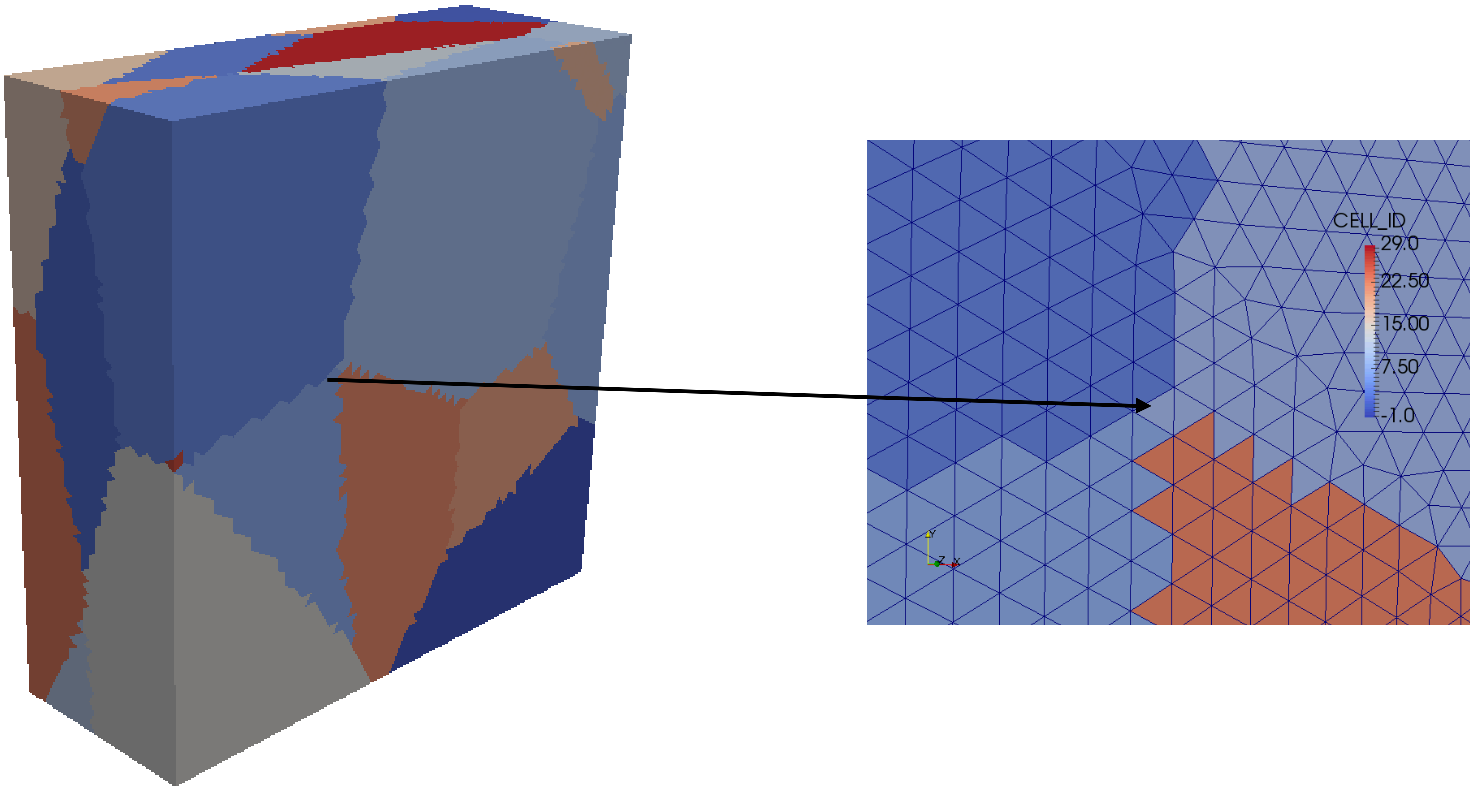
Grain orientations have spatial correlation



—— μ

- - - $\mu \pm \sigma$

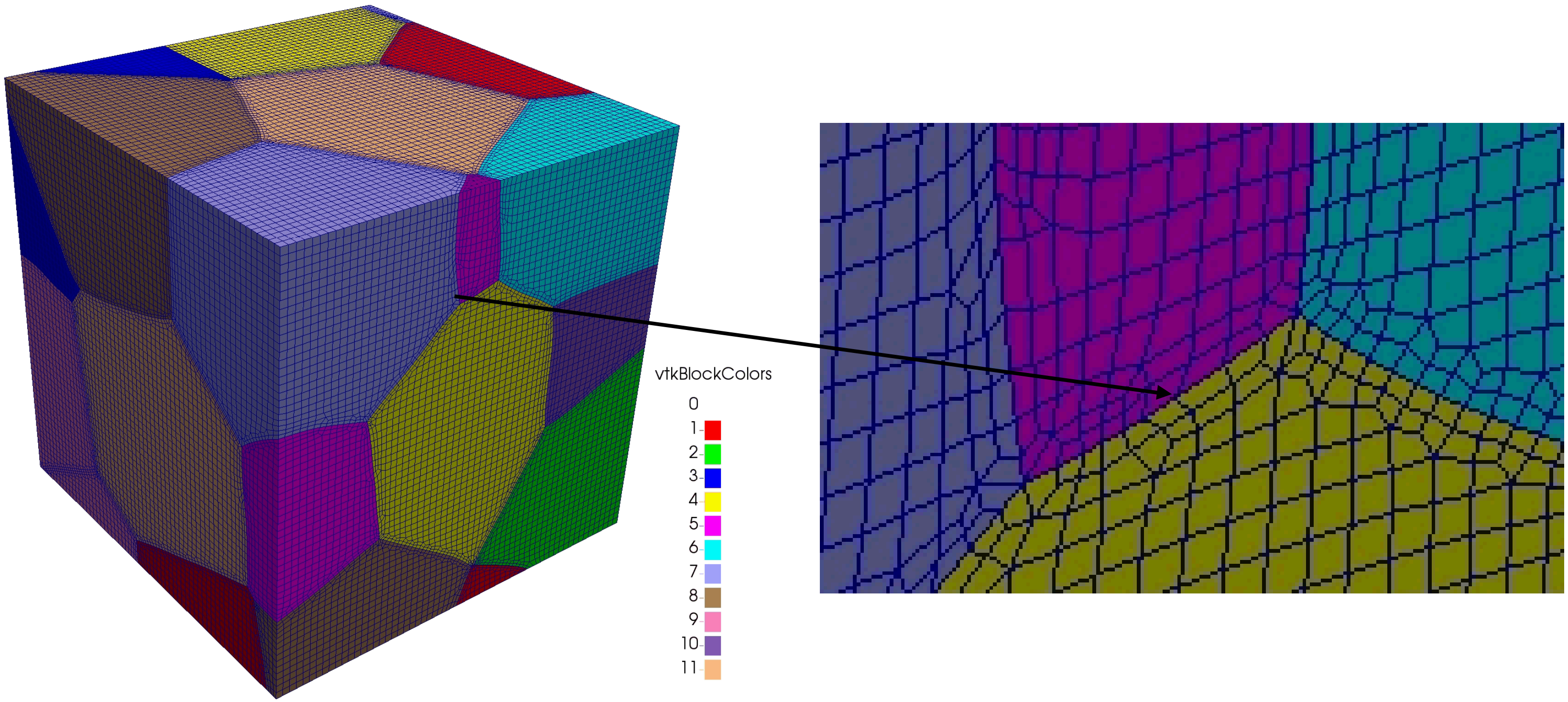
Meshing approaches



Simpler (Not grain aligned) approach:

- Conformal mesh at volume extents and ellipsoid inclusion
- Element boundaries will not align with grains (jagged grain boundary)

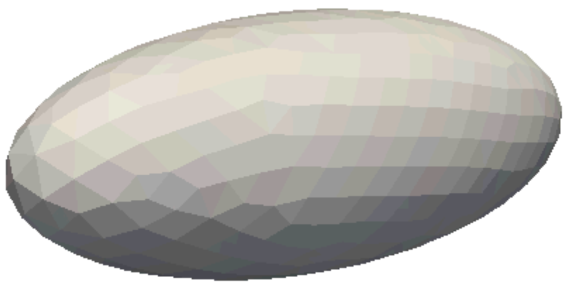
Meshing approaches

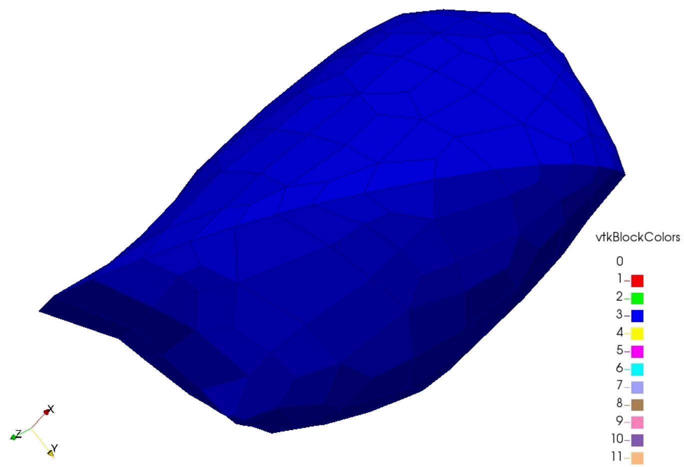


More expensive (Grain aligned) approach:

- Use meshing tool (Sculpt) to provide a hexahedral mesh that aligns with ellipsoid and grain boundaries
- Sculpt is an overlay-grid or mesh-first method
- Sculpt does not exactly align nodes with geometries (differences in ellipsoid size and shape are visible)

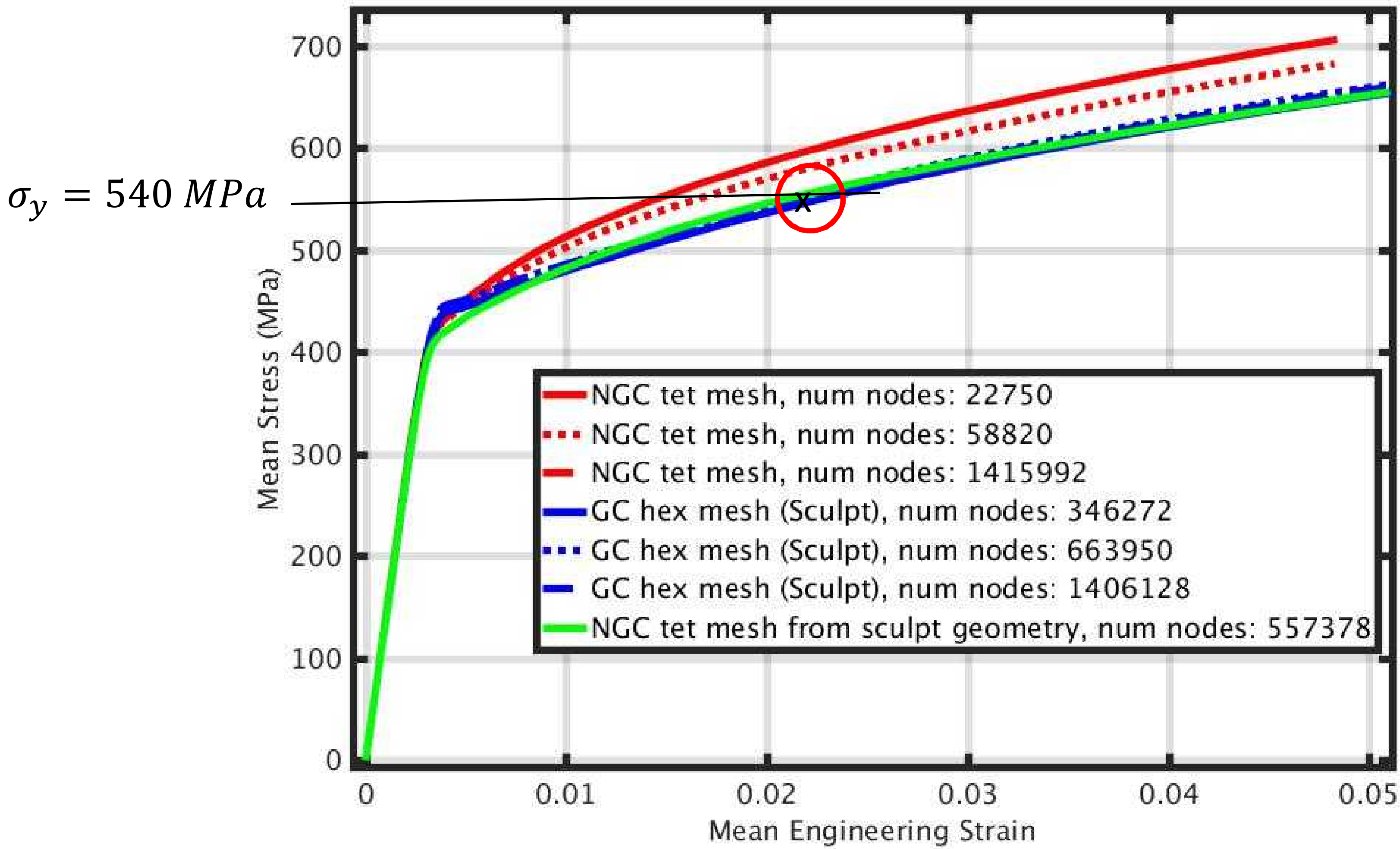
Inclusion geometry differences





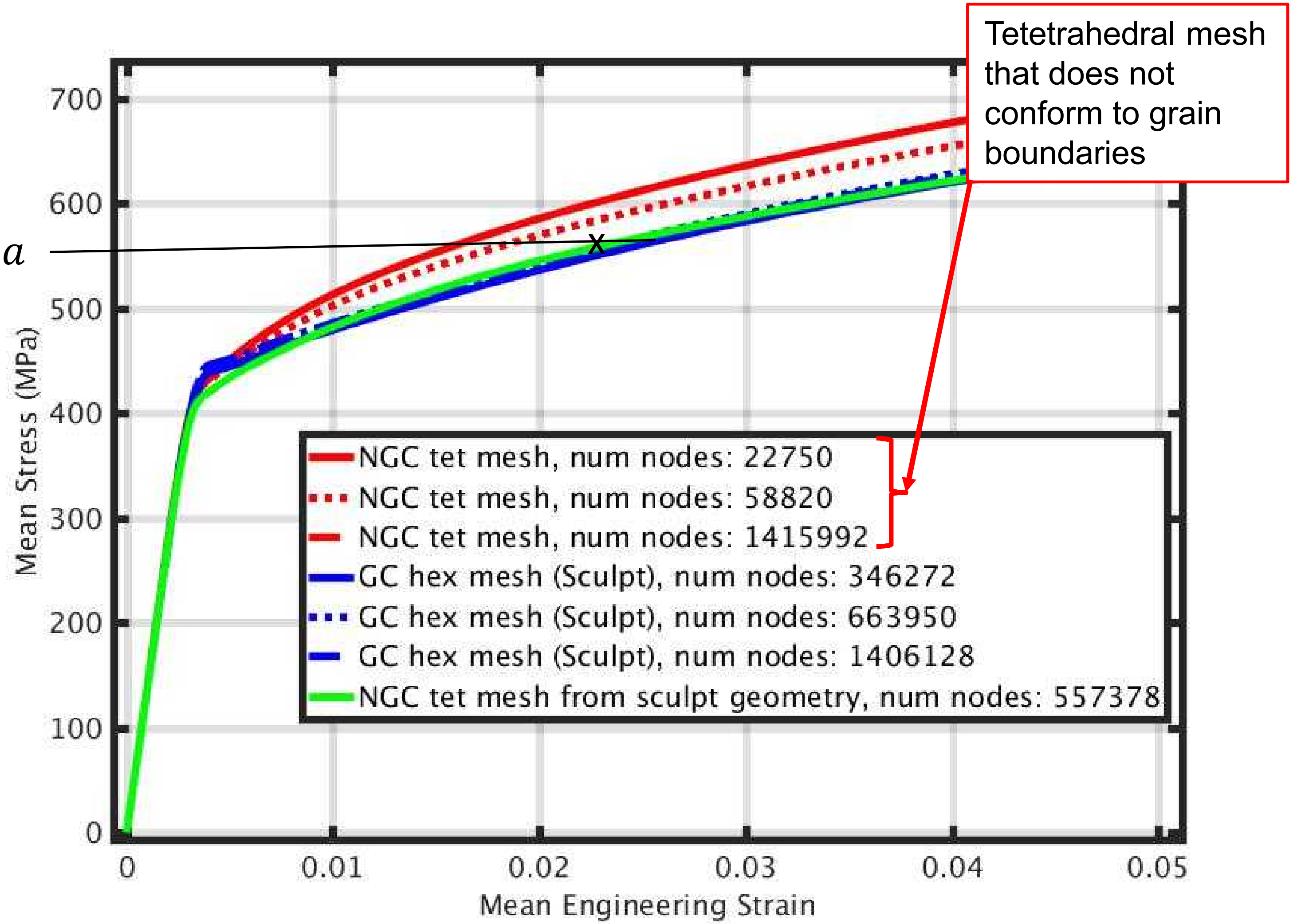
- Sculpt will not precisely adhere to geometry
- Small features (such as inclusion) can be poorly resolved
- Use 5x larger inclusion in following comparison
- Also extract sculpt inclusion geometry and mesh with tetrahedral elements for comparison (jagged grain boundaries)

Meshing consideration results

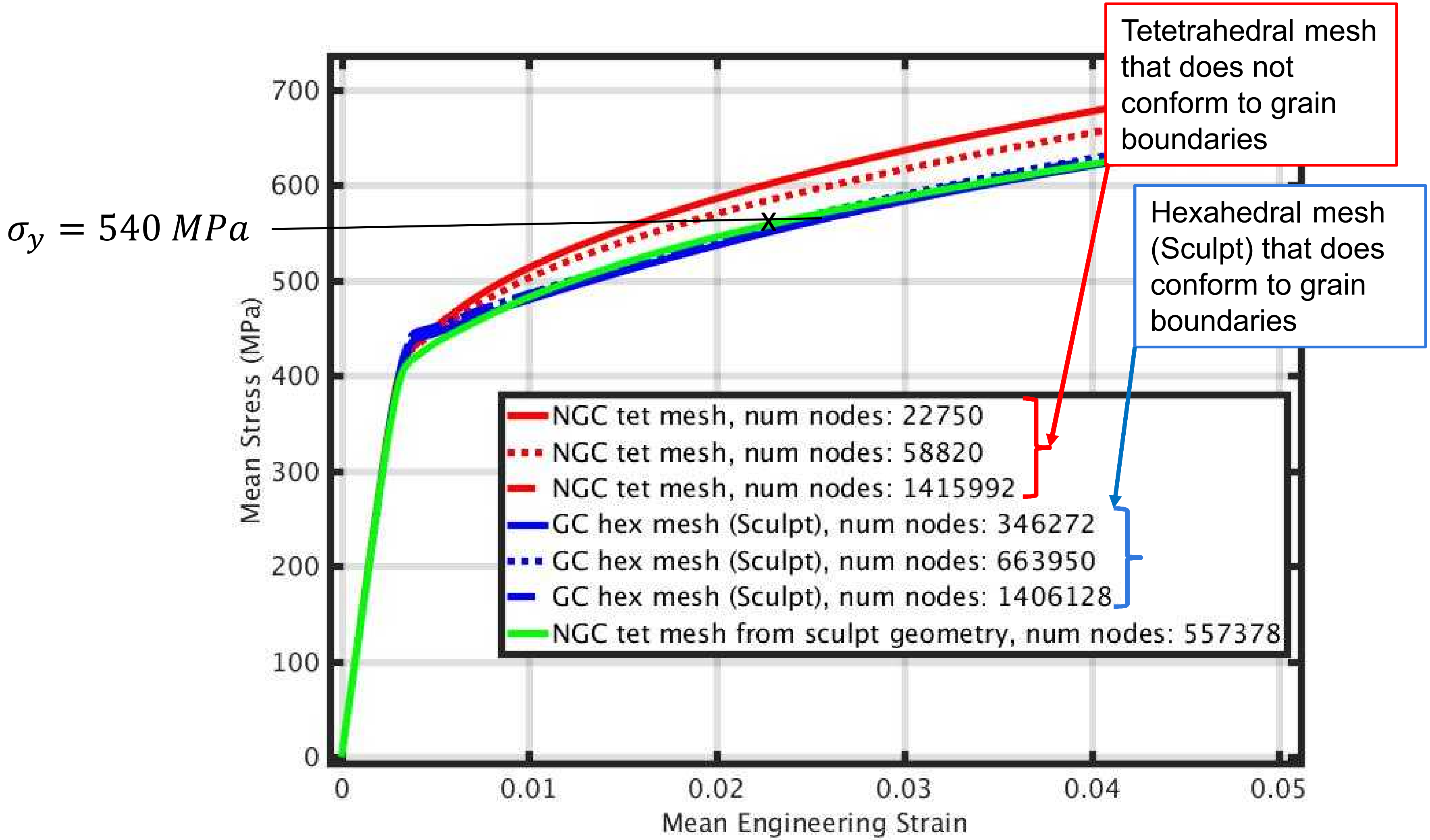


Meshing consideration results

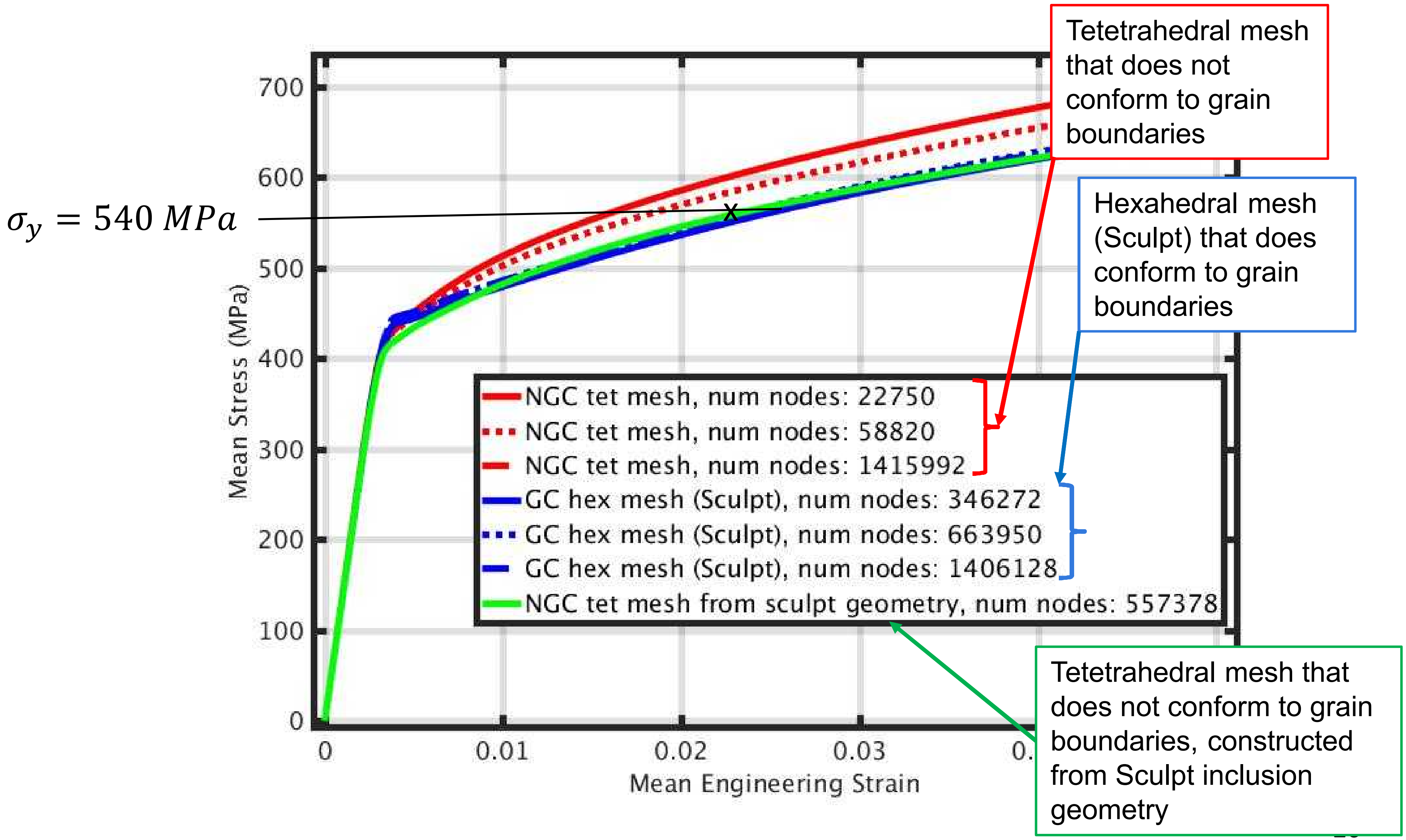
$\sigma_y = 540\ MPa$



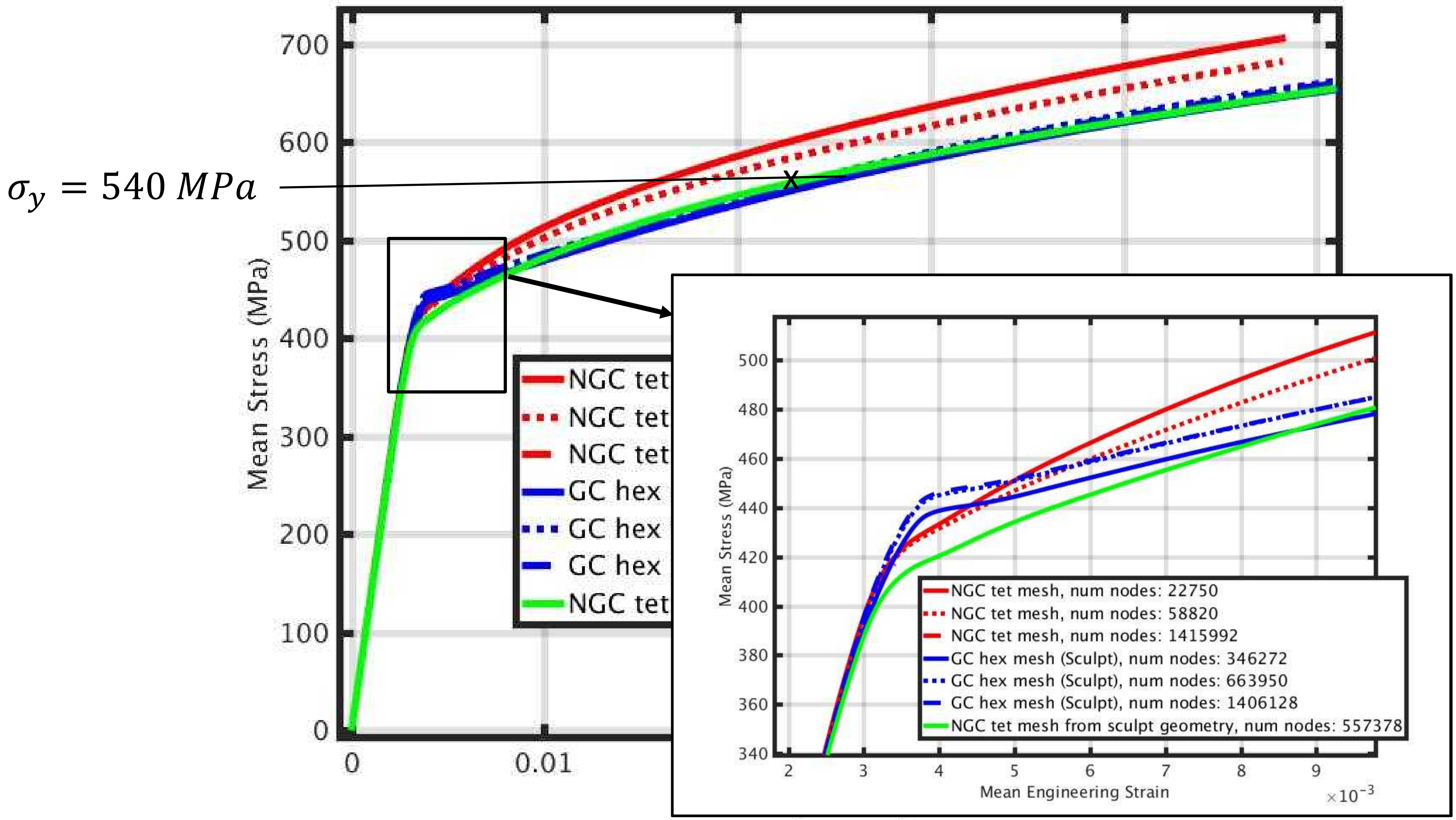
Meshing consideration results



Meshing consideration results

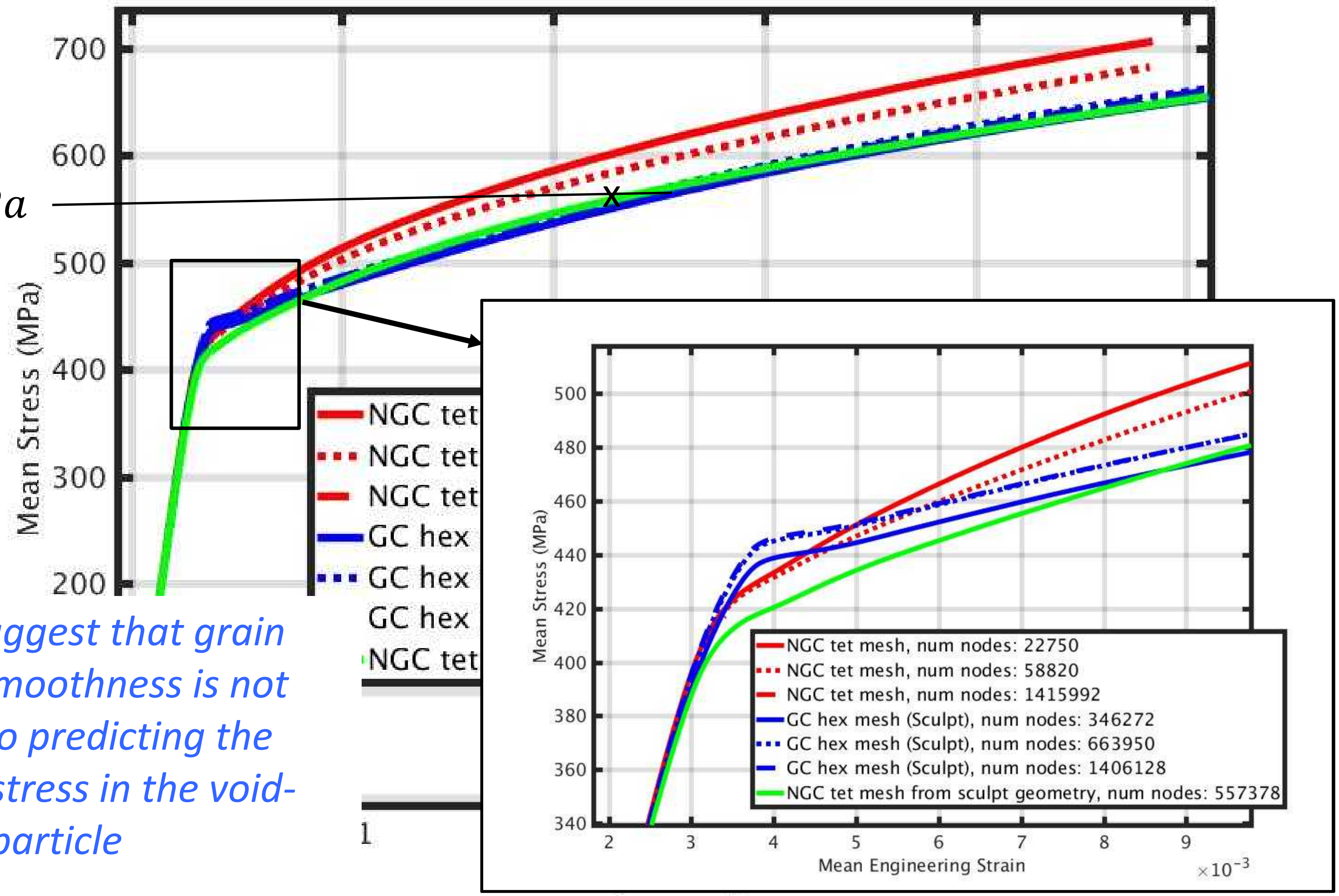


Meshing consideration results



Meshing consideration results

$\sigma_y = 540\ MPa$



Seems to suggest that grain boundary smoothness is not important to predicting the "ultimate" stress in the void-nucleating particle

Conclusions

- At a minimum submodeling appears necessary to estimate mean failure behavior at meso-scale
- With a high fidelity constitutive model at the engineering scale, submodeling holds promise for this work
- Concurrent (two-way) coupling may be necessary to accurately propagate higher moments (standard deviation) of the distribution of mean strains at failure
- Grain boundary smoothness (aligned element edges) is not important to predicting the "ultimate" stress in the void nucleating particle

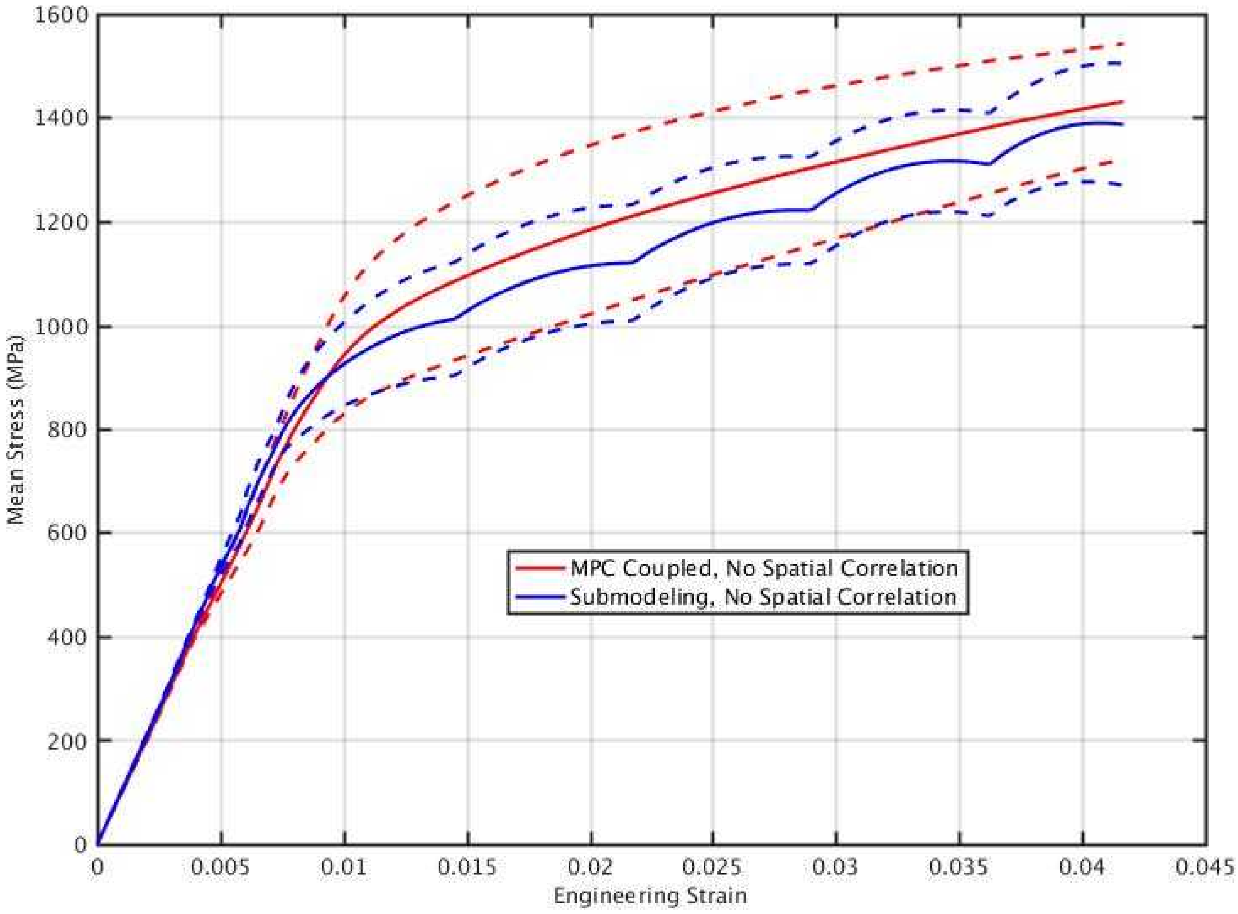
References

1. Pyle, Devin M., et al. "Effect of 3D grain structure representation in polycrystal simulations." *Computational Mechanics* 52.1 (2013): 135-150.
2. J. E. Bishop, J. M. Emery, C. R. Weinberger, R. V. Field and D. J. Littlewood (2015). Direct numerical simulations of macroscale structures with embedded polycrystalline microstructures and comparisons to homogenization theory. *Computational Methods in Applied Mechanics and Engineering*, 287, pp. 262-289.
3. J. M. Emery, R. V. Field, J. W. Foulk III, K. N. Karlson and M. D. Grigoriu (2015). Predicting laser weld reliability with stochastic reduced-order models. *International Journal for Numerical Methods in Engineering,* 103: pp. 914-936.
4. J. M. Emery and A. R. Ingraffea (2011). DDSim: Framework for Multiscale Structural Prognosis. In S. Ghosh and D. Dimiduk, editors, *Computational Methods for Microstructure-Property Relationships*. Springer NY. ISBN: 978-1-4419-0642-7
5. J. M. Emery, J. D. Hochhalter, P. A. Wawrzynek, G. Heber and A. R. Ingraffea (2009). DDSim: A hierarchical, probabilistic, multiscale damage and durability simulation system – Part I: Methodology and Level I. *Engineering Fracture Mechanics*, 76(10): pp. 1500-1530.
6. A. Ghahremaniezhad and K. Ravi-Chandar (2012). Ductile failure behavior of polycrystalline Al 6061-T6. *International Journal of Fracture*, 174: pp. 177-202.
7. A. Ghahremaniezhad and K. Ravi-Chandar (2013). Ductile failure behavior of polycrystalline Al 6061-T6 under shear dominant loading. *International Journal of Fracture*, 180: pp. 23- 39

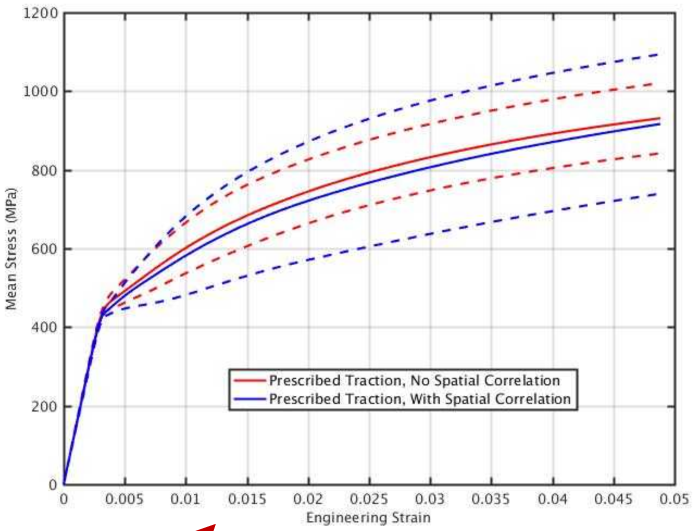
ADDITIONAL MATERIAL

Coupling Comparison

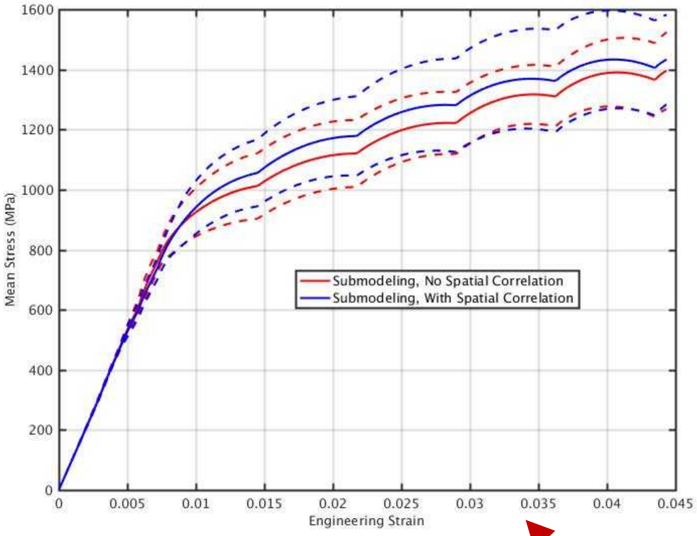
Grain orientations have no spatial correlation



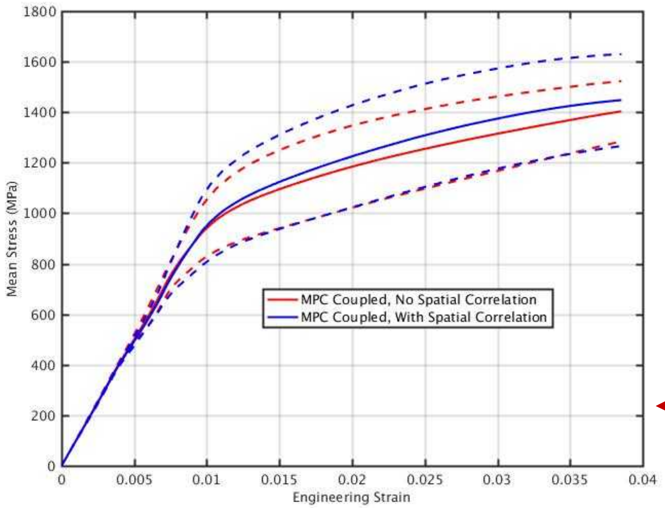
Grain orientation spatial correlation impact



Prescribed traction

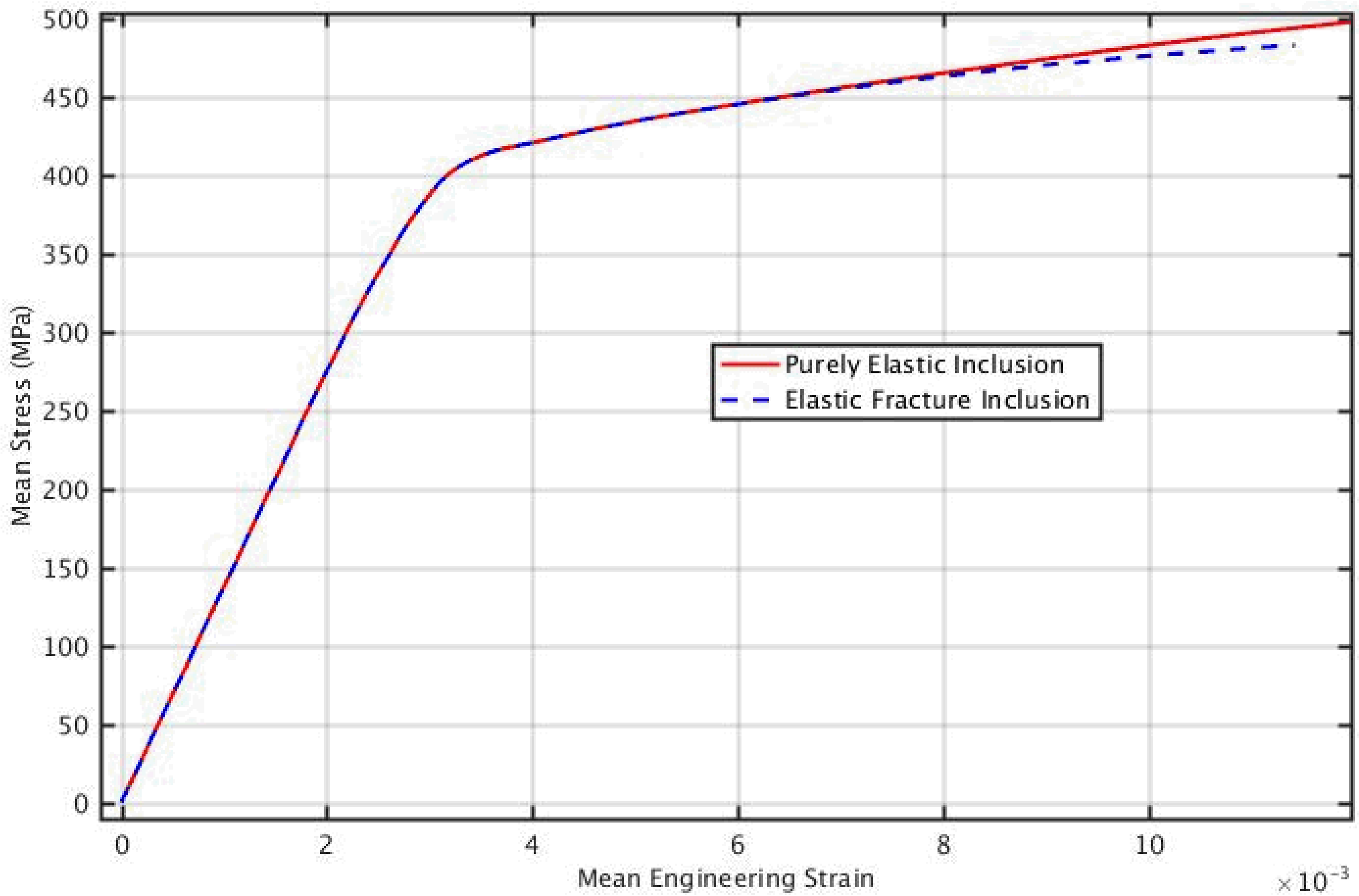


Submodeling



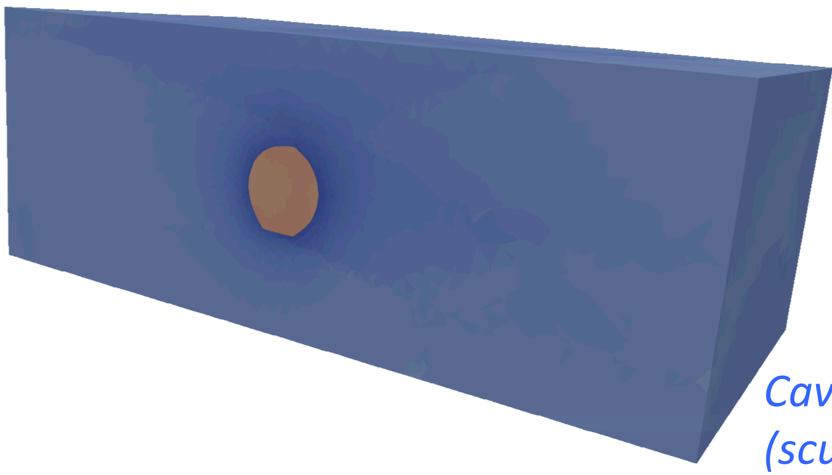
MPC Coupled

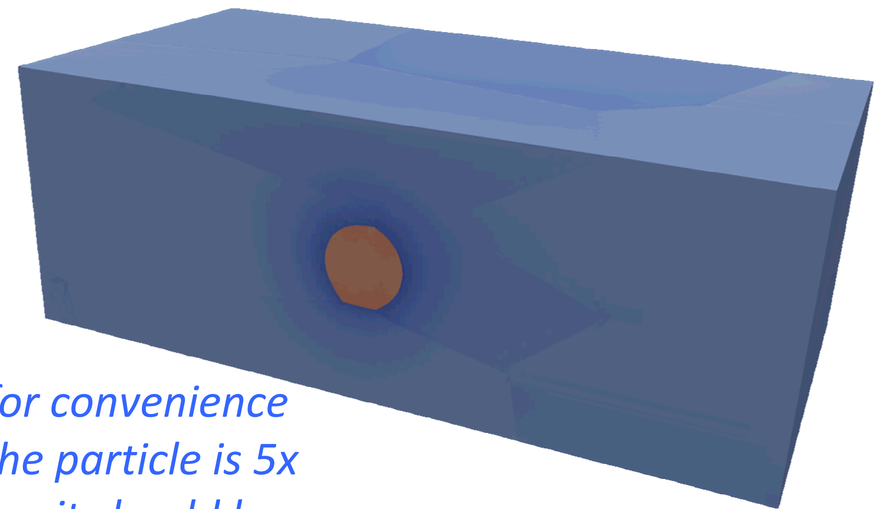
Inclusion Material Model



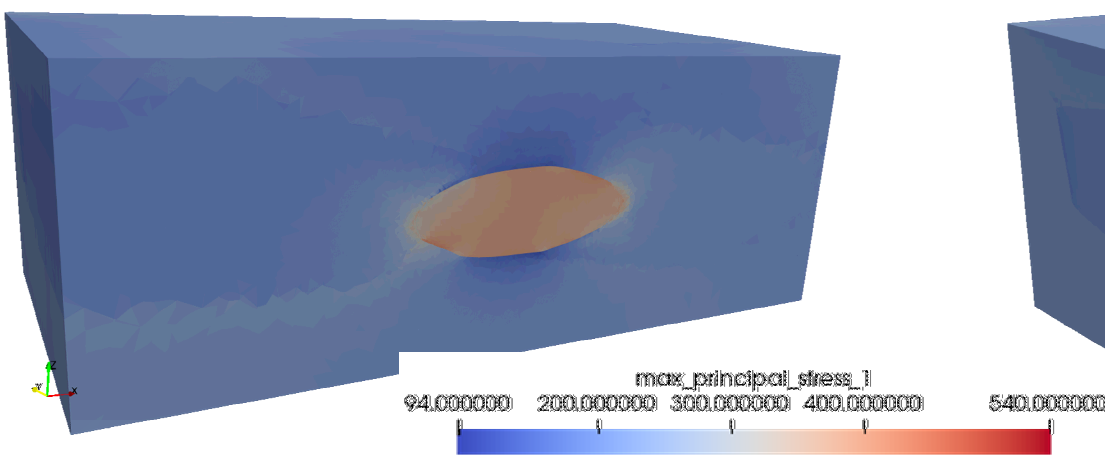
Computed stress in the particle

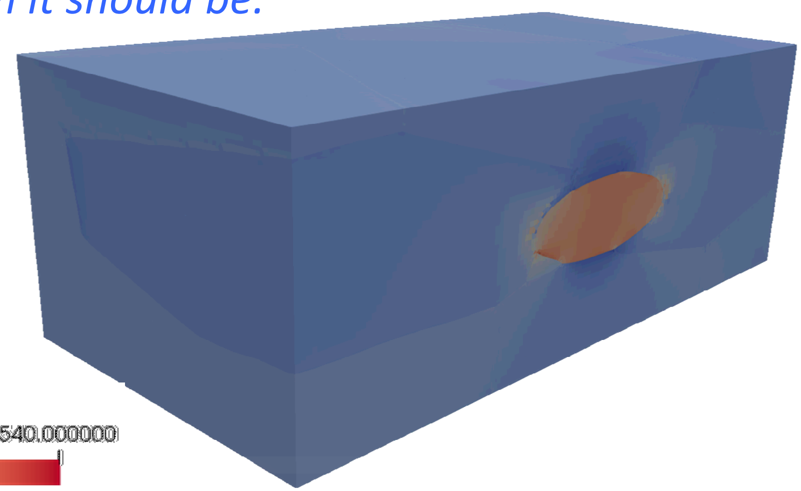
We sculpted the mesh and we overlayed tets on a mesh with the sculpted particle



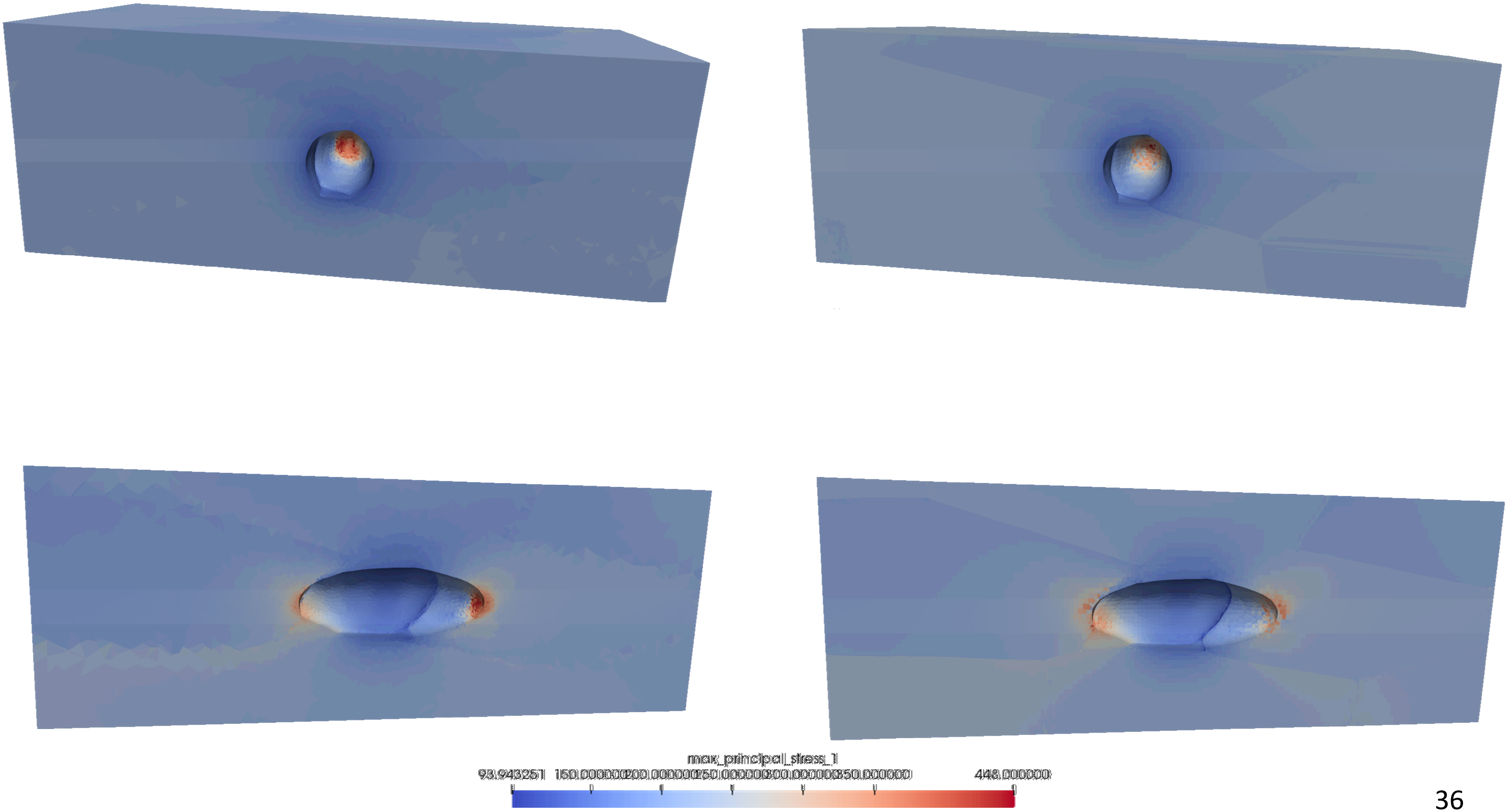


Caveat: for convenience (sculpt) the particle is 5x larger than it should be.





Computed stress nearby the particle



Computed stress in the particle