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Forward Propagation of Random Microstructural Features for Reliability Estimates of Engineering Structures

TMS 2018 Fracture: 65 Years after the Weibull Distribution and the Williams Singularity

Tuesday March 13, 2018

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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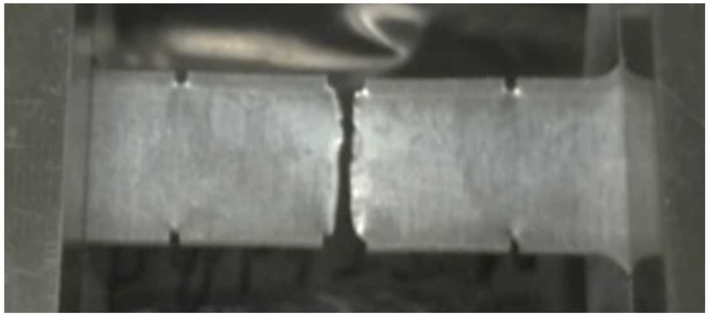
outline

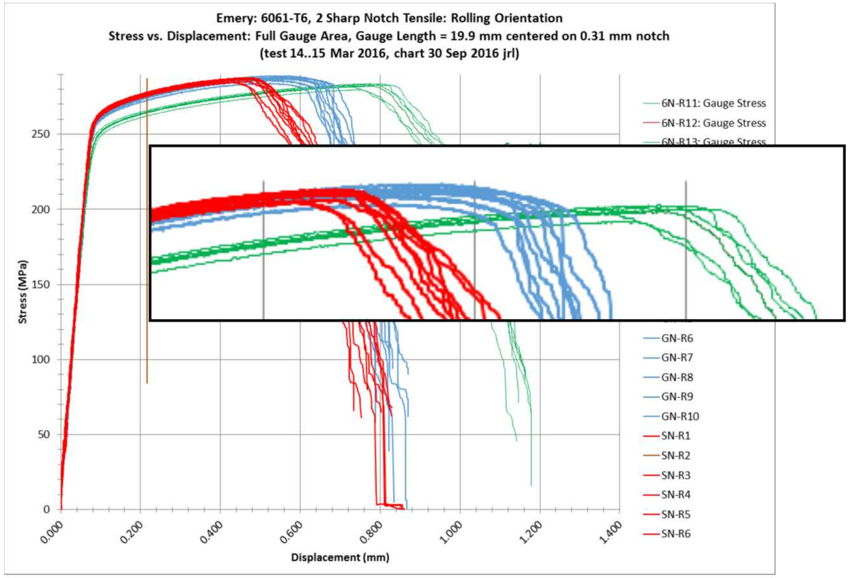
- Motivation: Why do multiscale? For uncertainty propagation
- Probability model for crystallographic orientation/texture
- Example 1: Load in a brittle inclusion within small polycrystal
  - Excursion – implications of meshing decisions
- Reduced-order model for texture
  - Example 2: Exploring RFROM w/ simple cubic-elastic plate
  - Example 1 revisited w/ RFROM
- Example 3: Coupled, multiscale analysis
- Summary

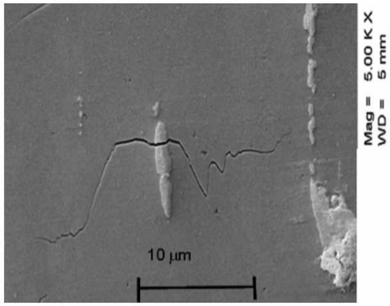
Multiscale In Situ Electron Microscopy Investigation of Deformation in Al 6061. Josh Kacher, Yung Suk Yoo, John Emery, Jay Carroll. Wednesday 3/14 2PM Rm 101C

Why do multiscale simulation? One reason: because structural reliability is dependent on ***random*** microstructure (among other sources of randomness).

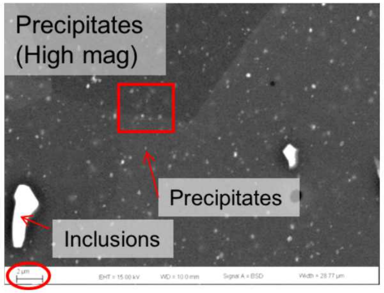


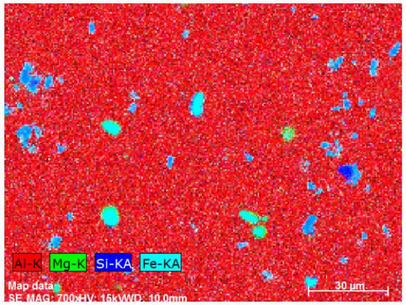
Engineering length scale (millimeters)

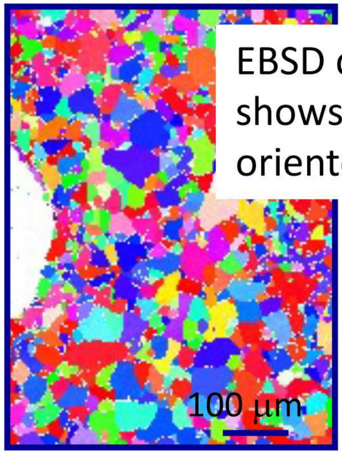




brittle particle







EBSD data shows randomly oriented grains

- Fine precipitates of Fe (~1 μm) throughout
- Larger inclusions of Mg_2Si and of Fe on the scale of 10 μm.

Microstructural length scale (μm)

randomly distributed brittle particles embedded in randomly oriented, anisotropic matrix

One multiscale calculation is necessary but not sufficient

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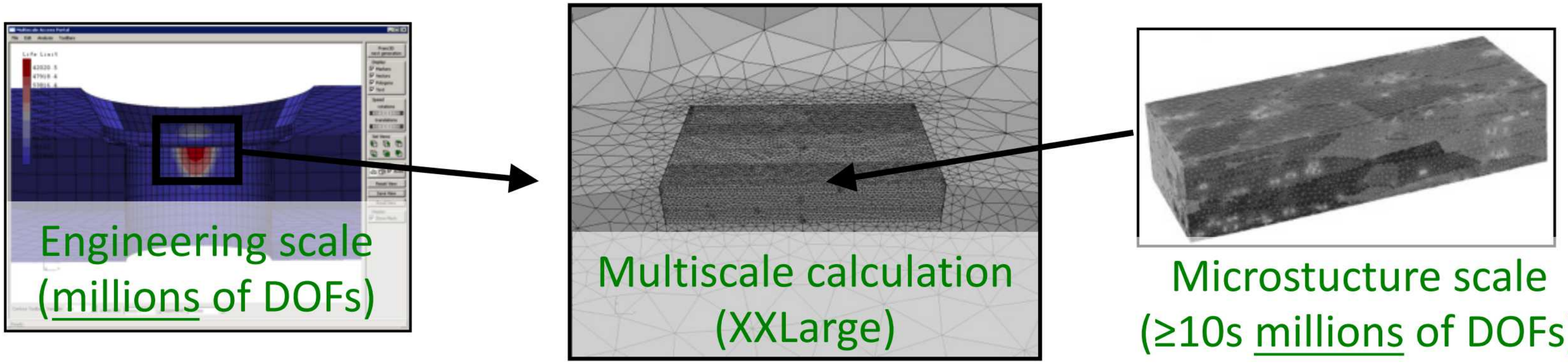
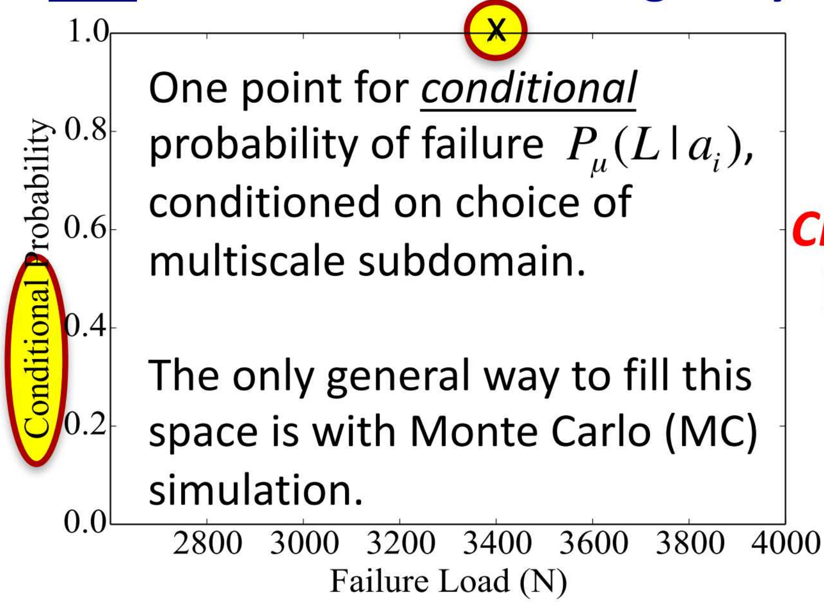


One multiscale calculation gives you this:

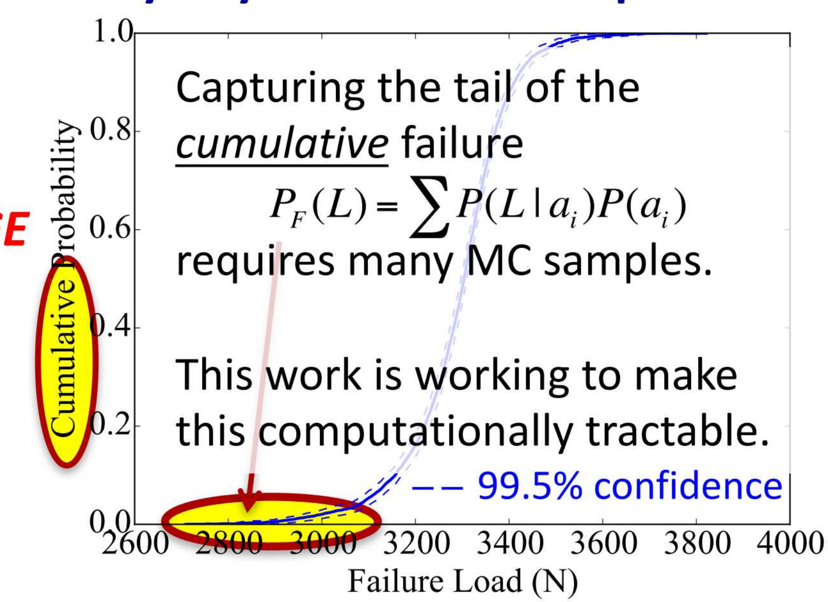


One point for *conditional* probability of failure $P_\mu(L \mid a_i)$, conditioned on choice of multiscale subdomain.

The only general way to fill this space is with Monte Carlo (MC) simulation.

OUR CHALLENGE

But you you'd like to compute this:



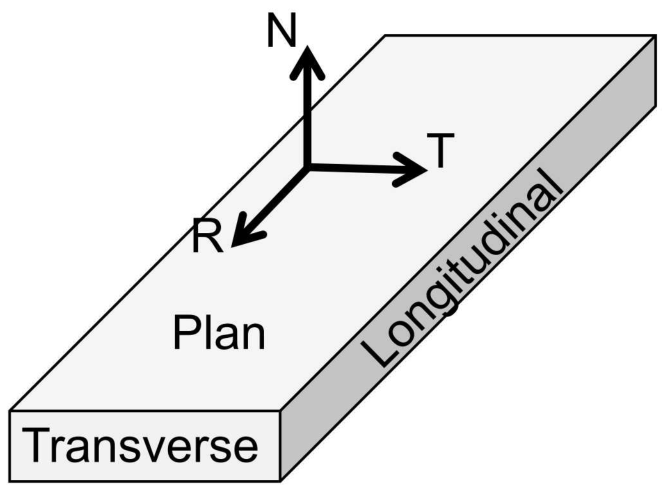
Capturing the tail of the *cumulative* failure

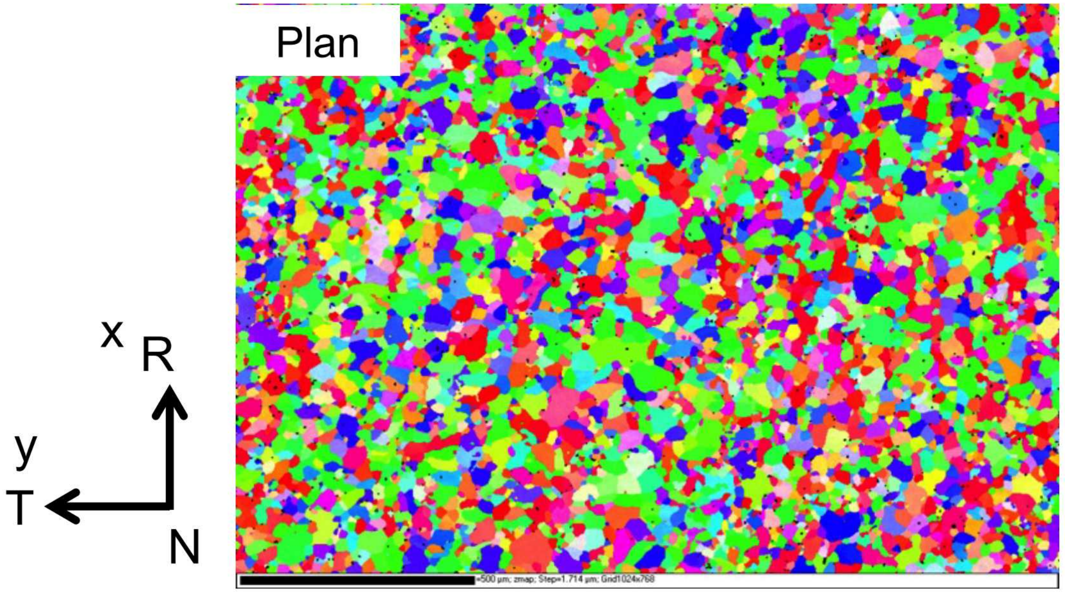
$$P_F(L) = \sum P(L \mid a_i) P(a_i)$$

requires many MC samples.

This work is working to make this computationally tractable.

AA6061-T6 EBSD on three planes shows pancake-shaped grains with mild texture



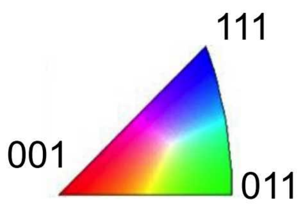


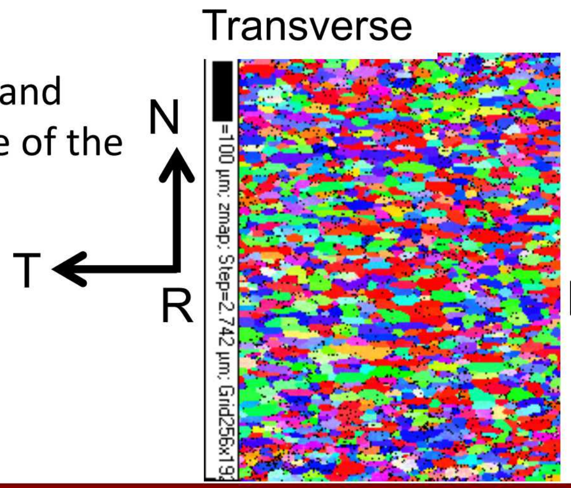
From Ghahremaninezhad & Ravi-Chandar, and confirmed for our material, mean grain size of the rolled 6061 microstructure:

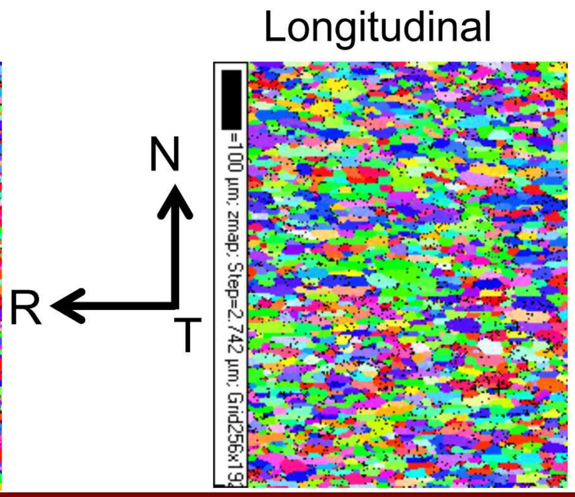
y-z mean 15 um

x-z mean 14 um

x-y mean 39 um







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Random Field Model for Texture

- Why? A probability model describing texture will be convenient, *e.g.*, for model reduction, rapid sampling etc.
- Let $\boldsymbol{\Theta}(\mathbf{x}) = (\Theta_1(\mathbf{x}), \Theta_2(\mathbf{x}), \Theta_3(\mathbf{x}))'$, $\mathbf{x} \in D \subset \mathbb{R}^3$, be a vector-valued random field model for the 3 Euler angles
- Following Arwade and Grigoriu (JEM 2004), model form

$$\boldsymbol{\Theta}(\mathbf{x}) = \boldsymbol{\mu} + \mathbf{a}\,\mathbf{Y}(\mathbf{x}) = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix} + \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix} \mathbf{Y}(\mathbf{x})$$

$$Y_k(\mathbf{x}) = h_k(G_k(\mathbf{x})) = F_k^{-1} \circ \Phi(G_k(\mathbf{x})),\ k = 1, 2, 3$$

$$\mathrm{E}[G_k(\mathbf{u})\, G_l(\mathbf{v})] = \rho_{kl}(\mathbf{u}, \mathbf{v})$$

  - μ_k and σ_k are the mean and standard deviations of Θ_k
  - F_k is related to the marginal CDF of Θ_k
  - $\boldsymbol{G} = (G_1, G_2, G_3)'$ is a vector-valued Gaussian random field with zero mean, unit variance, and correlation functions $\{ \rho_{kl} \}$

I’ll look at it, but I can’t today. My first question is this…how do you define the SROM? Let

T(x) = h[G(x)]

be a translation random field, where G is a homogeneous Gaussian random field, and h is a nonlinear mapping that is independent of x. G(x) is modeled as a Fourier series with random coefficients:

G(x) = \sum_{k=1}^r s_k (A_k sin(w_k x) + B_k cos(w_k x))

where A_k, B_k are correlated Gaussian random variables with zero mean and unit variance, and s_k, w_k are some constants.

Now we have talked and thought about the SROM for random fields in two ways:

(1) Define SROM w.r.t. T, that is, produce samples of a random field T_1(x), T_2(x), …, T_n(x), where n is large, then choose m < n of the samples that minimize the discrepancy between T and its SROM;

(2) Define SROM w.r.t. A and B, that is, produce samples of random vector (A_1, B_1), (A_2, B_2), …, (A_n, B_n), where n is large, then choose m < n of the samples that minimize the discrepancy between (A,B) and its SROM.

Are we using option (1) or (2) here? I’m cc’ing Brian so that he can chime in, too. Thanks.

Random Field Model – Calibration

1. Estimate mean and standard deviation functions, μ and **a**
2. Define spatial correlation functions
   - Can map correlation of G to correlation of Θ
   - Functional form: exponential or linear decay
     - Homogeneous, isotropic
     - Parameter estimates using least-squares, or user-specified
3. Select marginal distribution functions
   - Choose a functional form
     - Carefully to be consistent with physics
     - Beta distribution is a good choice
     - Parameter estimates using Method of Maximum Likelihood
   - Empirically-based
     - Requires a medium sized data set

Capturing spatial correlation

- A measure of the (average) linear dependence between two points in the field
  - Auto correlation function of Θ_1

    $$\mathrm{E}[\Theta_1(\mathbf{u})\Theta_1(\mathbf{v})]$$

  - Cross correlation between Θ_1 and Θ_2

    $$\mathrm{E}[\Theta_1(\mathbf{u})\Theta_2(\mathbf{v})]$$

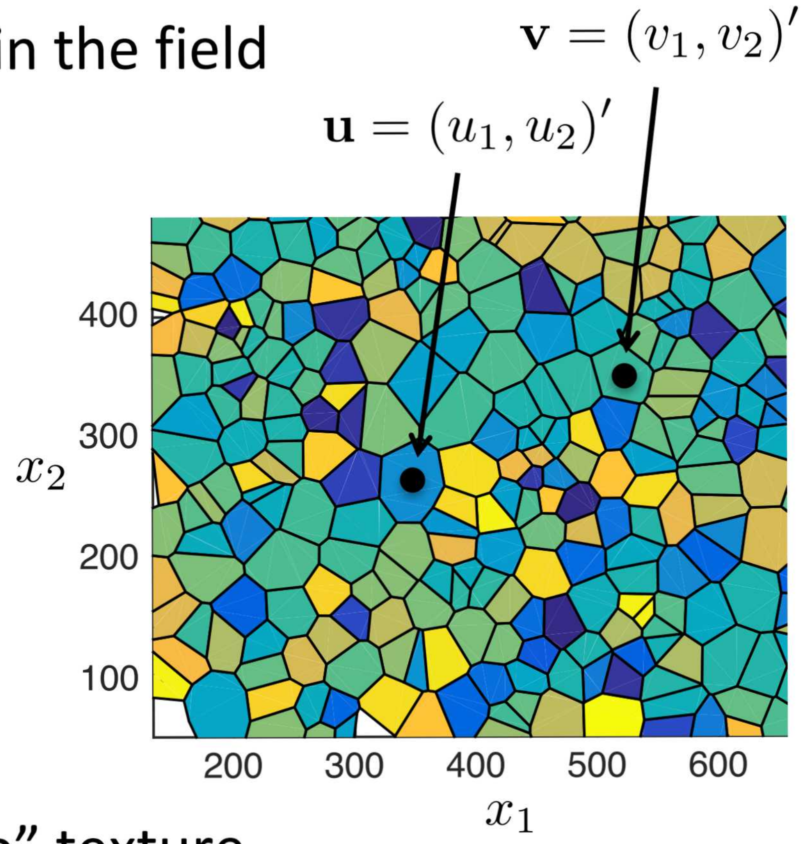
- Assumptions:
  - Statistically homogeneous

    $$\text{Depends on } (\mathbf{u}-\mathbf{v})$$

  - Statistically isotropic

    $$\text{Depends on } \|\mathbf{u}-\mathbf{v}\|$$

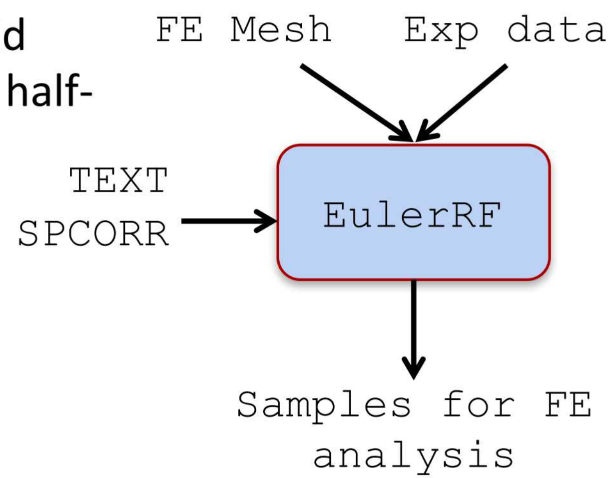
- Provides one way to model "micro" texture

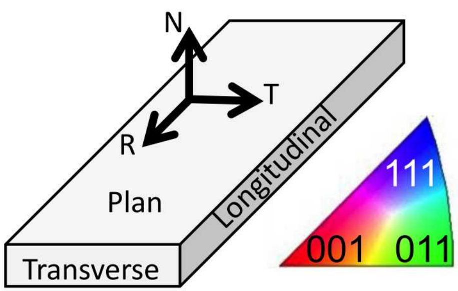


$$\xi_{kl}(\mathbf{u},\mathbf{v}) = \xi_{kl}(||\mathbf{u}-\mathbf{v}||) = \frac{\mathrm{Cov}(\Theta_k(\mathbf{u}),\Theta_l(\mathbf{v}))}{\sigma_k\sigma_l} \approx \xi(\eta) = \gamma_{kl}e^{-\alpha_{kl}\eta}, \quad k,l = 1,2,3$$

“EulerRF” Code

- Code to generate samples of Euler angle random field model for FE meshes, implemented in MATLAB (and half-way there with python implementation)
- Input:
  - Finite element mesh (grain geometry)
  - Texture data (EBSD data – AA6061 below)
  - User options for texture model
- Output: samples of no texture, macro- and micro-texture





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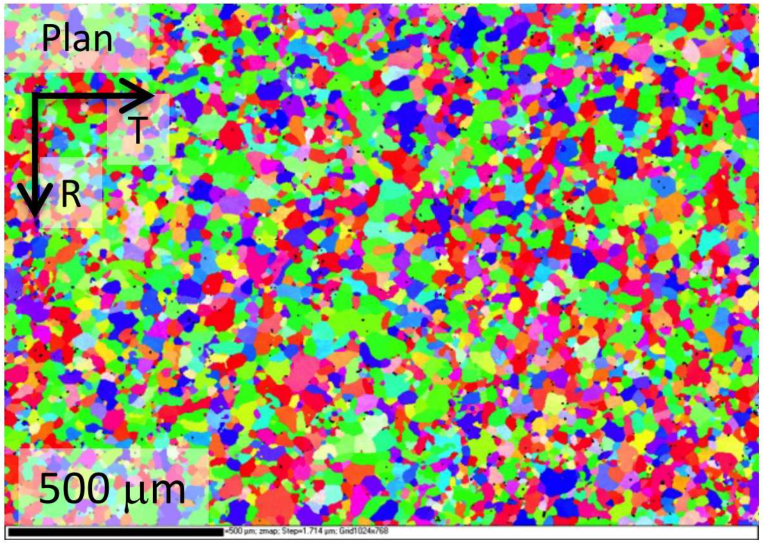
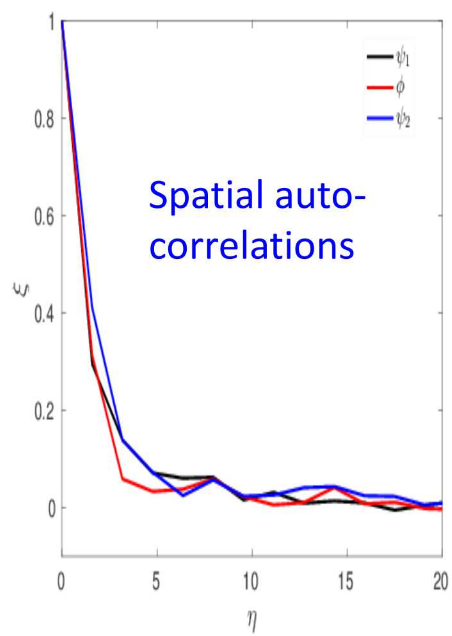
y-z mean 15 μm
x-z mean 14 μm
x-y mean 39 μm

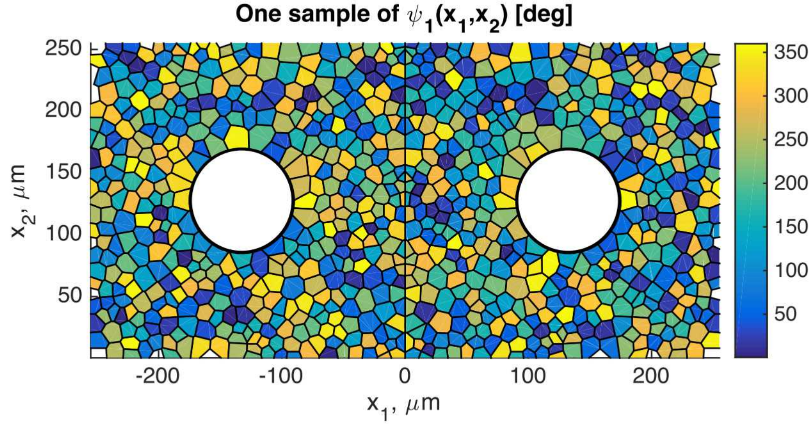


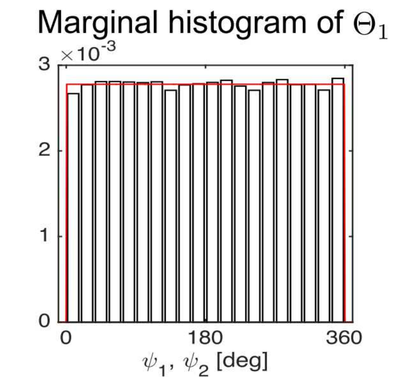
AA6061 T6 rolled plate



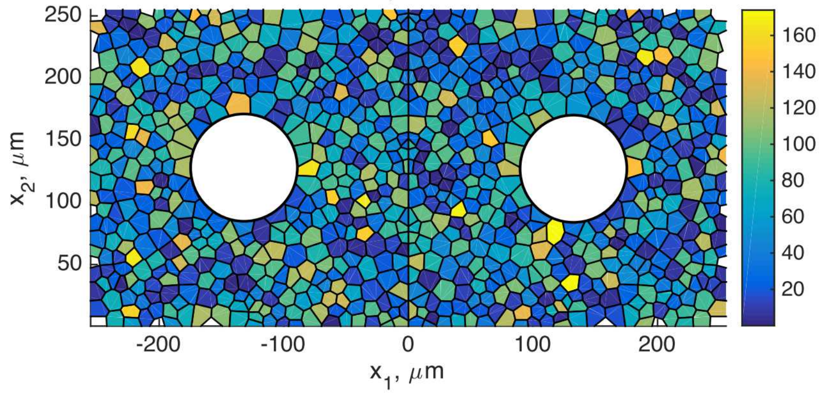
2D example from EulerRF

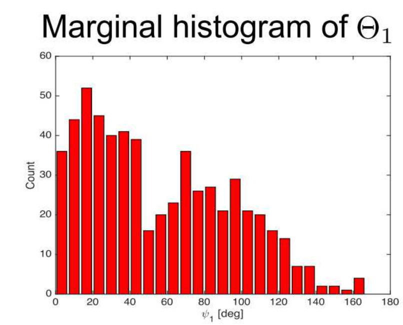
Zero texture, zero spatial correlation





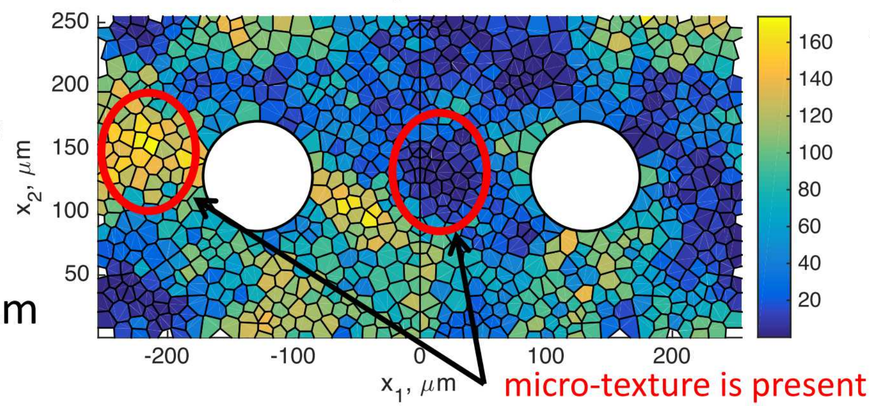
With macro-texture based on data file, zero spatial correlation

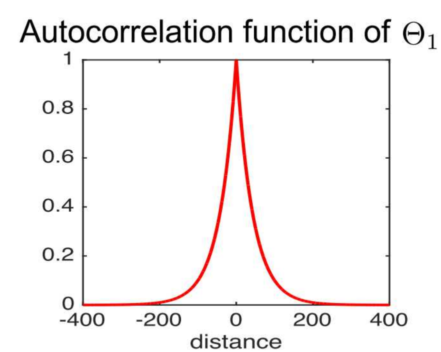




With micro-texture, *i.e*, including spatial correlation

- Texture based on data file
- Isotropic (exponential) spatial correlation with correlation length = 200 μm

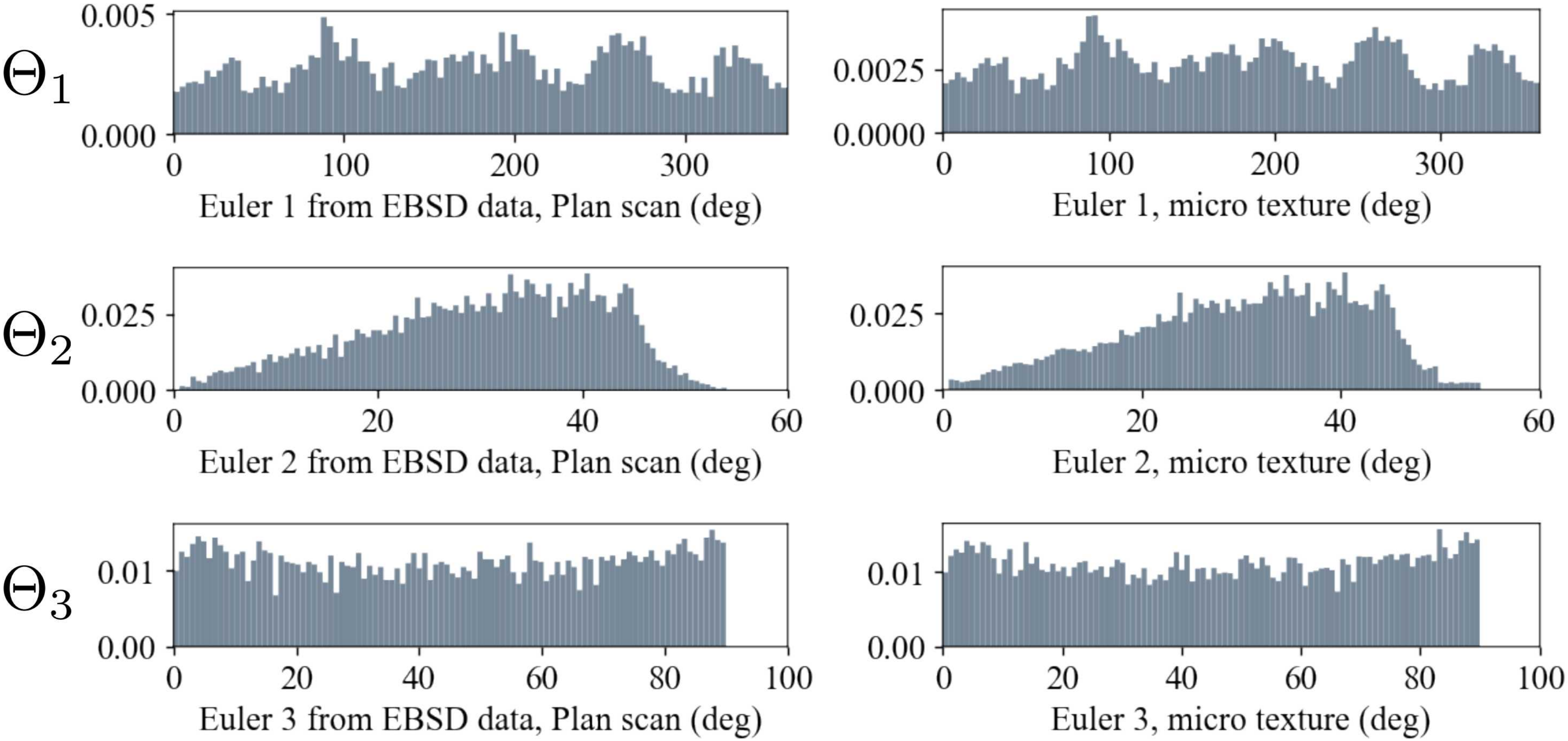




*** EBSD data for Ta wire*

Comparing texture – measured vs. model

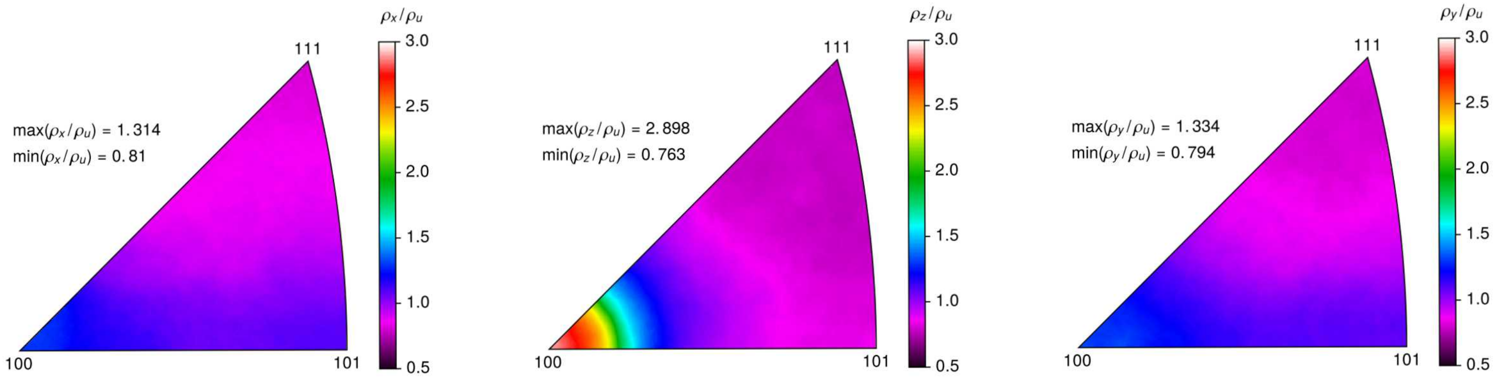
measured EBSD data | model data



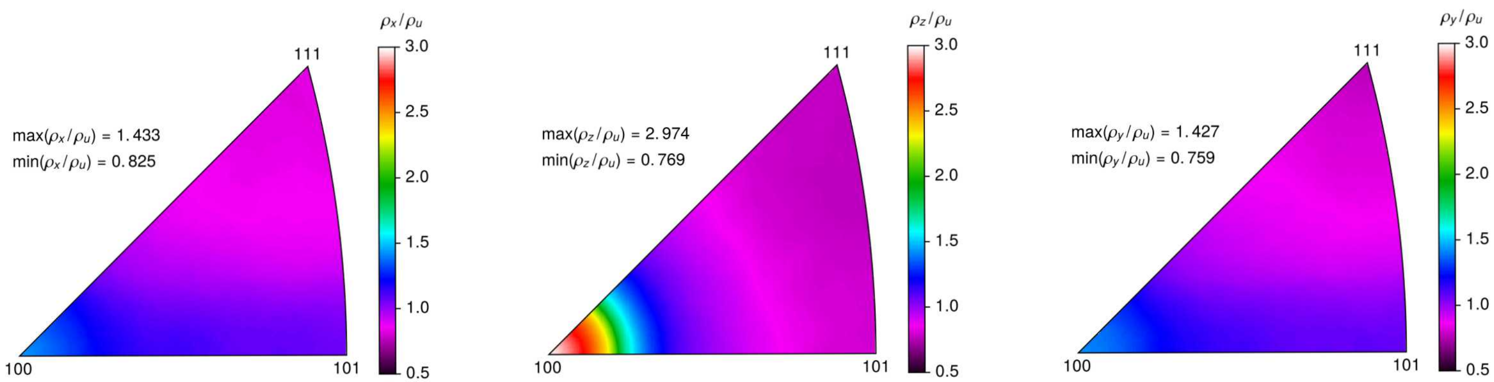
- Histograms drawn for the individual Euler angles

Inverse pole figure (IPF) comparing EBSD to eulerRF samples

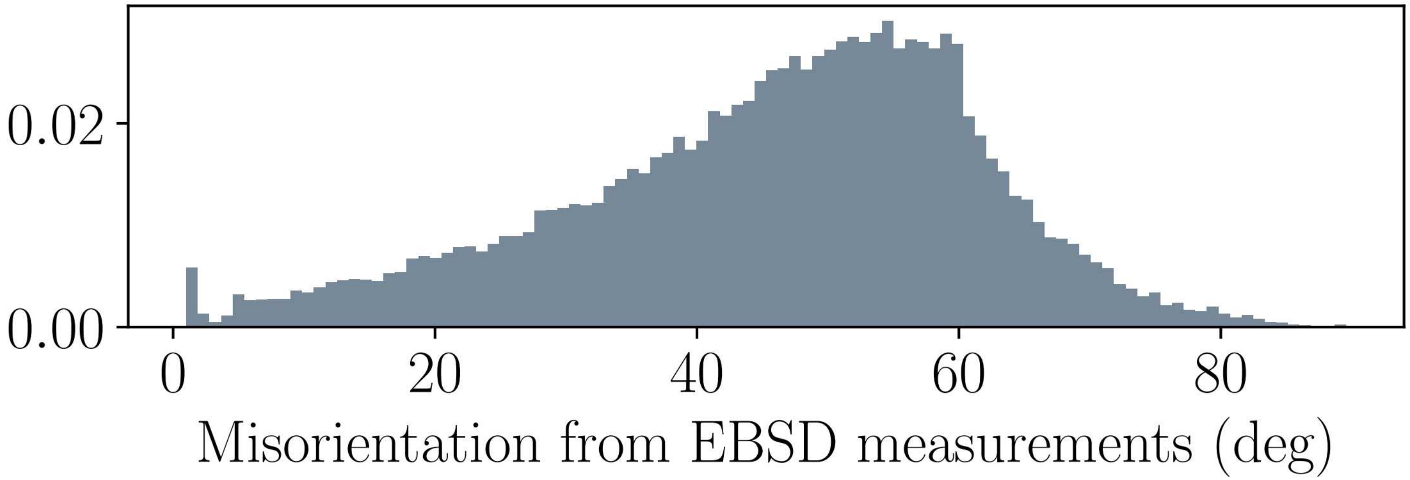
measured EBSD data

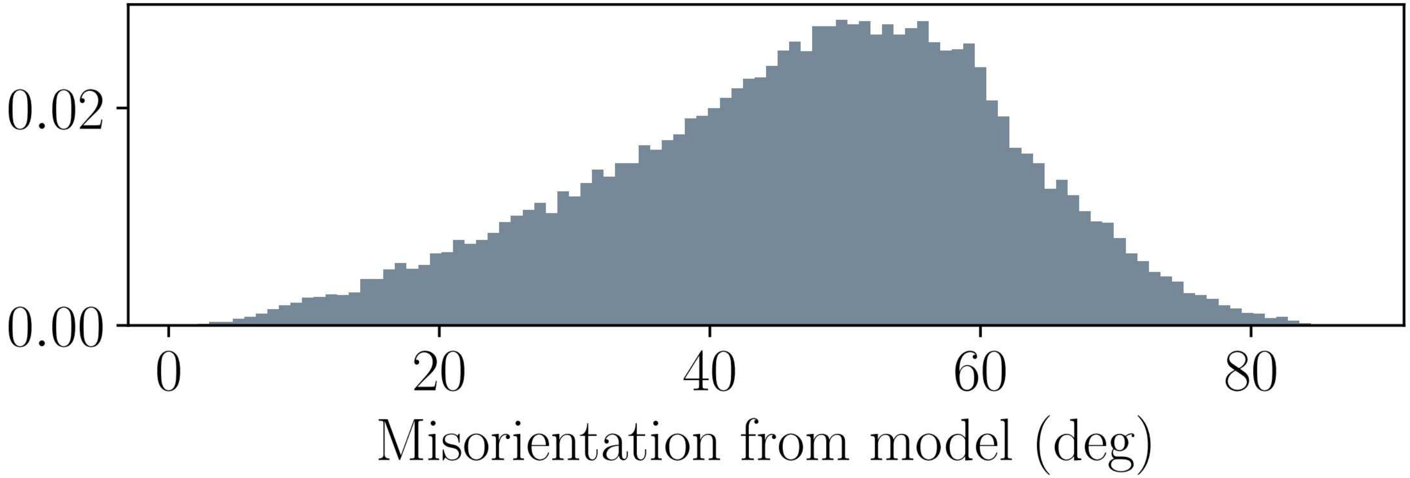


model



Misorientation $\Theta_{mis} = min \left| arccos\left(\frac{tr(g_B g_A^{-1} O) - 1}{2}\right) \right|$





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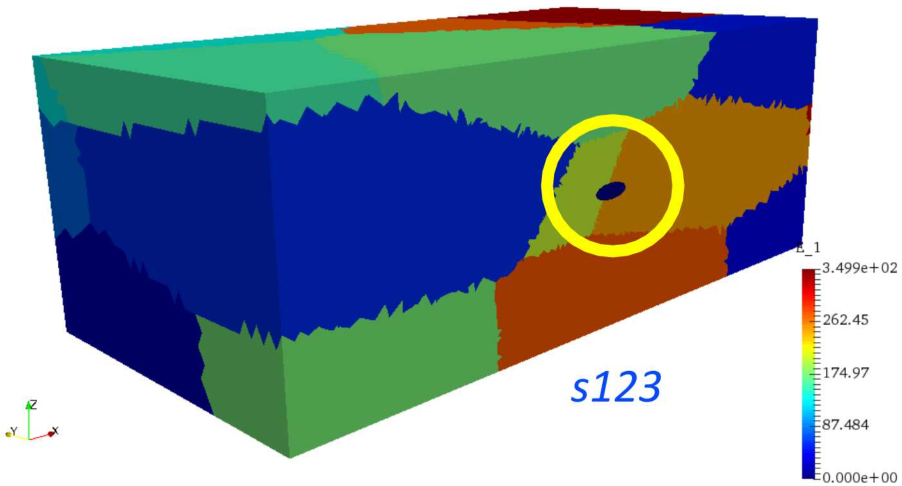
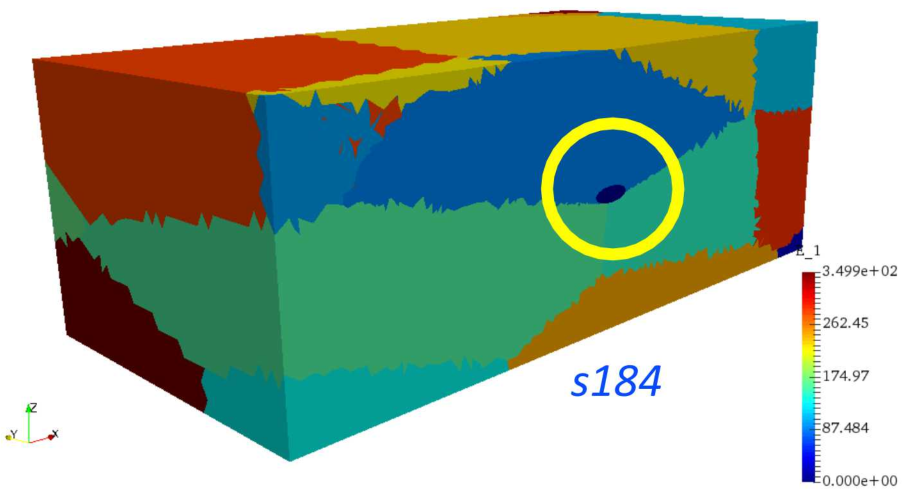
A small polycrystal with brittle inclusion

- AA6061 T6 rolled plate
- Embed an ellipsoidal particle, 5 x 1.8 μm
- Coherent, geometry-obeying mesh at particle/matrix interface, overlay geometry otherwise
- 2 morphologies w/ ~27 grains, s123 & s184
- 200 samples of macro-texture & 55 samples of micro-texture
- Assumed elastic mechanical properties for particle (pure iron)
  - E = 211 GPa, ν = 0.29
  - Strength 540 MPa
- Assumed perfect and rigid particle/matrix interface bond





Cross-sections through major-axis of ellipsoid

Crystal plasticity formulation

- A simple crystal plasticity formulation (Matous and Maniatty 2004):

$$\mathbf{L}^p = \sum_{\alpha=1}^{12} \dot{\gamma}^\alpha \, \mathbf{P}^\alpha$$

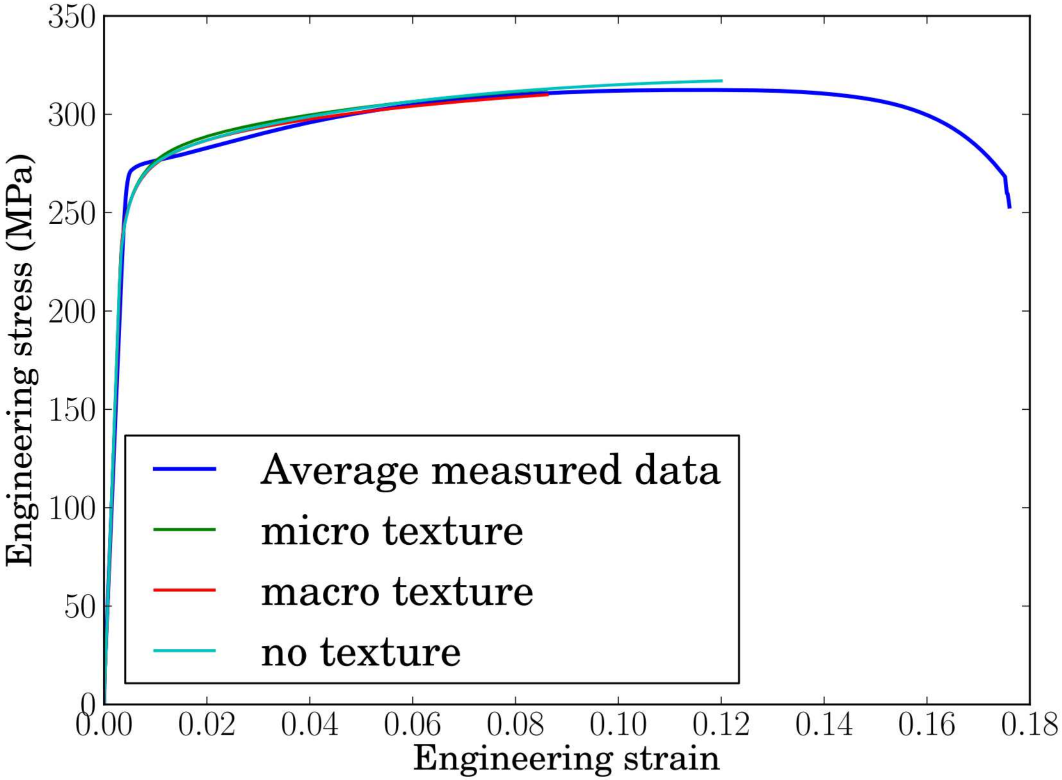
$$\mathbf{P}^\alpha = \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha$$

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{g^\alpha} \right|^{1/m} \operatorname{sign}(\tau^\alpha)$$

$$\dot{g} = G_0 \left(\frac{g_{s_0} - g}{g_{s_0} - g_0} \right) \dot{\gamma}$$

$$\dot{\gamma} = \sum_{\alpha=1}^{12} |\dot{\gamma}^\alpha|$$

	no texture	micro texture	macro texture
g_0	110.6	114.0	115.2
g_{s_0}	169.4	172.8	174.7
G_0	116.6	116.6	116.6
m	0.01	0.01	0.01



Watch mean, first-principal stress in the particle

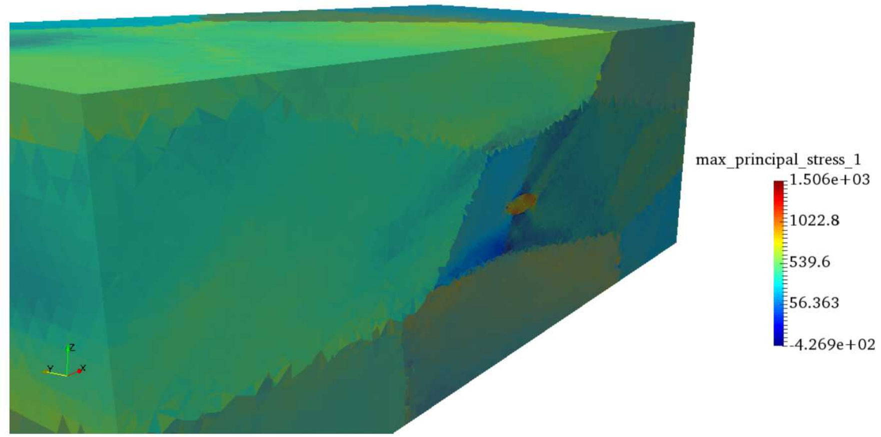
Assuming elastic and brittle, monitor the mean (or max) first-principal stress in the particle.

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

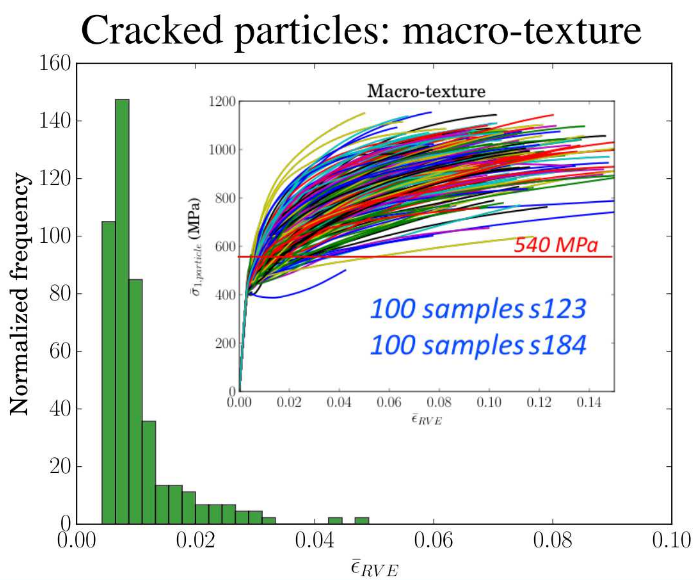
$$S = \{\bar{\epsilon}_{RVE} \in \mathbb{R}^{+} : g(\bar{\epsilon}_{RVE} \leq 0\}$$

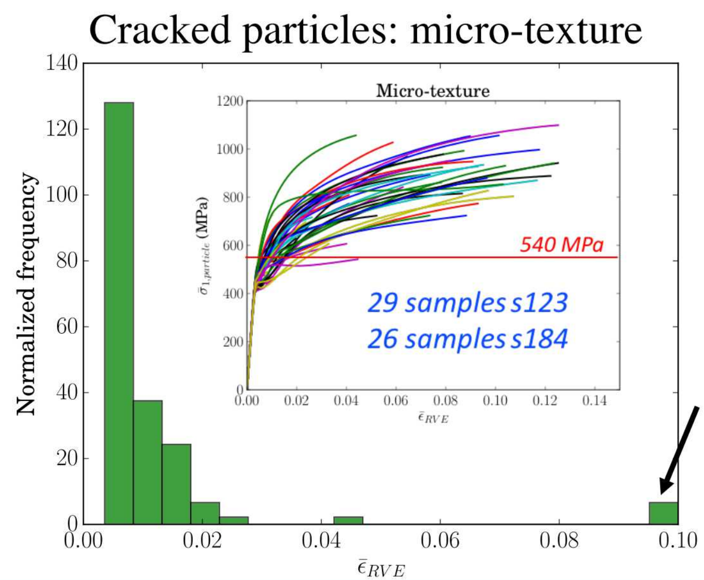
$$g(\bar{\epsilon}_{RVE}) = \bar{\sigma}_{p,cr} - \bar{\sigma}_{p}(\bar{\epsilon}_{RVE})$$

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



Maximum principal stress contour for one sample



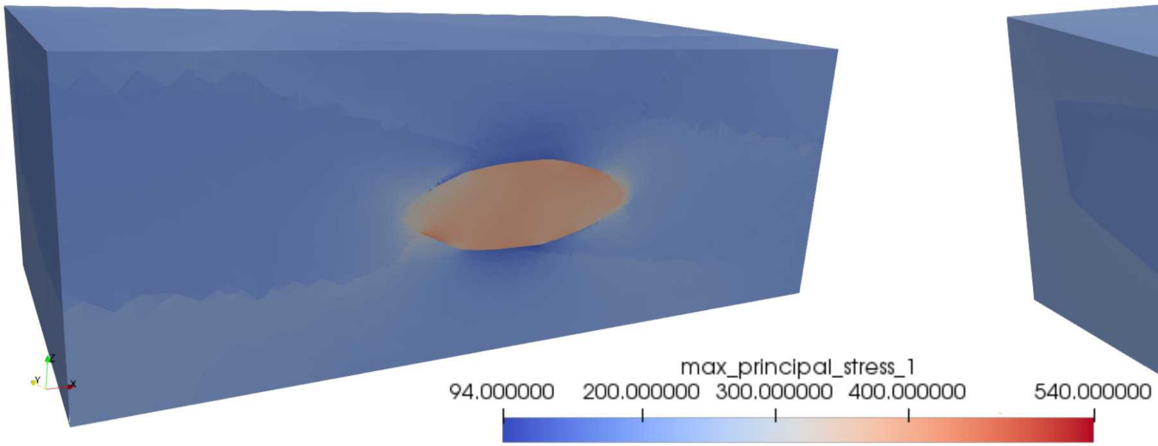


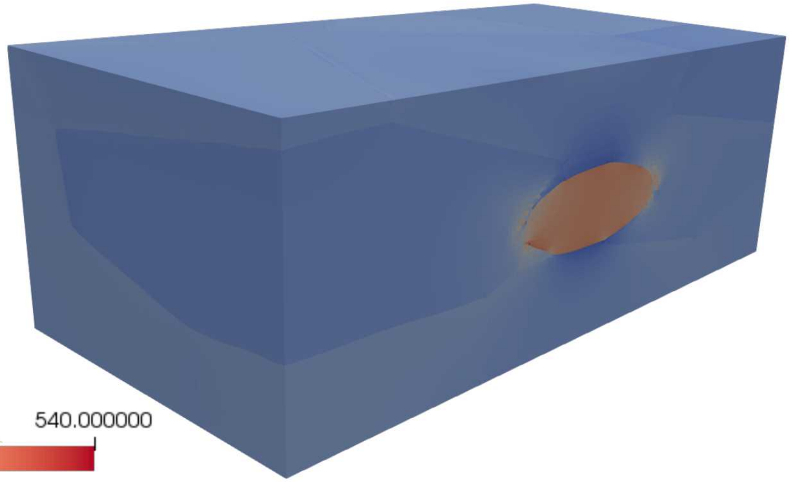
Particles that did not crack within simulated deformation

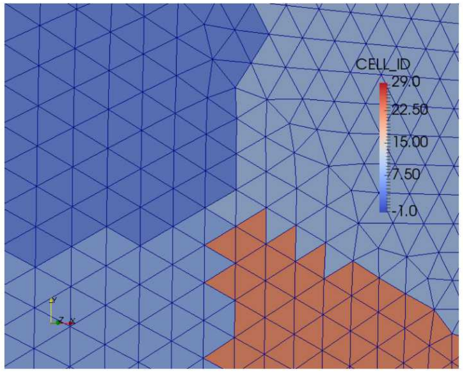
Study treatments of grain boundary

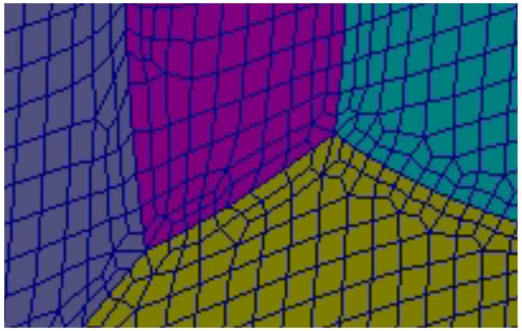
Conformally mesh geometry of particle then overlay grain orientation on existing mesh

Using Sculpt [ref], conform mesh to particle and grain geometry

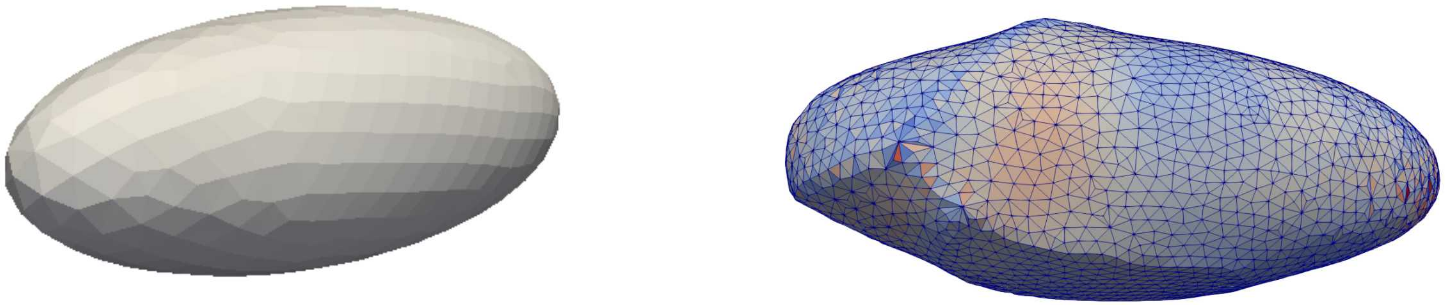






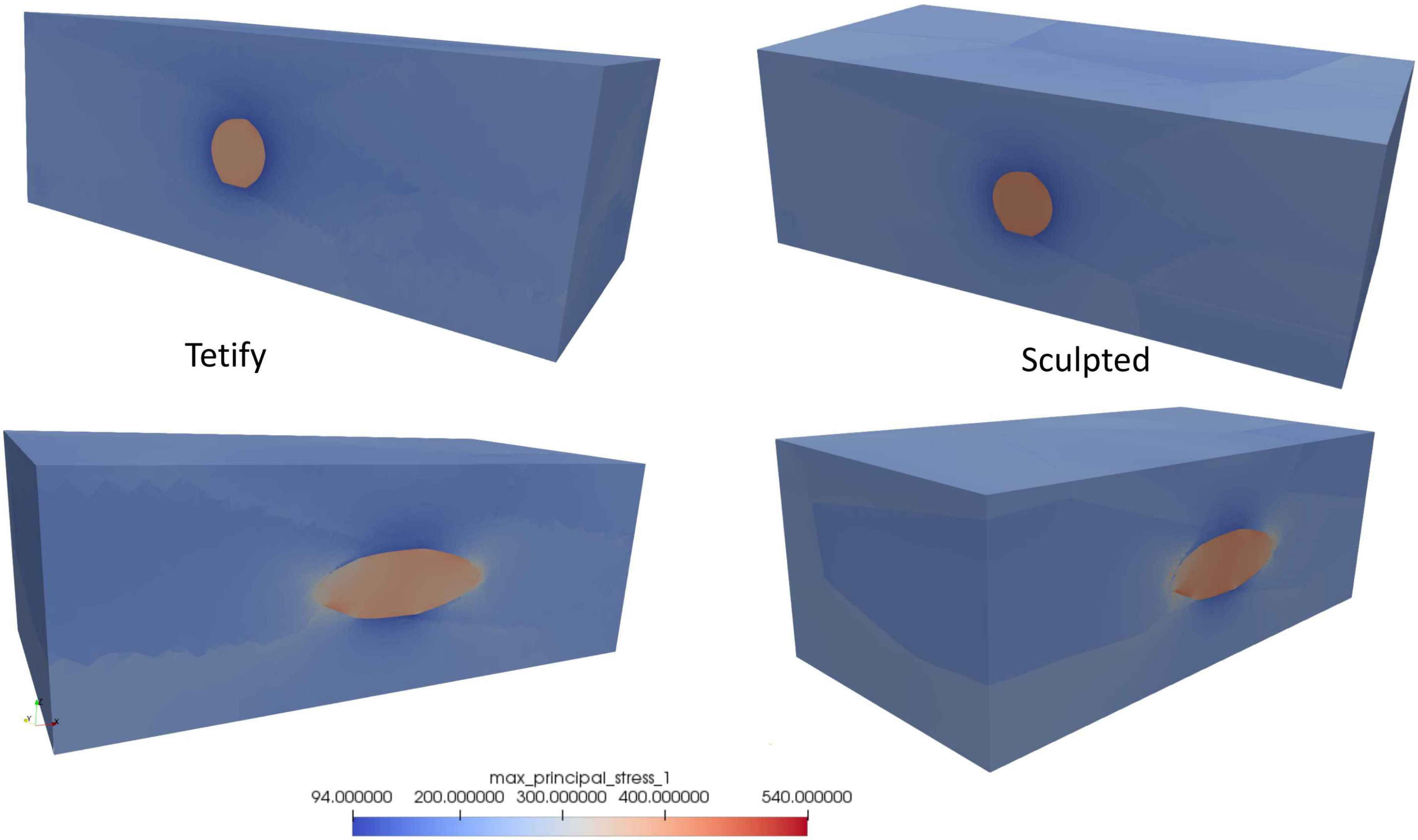


Inclusion geometry differences



- Sculpt [a Cubit tool, Steve Owen] will not precisely adhere to geometry
- Small features (such as inclusion) can be poorly resolved
- Used 5x larger inclusion in following comparison
- For apples-to-apples particle geometry, extract Sculpt inclusion geometry and mesh with overlay tetrahedral elements for comparison

Computed stress in the particle



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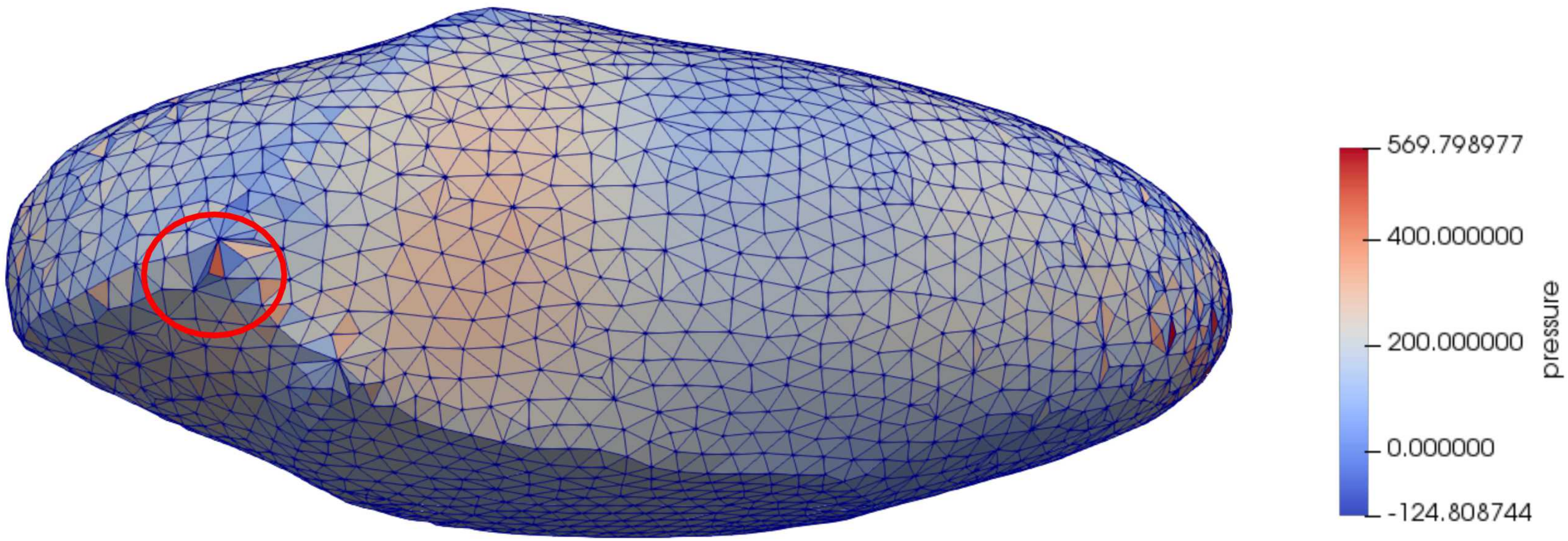
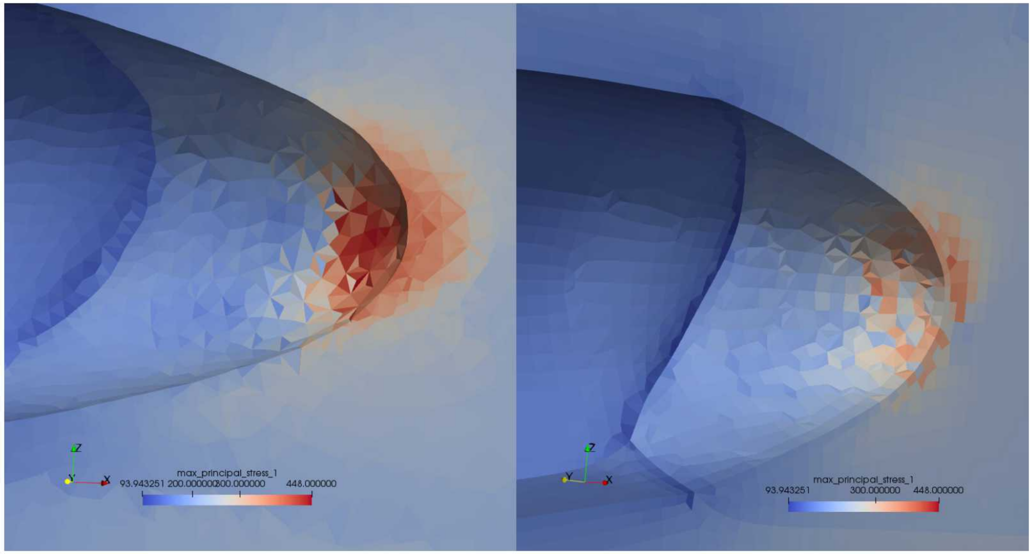
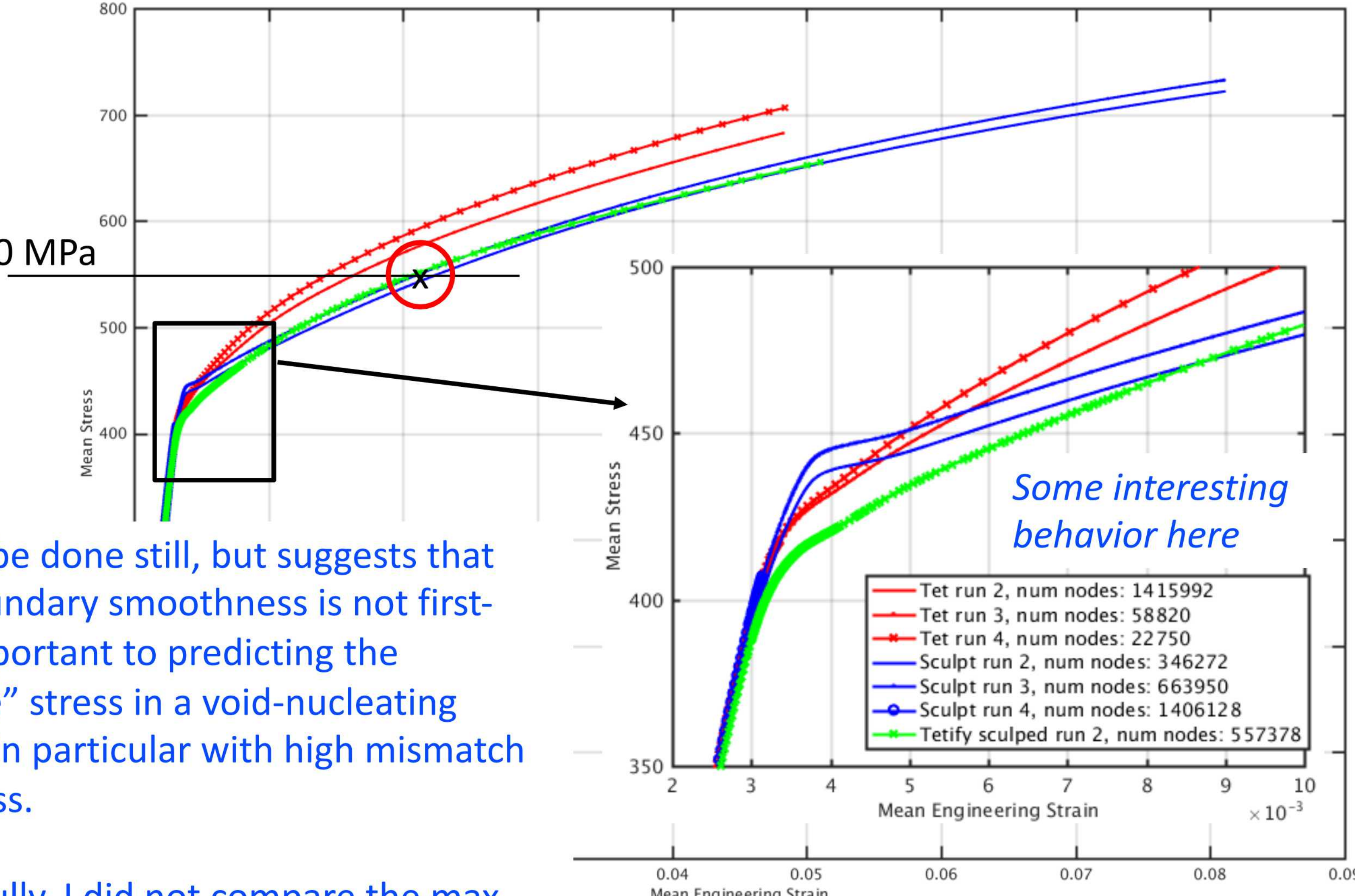




Mean stress in the particle



Some interesting behavior here

Work to be done still, but suggests that grain boundary smoothness is not first-order important to predicting the "ultimate" stress in a void-nucleating particle, in particular with high mismatch in stiffness.

*Regretfully, I did not compare the max stress in the particle.

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Stochastic reduced-order model (SROM)

To develop a model that optimally represents the uncertainty in the input we choose a discrete random variable $\tilde{\boldsymbol{\Theta}}$ (Grigoriu, JCP 2012). The SROM is then defined by the collection $\left(\tilde{\boldsymbol{\theta}}_k, \tilde{p}_k\right)$ k = 1, …, n that minimizes an objective function of the form:

$$\underbrace{\max_{1\le r\le \bar{r}} \max_{1\le s\le d} \alpha_{s,r} |\tilde{\mu}_s(r) - \hat{\mu}_s(r)|}_{\text{moments}} + \underbrace{\max_{x} \max_{1\le s\le d} \beta_s |\tilde{F}_s(x) - \hat{F}_s(x)|}_{\text{cumulative distribution}} + \underbrace{\zeta_{s,t} \max_{s,t} |\tilde{c}(s,t) - \hat{c}(s,t)|}_{\text{correlation}}$$

Estimates of SROM statistics given SROM sample size n

$$\tilde{\mu}_s(r) = \mathrm{E}[\tilde{\Theta}_s^r] = \sum_{k=1}^{n} p_k\,(\tilde{\theta}_{k,s})^r$$

$$\tilde{F}_s(x) = \Pr(\tilde{\Theta}_s \le x) = \sum_{k=1}^{n} p_k\,1(\tilde{\theta}_{k,s} \le x)$$

$$\tilde{c}(s,t) = \mathrm{E}[\tilde{\Theta}_s\,\tilde{\Theta}_t] = \sum_{k=1}^{n} p_k\,\tilde{\theta}_{k,s}\,\tilde{\theta}_{k,t}$$

Estimates of sample statistics given q samples of $\boldsymbol{\Theta}$

$$\hat{\mu}_s(r) = \sum_{i=1}^{q} (1/q)(\theta_{i,s})^r$$

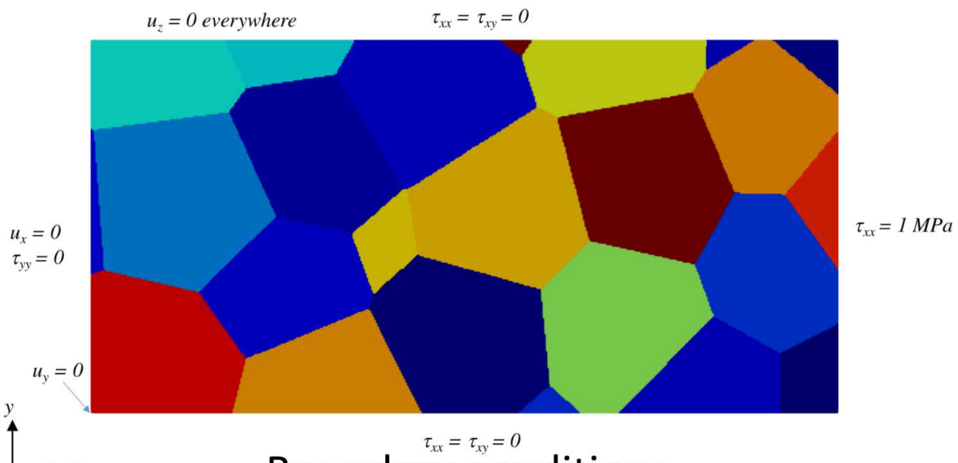
$$\hat{F}_s(x) = \sum_{i=1}^{q} (1/q)1(\theta_{i,s} \le x)$$

$$\hat{c}(s,t) = \sum_{i=1}^{q} (1/q)\theta_{i,s}\,\theta_{i,t}$$

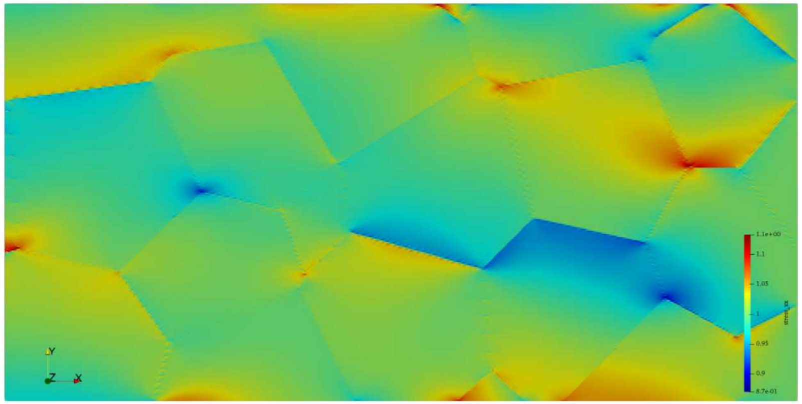
with n << q and $\alpha,\ \beta,\ \zeta > 0$ are weights and subject to probabilities $\tilde{p}_k \ge 0$ and $\sum_k \tilde{p}_k = 1$.

Cubic elasticity in a polycrystal

- Plane strain plate dimensions: 240 µm x 120 µm x 0.5 µm.
- Cubic-elastic pure aluminum; average grain size is approximately 40 µm.
- Voronoi tessellation, so that there are 26 grains in this specimen -- locked morphology.
- Suppose that the plate has stringent design requirements for extension displacement when loaded longitudinally, so developing the probability law for apparent modulus of elasticity E_{app} can be used to quantify failure.
- We generate "truth" data by FE simulation, varying crystallographic orientation using our models and calibrated to our AA6061 T6 EBSD data, with 10,000 instantiations of non-textured, macro-textured and micro-textured crystals.
- We developed a random-field reduced-order model (RFROM) for the textures and here we use them to quantify the apparent modulus of the plate.



Boundary conditions



First principal stress contour

Predicted performance

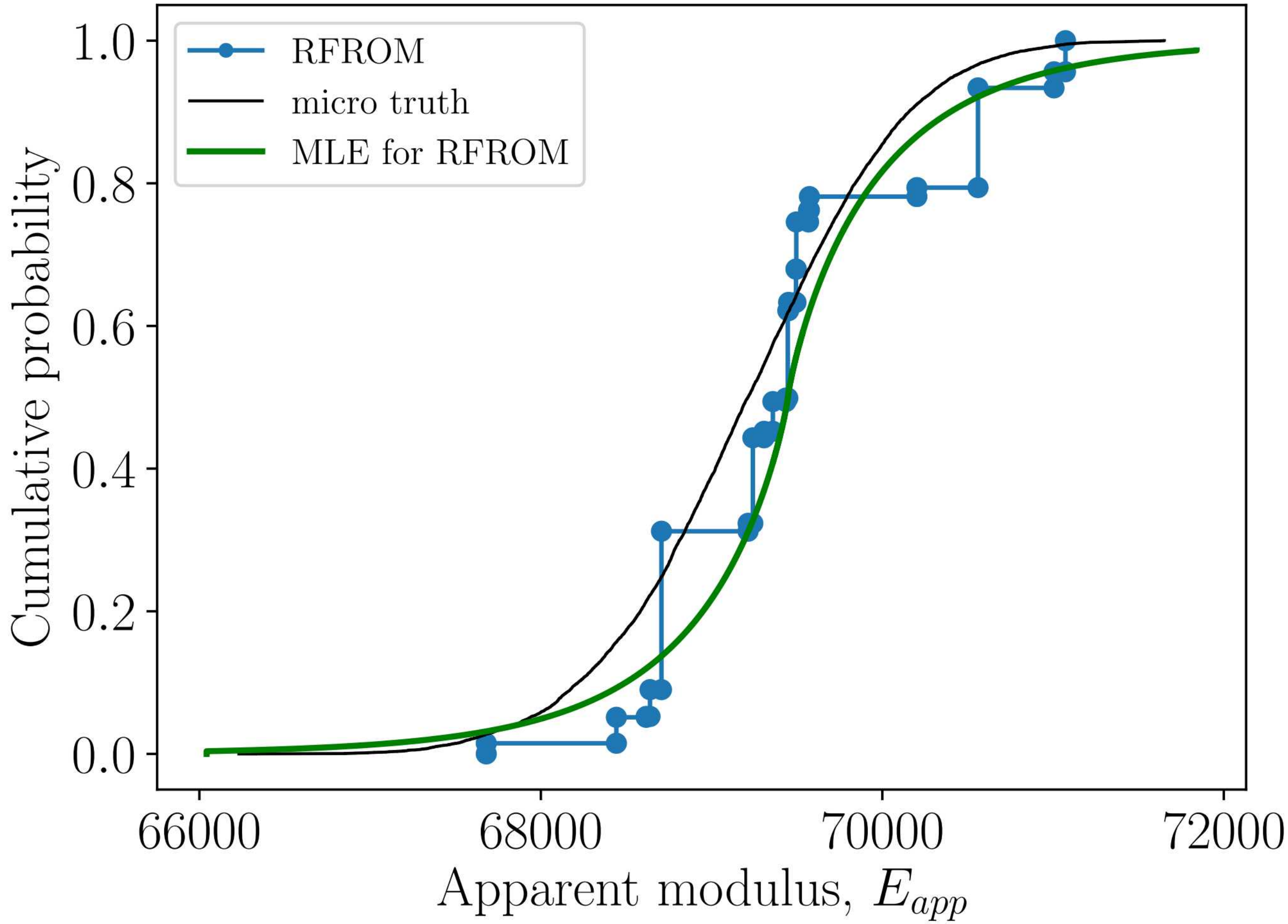
The following plots show the cumulative distribution function for apparent modulus. There are 3 lines plotted:

- RFROM – Plot the CDF estimated from the reduced order model.
- truth – Plot the CDF estimated from the 10,000 truth simulations.
- MLE for RFROM – Estimate the CDF using maximum likelihood estimates with likelihood function constructed as:

$$\mathcal{L} = \prod_{i=1}^{m} \tilde{f}(E_{app}|\theta)^{np_i}$$

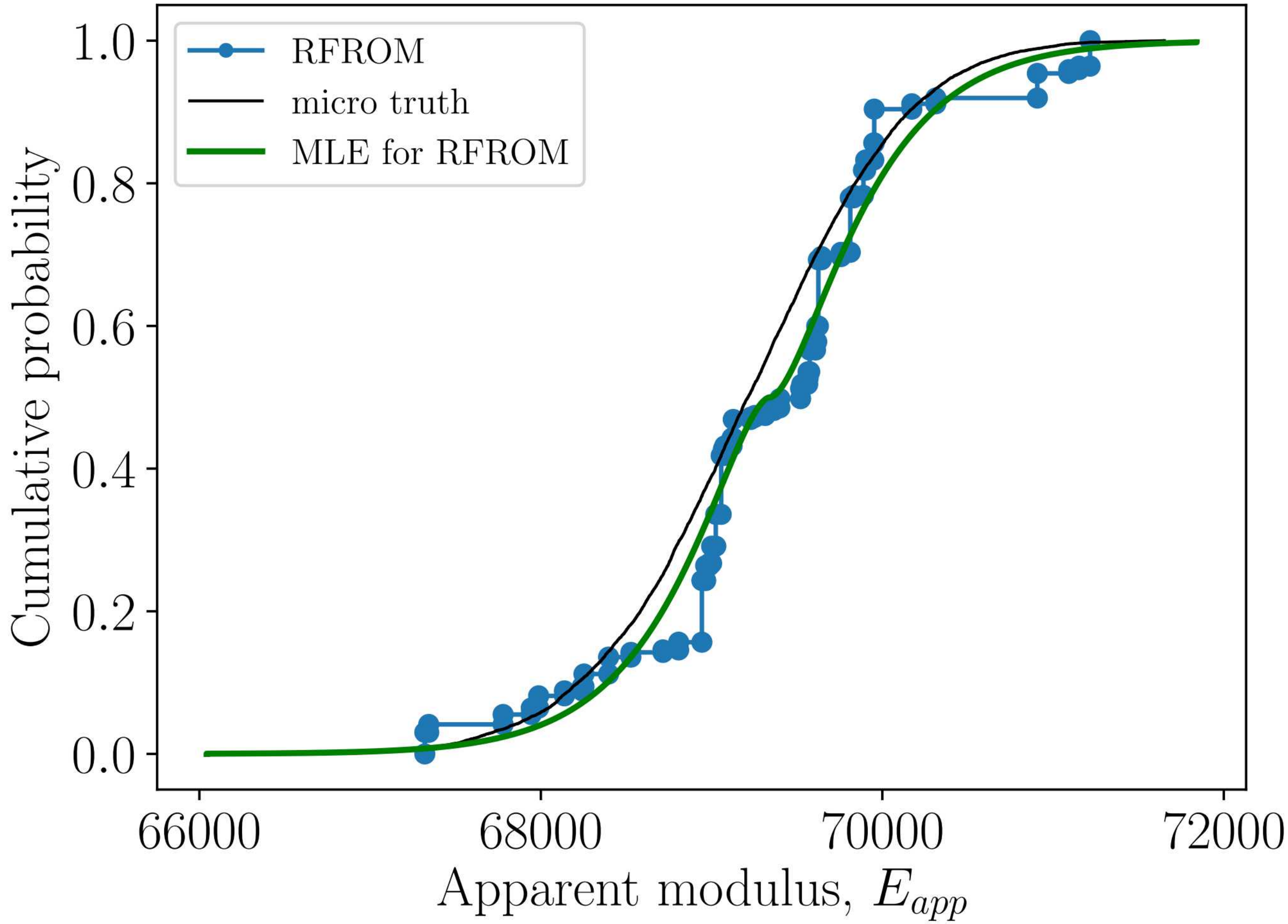
m = RFROM samples
E_{app} = Apparent modulus
$\boldsymbol{\theta}$ = CDF parameters
n = arbitrary integer > 1
p_i = probability of RFROM sample i

Micro texture, RFROM m = 20



**it's not very good, but it's "cheap"*

Micro texture, RFROM m = 50

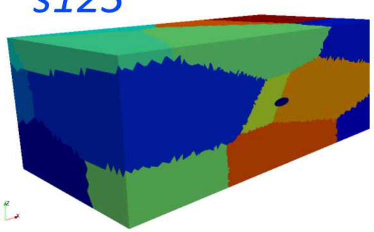


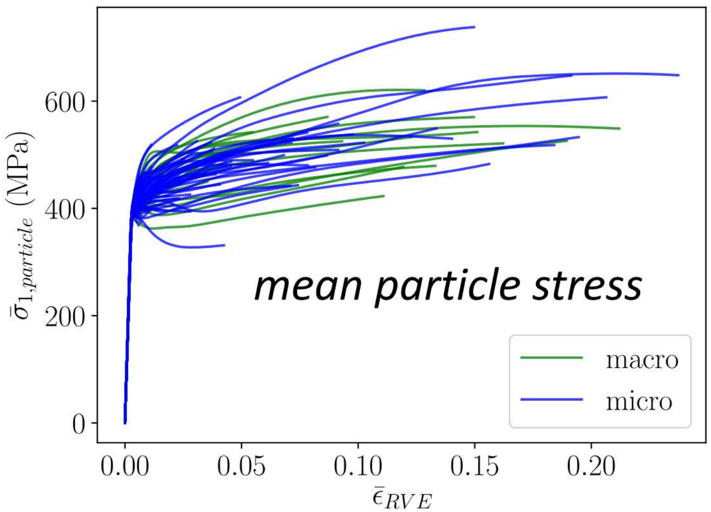
**it's better, and reasonably $$*

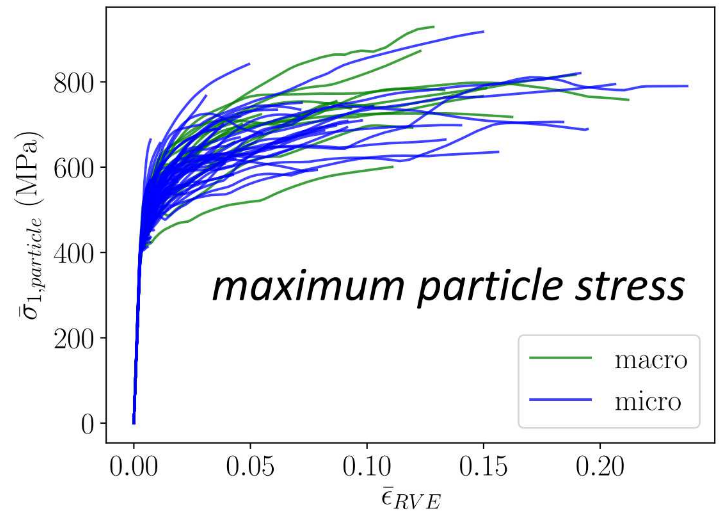
Allow plasticity in our particle w/ SROM m = 20

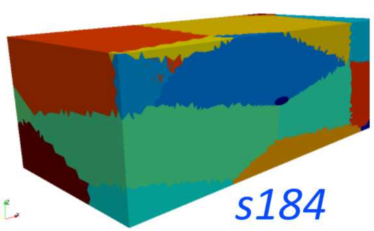
$$\bar{\sigma}(\bar{e}_p) = \sigma_y + A\bar{e}_p^n \quad \sigma_y = 300 \text{ MPa} \quad A = 333 \text{ MPa} \quad n = 0.15$$

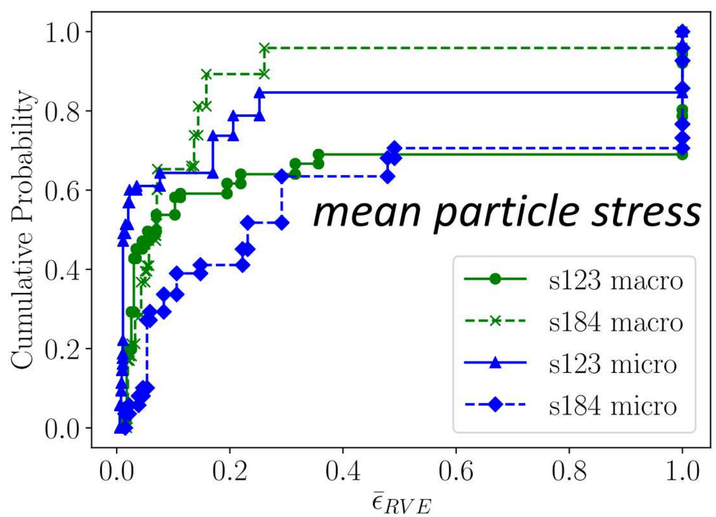
s123

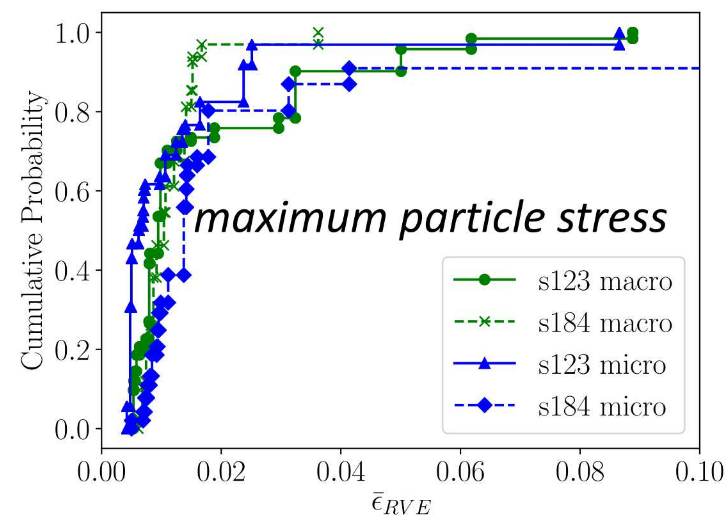












~26 hours on 128, 2.1GHz procs w/4GBRAM

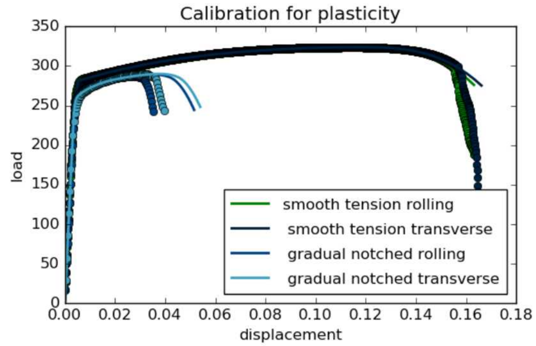
outline

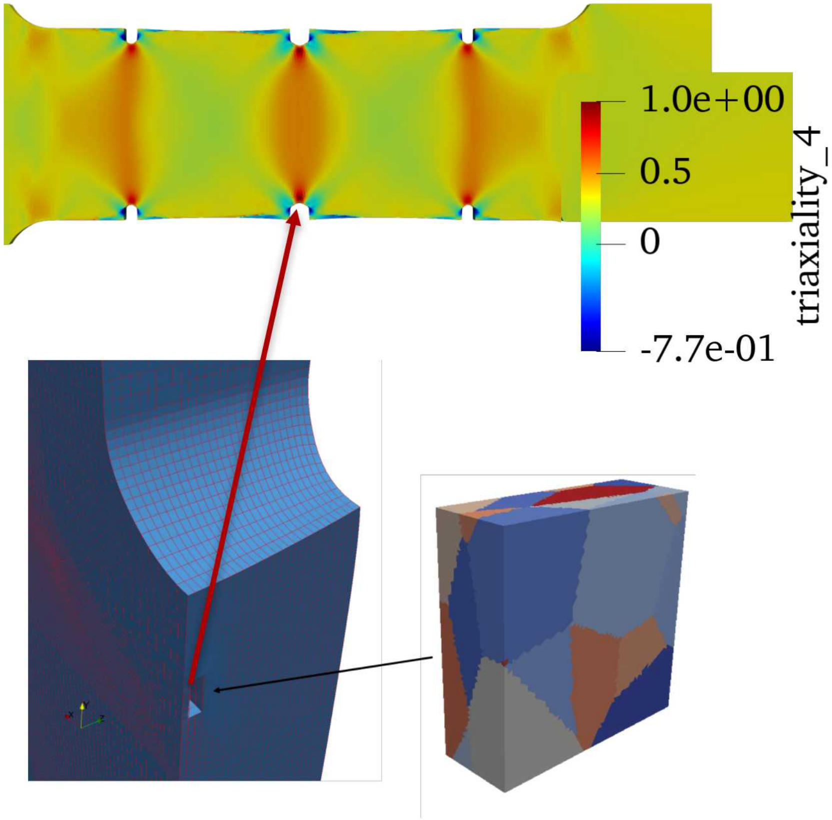
- Motivation: Why do multiscale? For uncertainty propagation
- Probability model for crystallographic orientation/texture
- Example 1: Load in a brittle inclusion within small polycrystal
  - Excursion – implications of meshing decisions
- Reduced-order model for texture
  - Example 2: Exploring RFROM w/ simple cubic-elastic plate
  - Example 1 revisited w/ RFROM
- Example 3: Coupled, multiscale analysis
- Summary

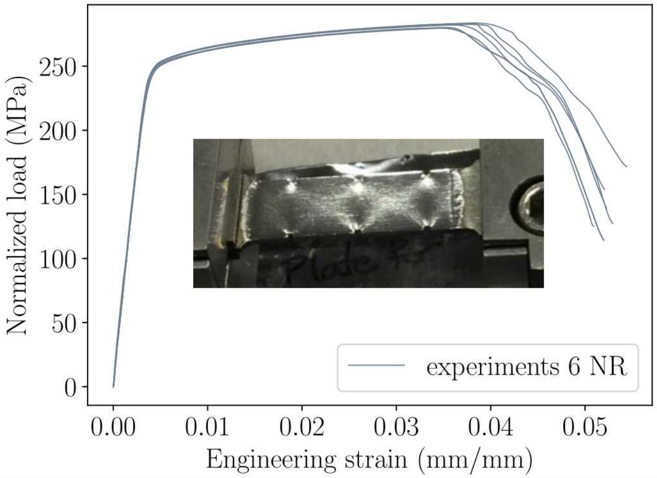
Couple multiscale w/ second-phase particle

- The polycrystal with brittle inclusion is embedded in a “component” at the point of highest triaxiality and concurrently coupled using multi-point constraints.
- The component model uses Hill plasticity, calibrated to tension/notched tension data.
- Simulations conducted for 20-sample RFROM

parameter	value
R11	1.00e-00
R22	8.07e-01
R33	8.00e-01
R12 = R23 = R31	9.50e-01
yield (MPa)	2.80e+02
hardening (MPa)	1.16e+02
recovery	1.11950e+01
damage exponent	9.875

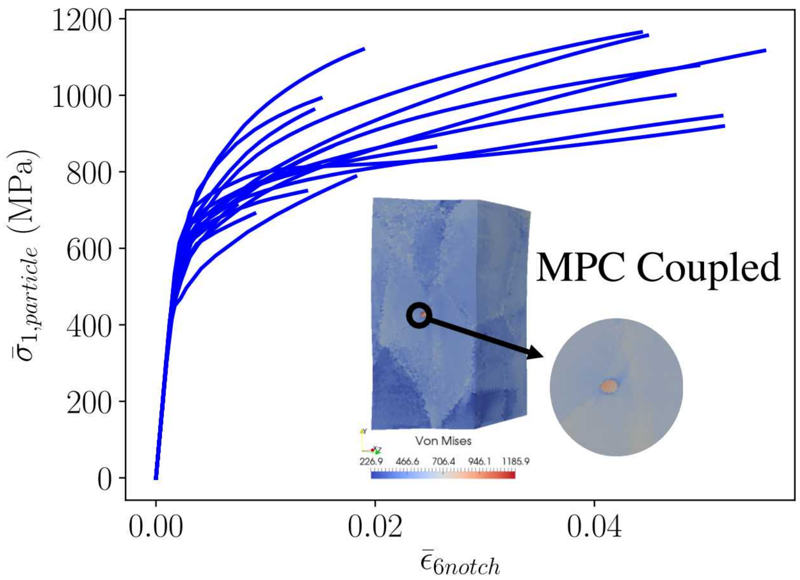


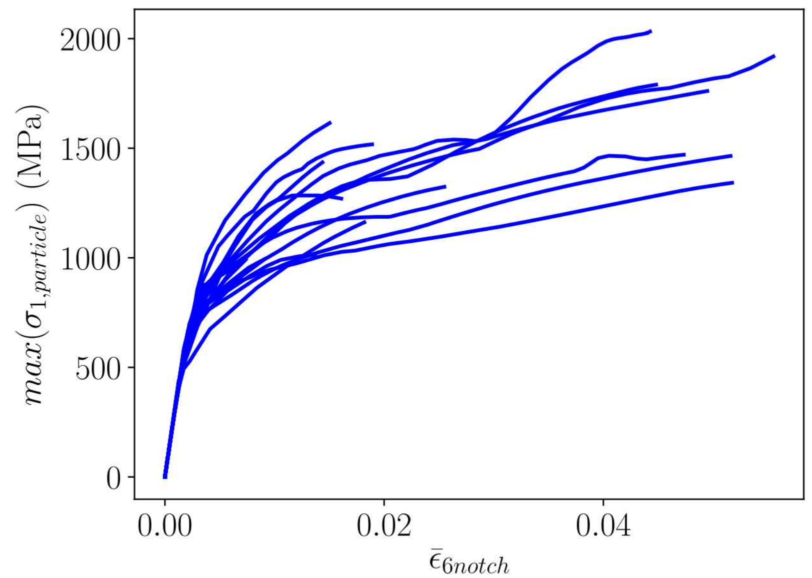


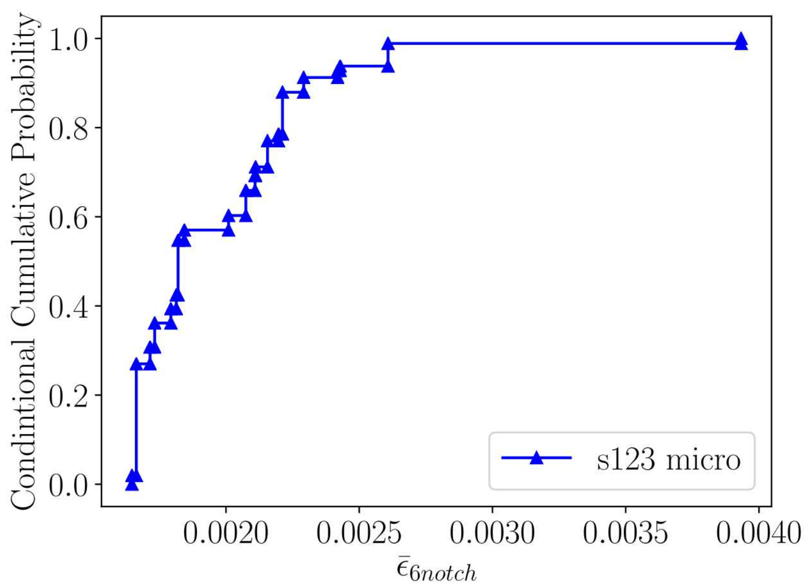


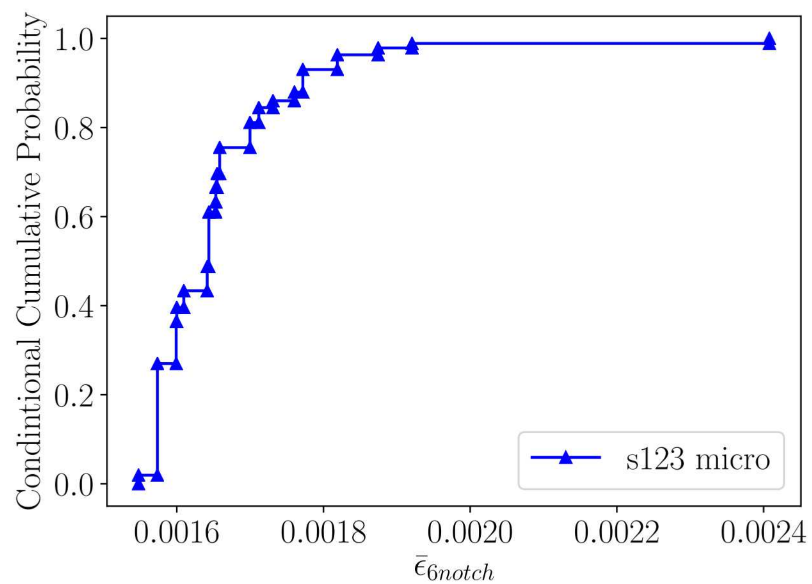
Statistics of particle load

Sandia National Laboratories



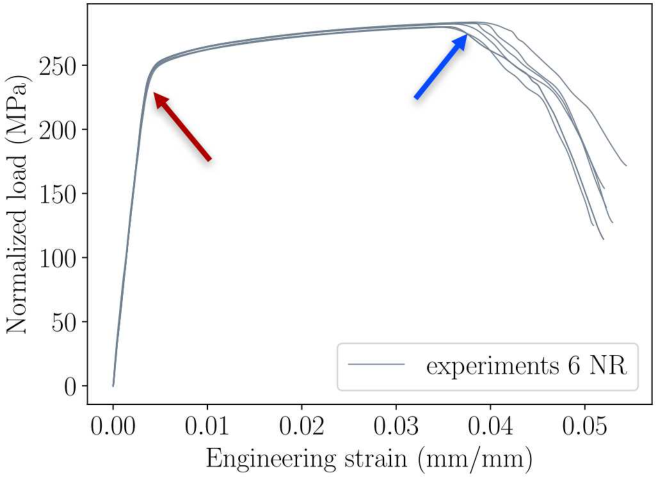






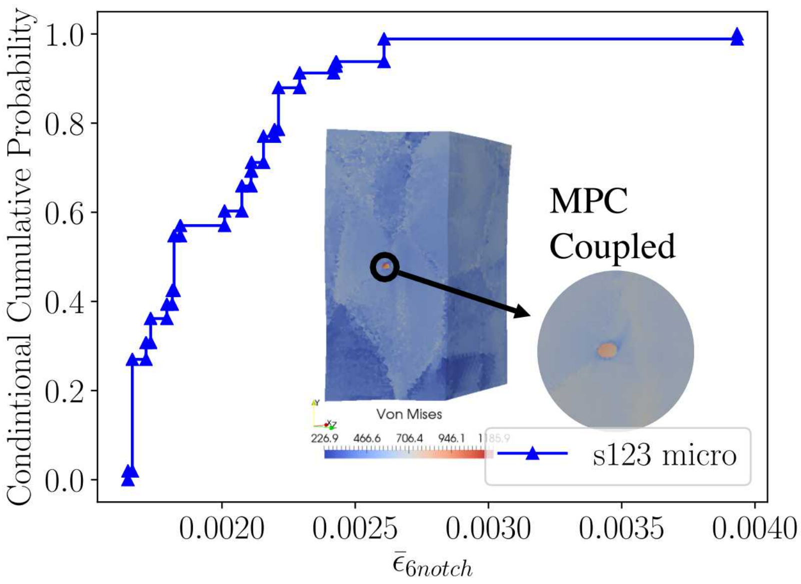
On Validation – room for improvement

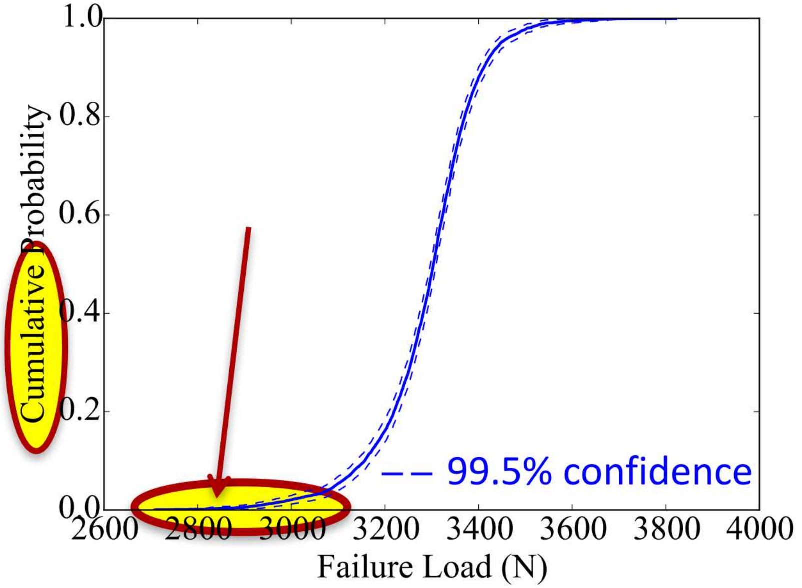
- Predicted load in our brittle particle suggests fracture in the applied strain range 0.001 - 0.004. Very early in the load history.
- Of 6 specimens tested, initiation/fracture occurs in a range of 0.034 – 0.042.
- No dissipation mechanism for the particle in the multiscale model. We saw a broadening of the predicted particle load in the meso-scale simulations when we introduced some yielding in the particle.
- Practically, validating this model is a challenge. How to observe when one particle breaks *in situ*? Future work will adopt a field of particles (using our random field model) and damage, motivated by the observation of bi-modal particle/inclusion size.
- Physically, this work is over-simplified
  – one particle ~30 grains is not statistically representative.
- Crystal plasticity models requires further investigation.



Summary

- Developed and demonstrated our random field model for crystal texture that maintains spatial correlation and reproduces various properties of texture
- Using the random field model, we built a reduced-order model to expedite uncertainty propagation
- The RFROM is efficient for simple elastic problems and beneficial for multiscale calculations
- Quite a lot of work required for validation of multiscale calculations





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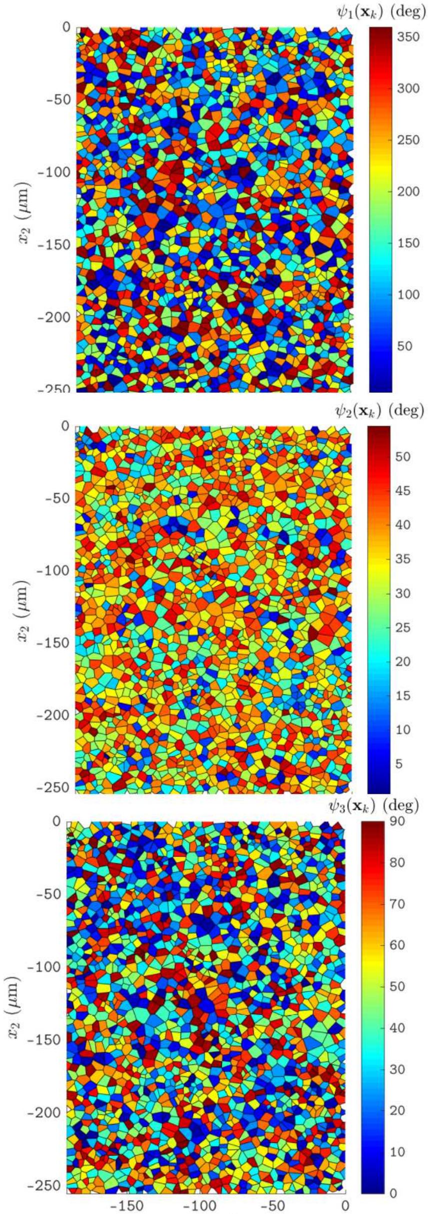
Backup slides

Experimental Data

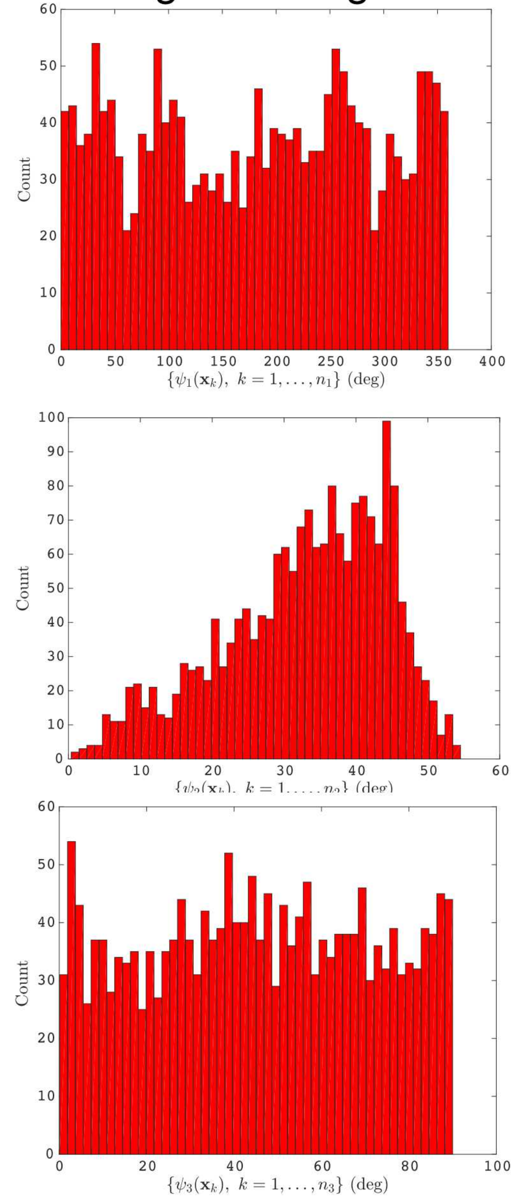
Angle 1: Θ_1

Angle 2: Θ_2

Angle 3: Θ_3

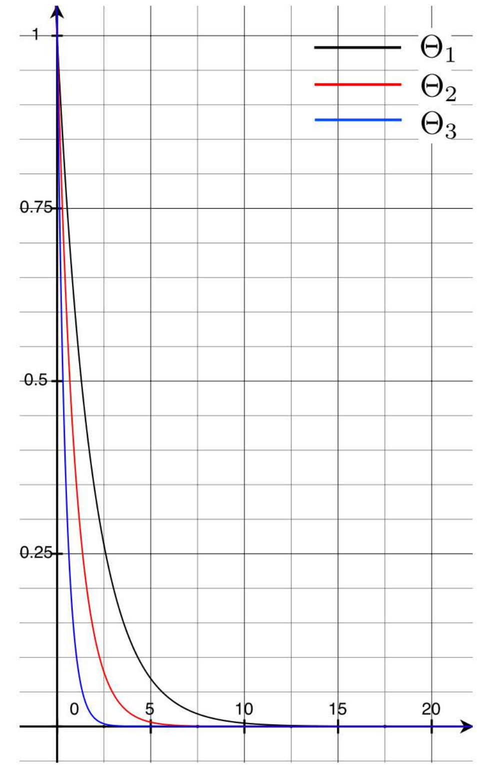


Marginal histograms



Estimated auto-correlations

$$\xi(\eta) = \gamma_{kl} e^{-\alpha_{kl}\eta}$$

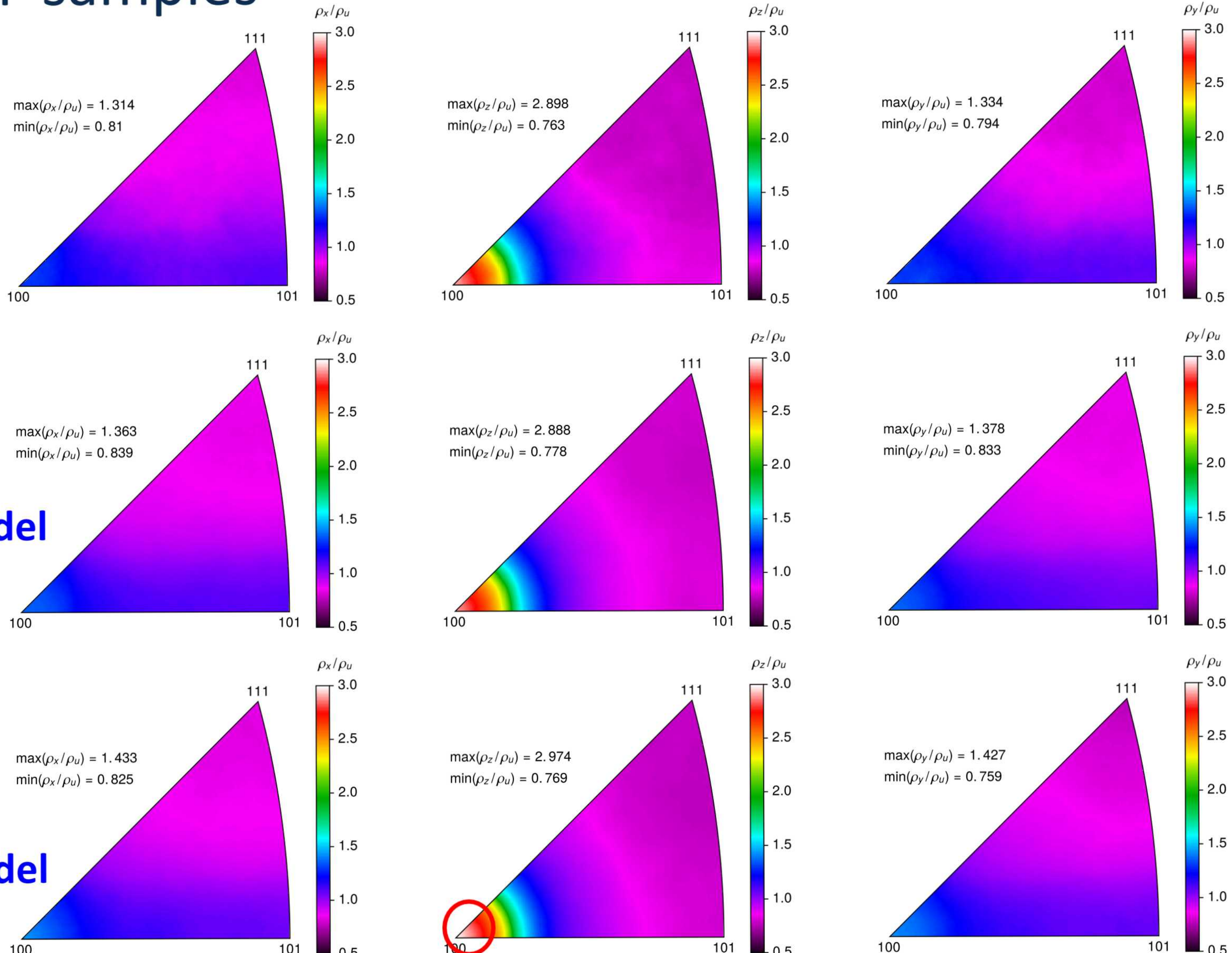


Inverse pole figure (IPF) comparing EBSD to eulerRF samples

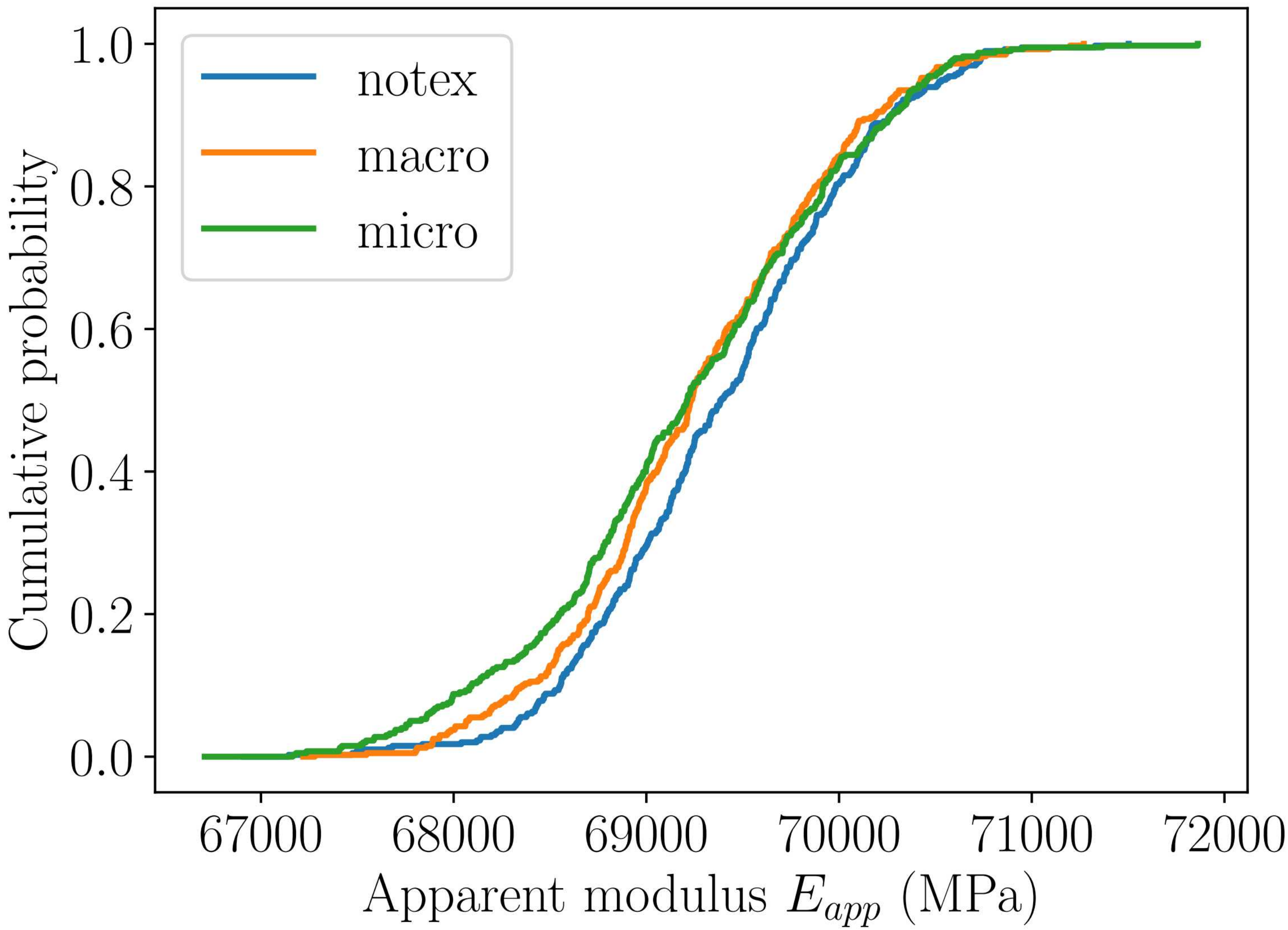
measured EBSD data

macro-texture model

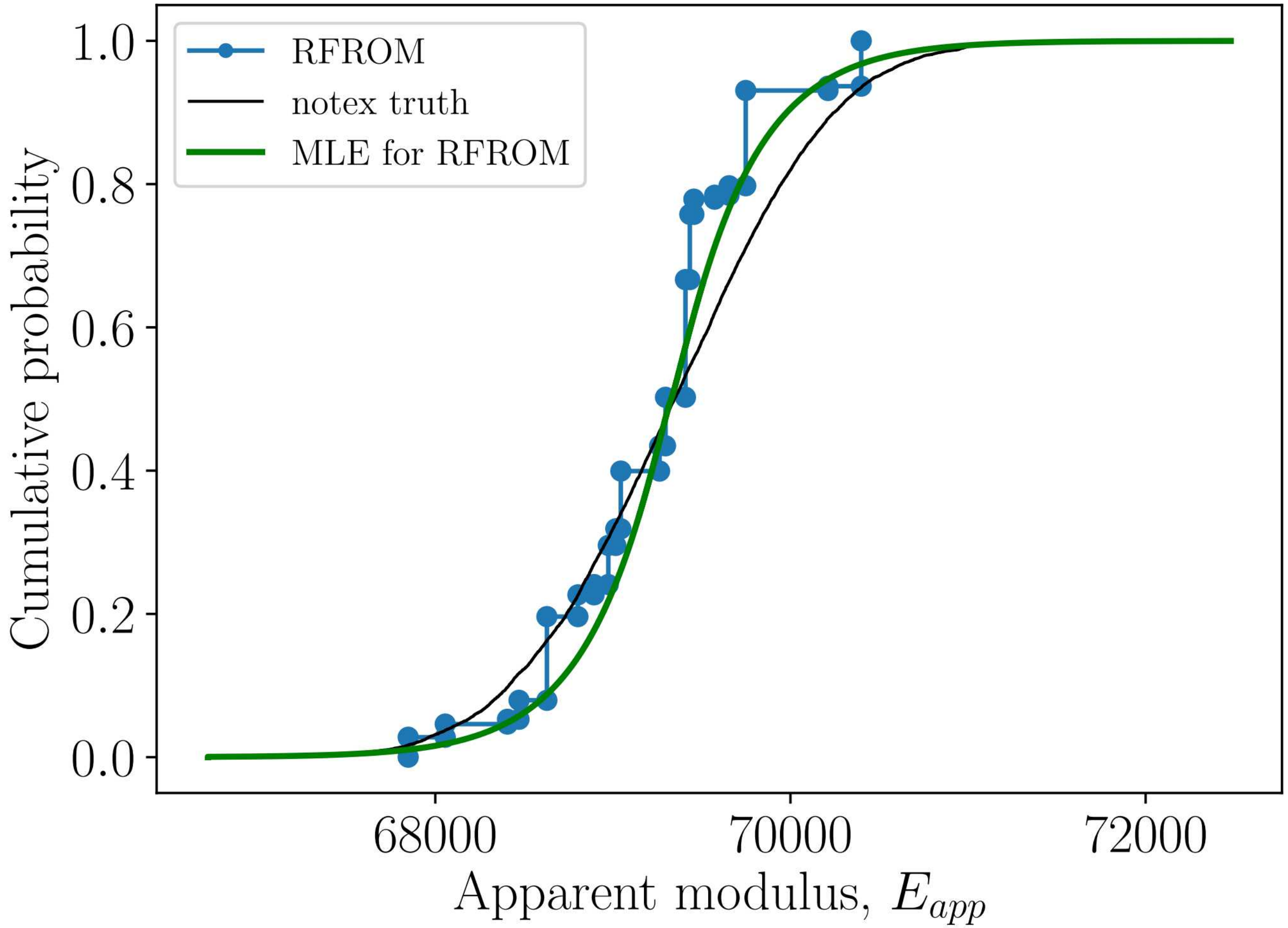
micro-texture model



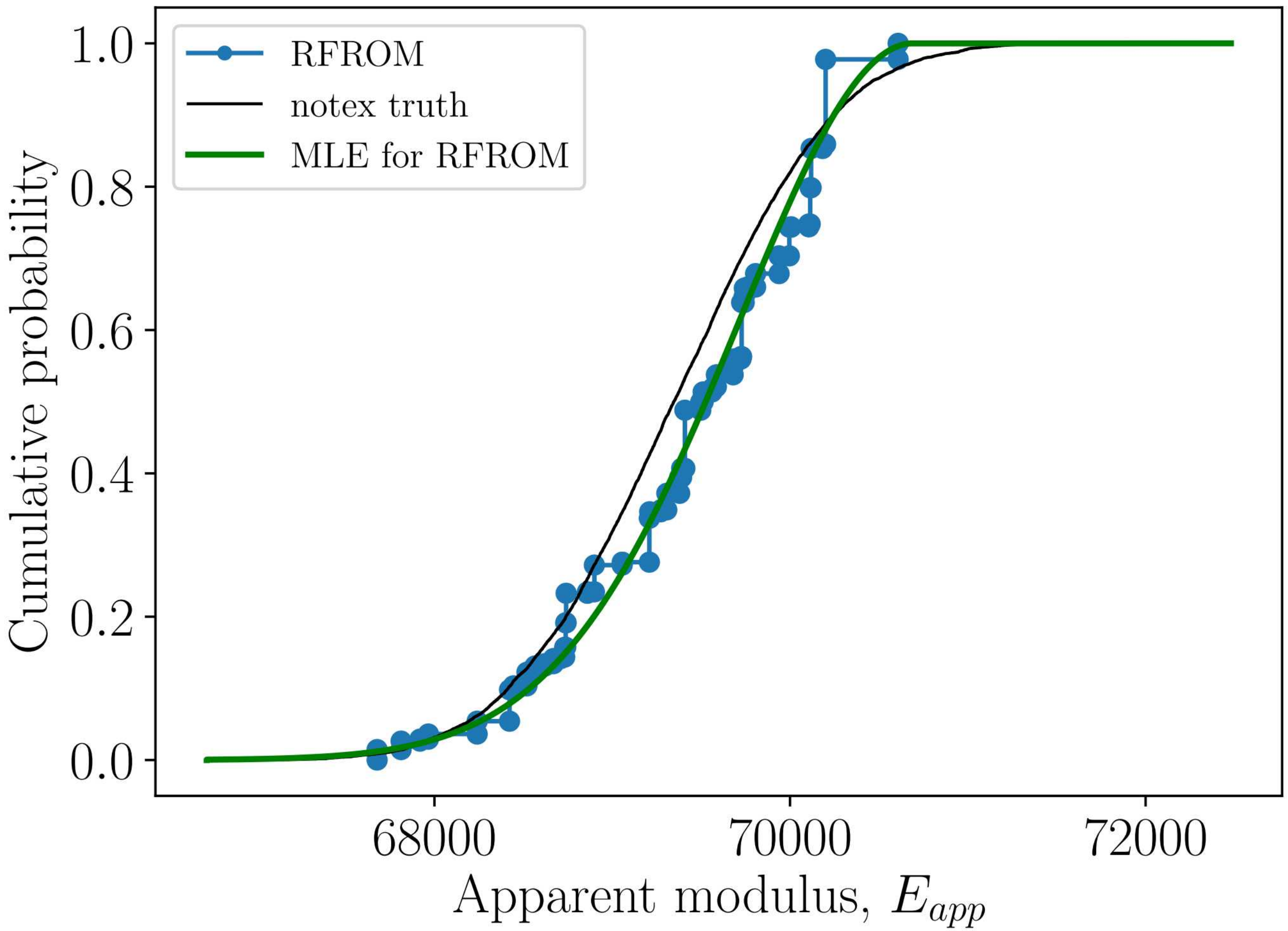
Comparing texture models for cubic elasiticity



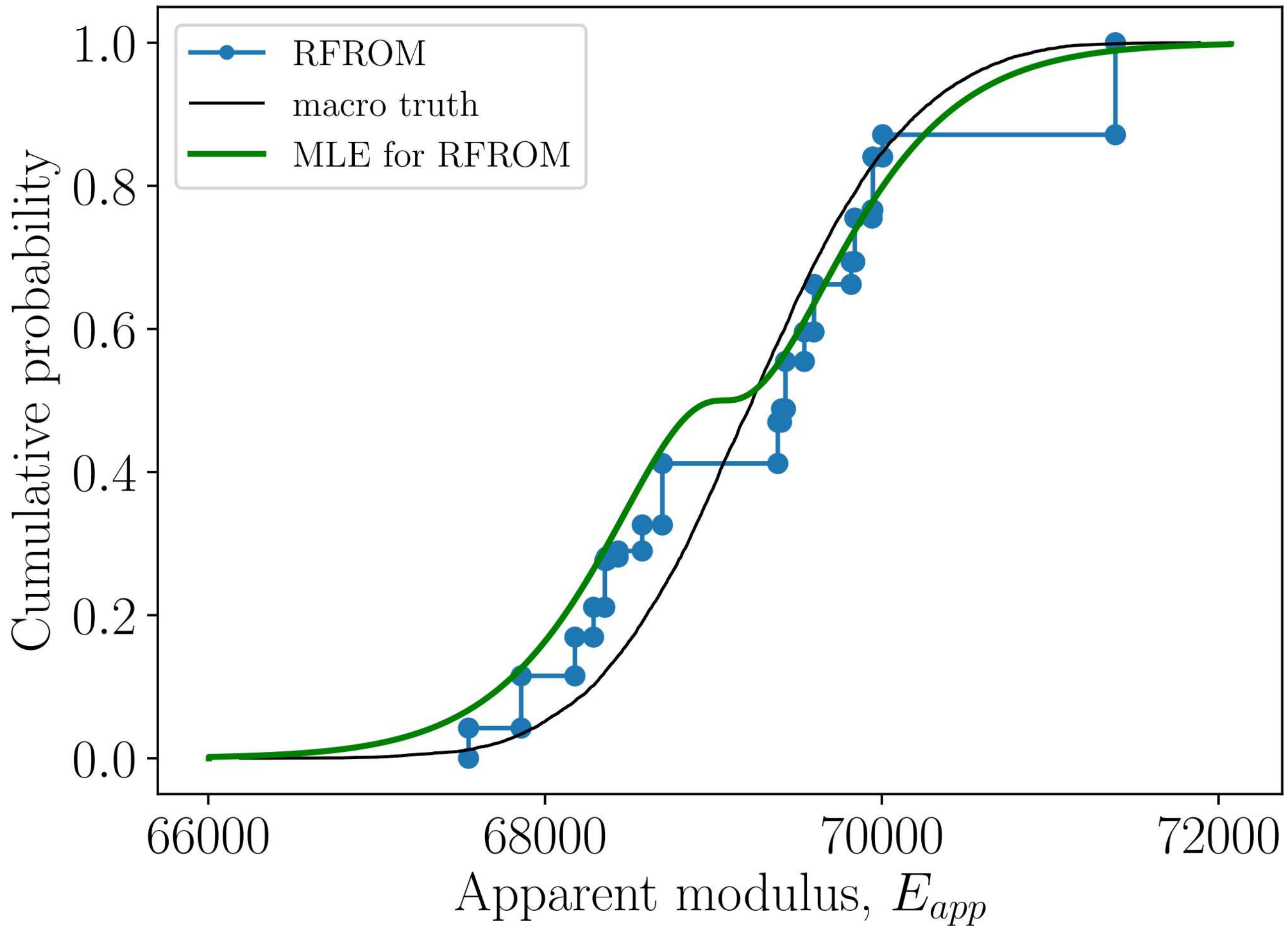
No texture, RFROM m = 20



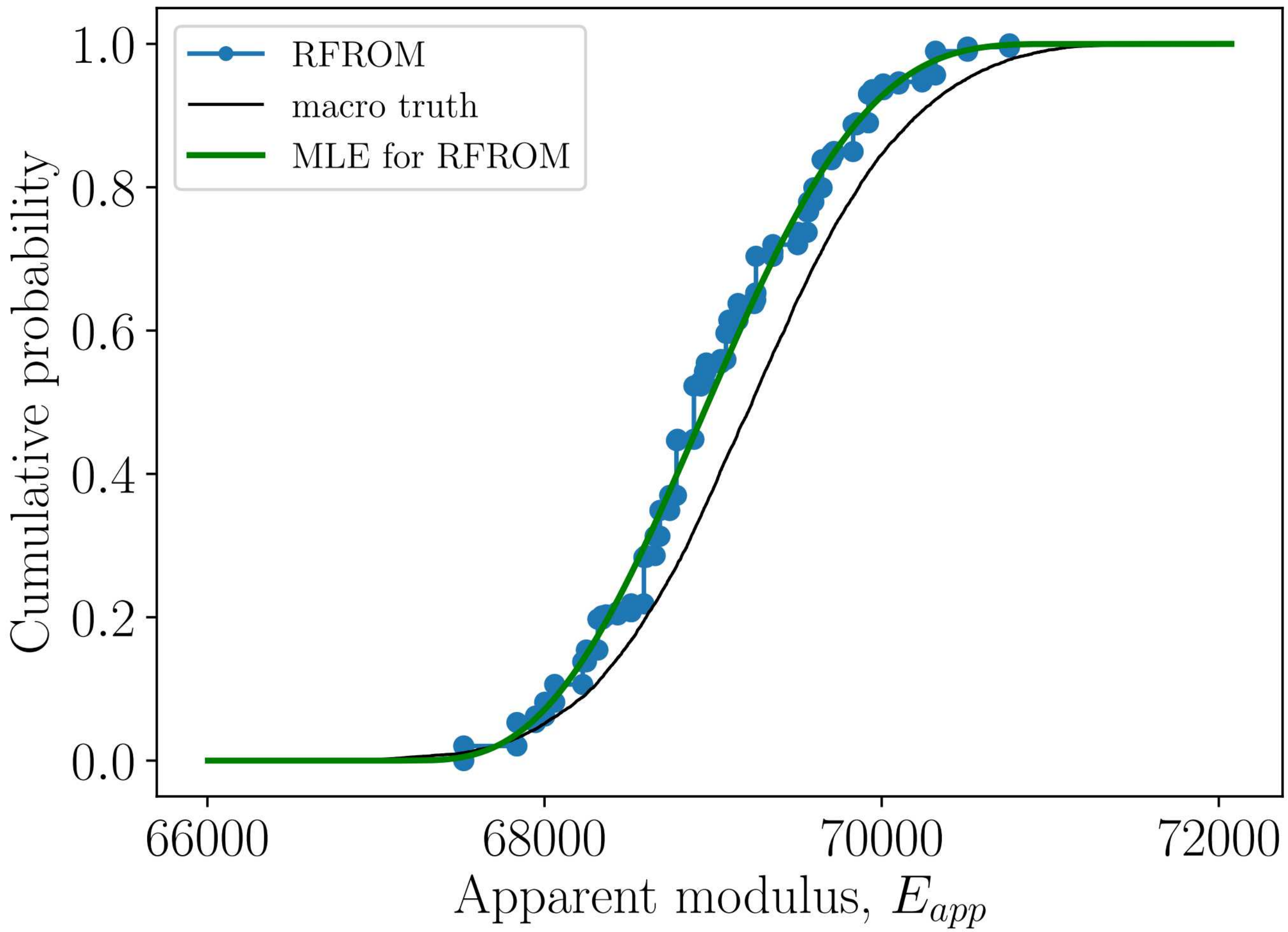
No texture, RFROM m = 50



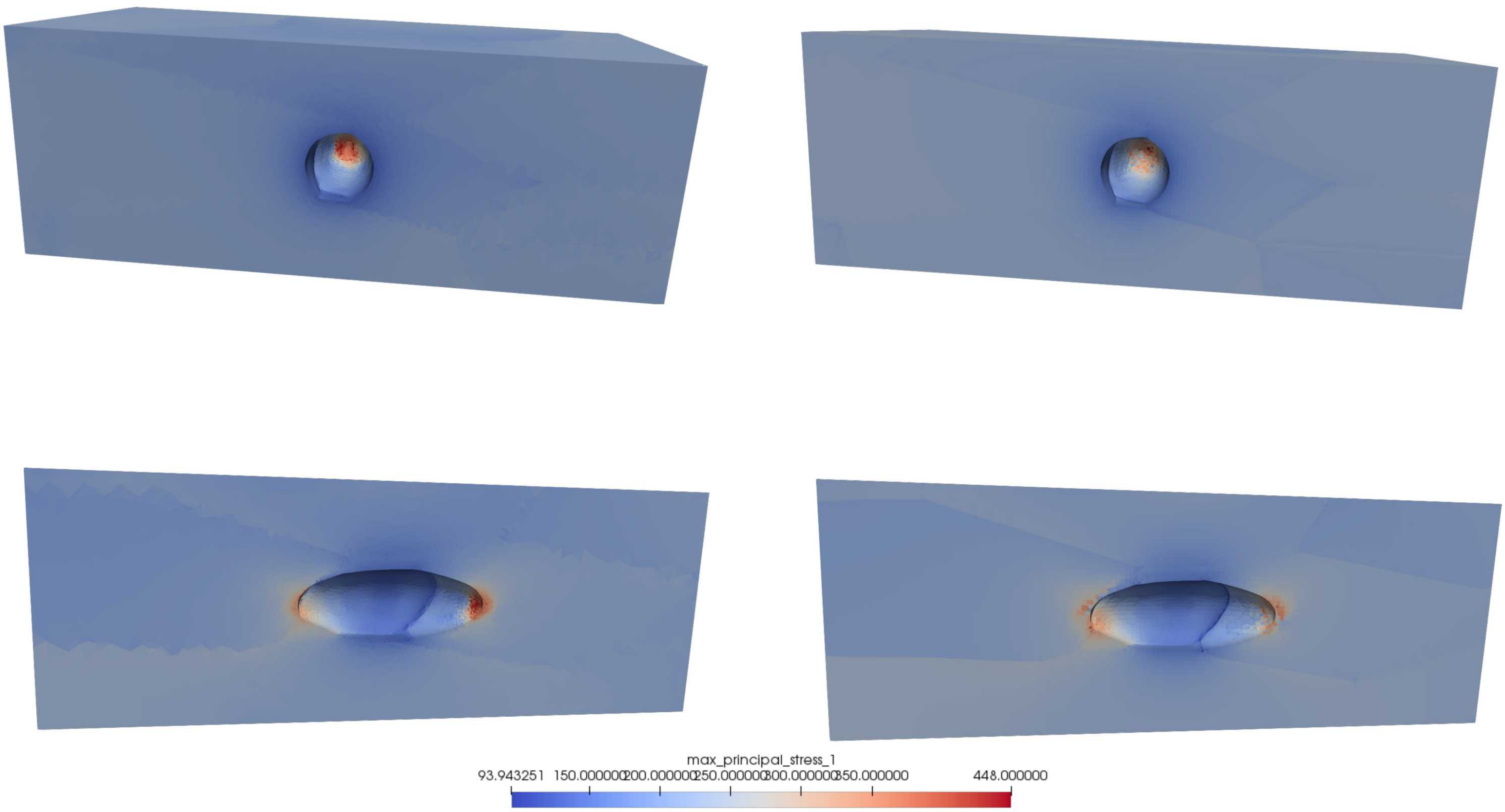
Macro texture, RFROM m = 20



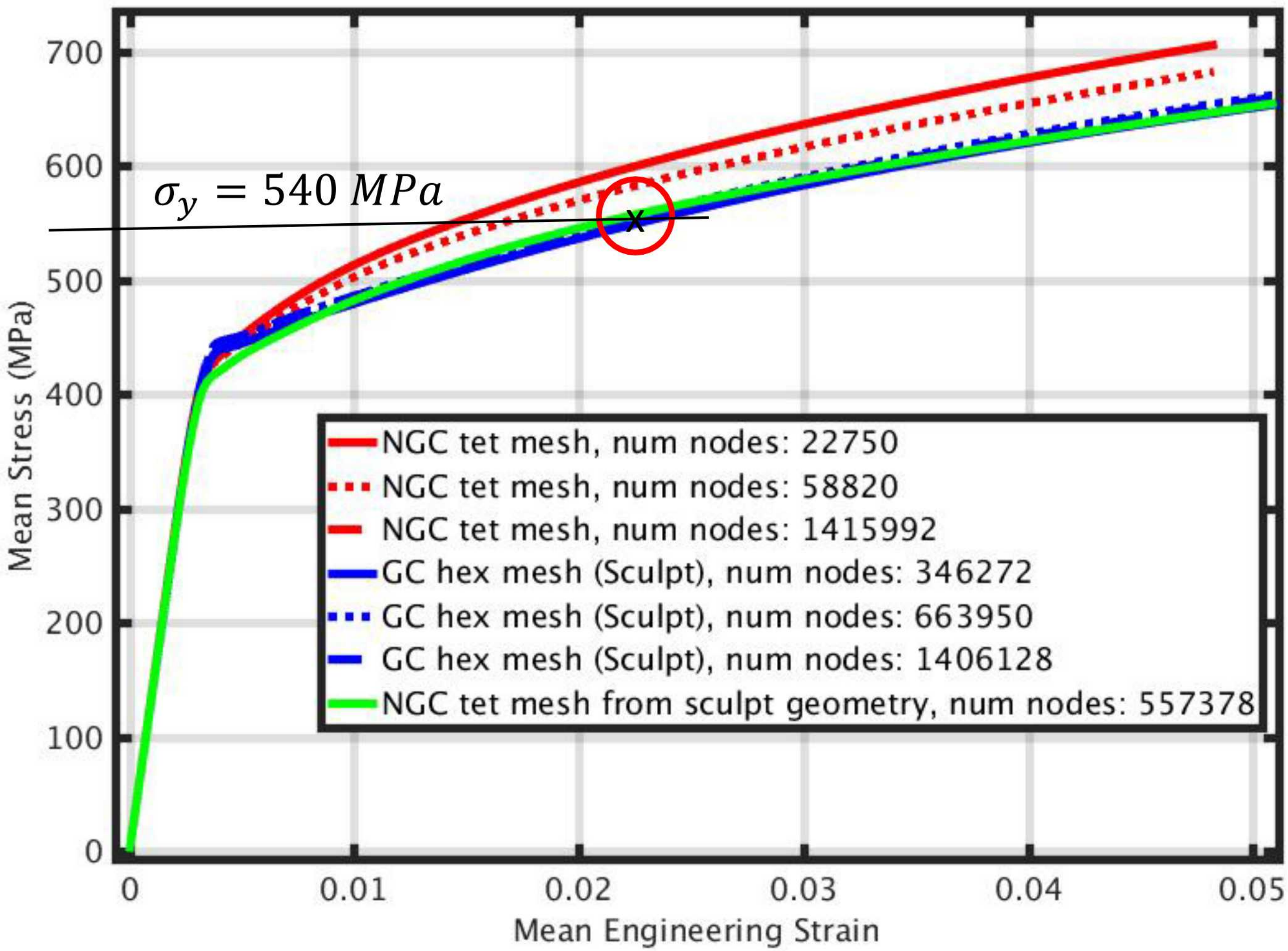
Macro texture, RFROM m = 50



Computed stress nearby the particle



Meshing consideration results



Random-field, reduced-order model

Let $\tilde{\boldsymbol{\Theta}}(\mathbf{x}) = \{\tilde{\boldsymbol{\theta}}(\mathbf{x})^{(1)}, \ldots, \tilde{\boldsymbol{\theta}}(\mathbf{x})^{(m)}\}$ be the SROM of $\boldsymbol{\Theta}(\mathbf{x})$

probabilities $(\tilde{p}^{(1)}, \ldots, \tilde{p}^{(m)})$ $\quad \tilde{p}^{(i)} \geq 0 \; \forall \; i, \; i = 1, \ldots, m$, and $\sum_{i=1}^{m} \tilde{p}^{(i)} = 1$

$(\tilde{\boldsymbol{\theta}}^{(i)}, \tilde{p}^{(i)}), \; i = 1, \ldots, m$