

Stochastic Multiscale Analysis and Design of Engine Disks

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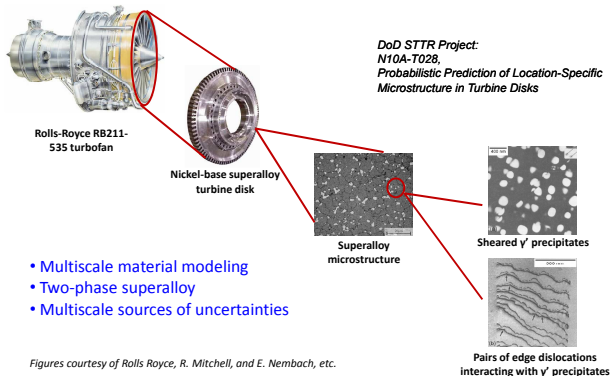
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Motivation

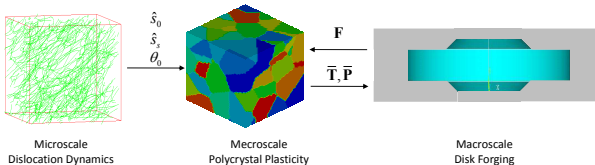
- Develop probabilistic modeling methods predicting location dependent microstructure and properties in nickel-based superalloy turbine disks.
- Issues: Property variability of turbine disk due to high-dimensional multiscale sources



The Big Picture of Multiscale Modeling

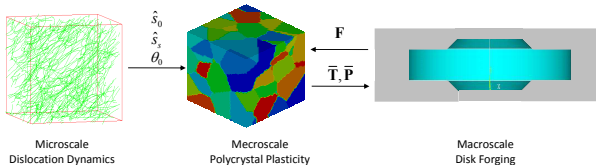
Modeling Methodologies:

- Microscale: Dislocation dynamics
- Mesoscale: Crystal plasticity
- Macroscale: Finite element analysis based multiscale forging



The Big Picture of Multiscale Modeling

Linking Strategy:



- **Micro-Mesoscale:** Regression model that passes constitutive parameters from microscale to mesoscale.
- **Meso-Macroscale:** Homogenization methods exchanging information between both scales. Working with discrete polycrystal aggregates.

Uncertainties propagate within each scale and across scales (e.g. processing and microstructure uncertainties)

Uncertainties in Microscale DD Simulation of Precipitation Hardened Nickel-based Superalloys

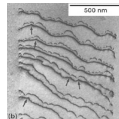
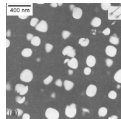
The properties of high performance superalloys are controlled by the γ' precipitates coherently embedded in the γ matrix. A force is exerted on a dislocation when it is creating or recovering an anti-phase boundary (APB). The force per unit length on dislocation is

$$F = \chi_{APB}$$

Dislocation dynamics (DD) simulation is adopted to investigate the hardening mechanism in microscale.

Primary factors determining strength of superalloys

- Volume fraction of γ' precipitates
- Precipitate size and spatial distribution
- Anti-phase boundary energy density (χ_{APB}) distribution



Precipitate Size Distribution in Aged Alloys

Aging of precipitation hardened alloys leads to particle coarsening. In order to match the case of an Ostwald ripened crystal, the particles are chosen to be spherical with a radius distribution following a WLS distribution.

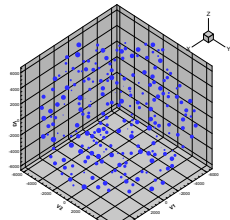
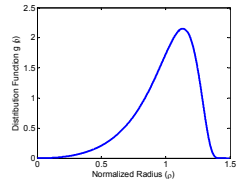
The distribution of normalized particle radius ρ ($\rho = \frac{r}{r_m}$, r_m is the mean radius) follows

$$g(\rho) = \frac{4}{9} \rho^2 \left(\frac{3}{3 + \rho} \right)^{\frac{7}{3}} \left(\frac{1.5}{1.5 - \rho} \right)^{\frac{11}{3}} \exp \left(\frac{\rho}{\rho - 1.5} \right).$$

for $0 \leq \rho < 1.5$,

$g(\rho) = 0$, for $\rho > 1.5$

The spatial distribution is totally random without overlap.



Linking Between Mesoscale and Microscale

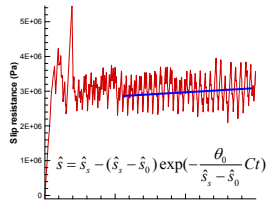
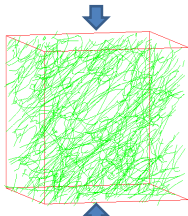
Hardening law in mesoscale crystal plasticity constitutive model

$$\hat{s}(\tau) = \hat{s}(t) + \theta_0 \left(\frac{\hat{s}_s - \hat{s}(t)}{\hat{s}_s - \hat{s}_0} \right) \sum_{\beta \in \text{Active}} |\Delta\gamma^\beta|$$

When constant strain rate is applied, $\sum_{\beta \in \text{Active}} |\Delta\gamma^\beta|$ is also a constant C . Integrating the hardening law with respect to time, we can modify it as

$$\hat{s}(t) = \hat{s}_s - (\hat{s}_s - \hat{s}_0) \exp\left(-\frac{\theta_0}{\hat{s}_s - \hat{s}_0} Ct\right)$$

Extracting the slip resistance \hat{s} relationship with time t from DD simulations, we can coarse grain and compute the parameters \hat{s}_0 , \hat{s}_s , and θ_0 needed in the mesoscale.



Maximum Entropy Principle to Estimate Material Parameters

- Given a specific configuration, we can fit the three parameters by conducting an one time simulation. However, the parameters obtained are different in DD simulations that started from distinct configurations (different precipitate realization, APB energy densities, volume fraction of γ' phase, ...).
- These material parameters are treated as random variables inducing variability of the mechanical properties of the microstructure at meso-scale.
- Conduct N DD simulations with different configurations. Then compute the first n moments of these parameters using Monte Carlo methods.

$$E(x^k) = \sum_{i=1}^N x_i^k = M_k, k = 1, 2, \dots, n$$

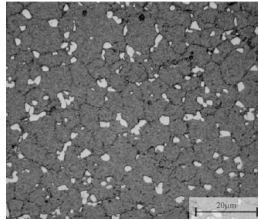
- Use MaxEnt to compute the distribution of the parameters satisfying the constraints.

$$p(x) = \frac{\exp(-\sum_{k=1}^n \lambda_k x^k)}{Z}, Z = \int \exp(-\sum_{k=1}^n \lambda_k x^k) dx$$

- These distributions are our stochastic input model on the mesoscale.

Representation of Two-phase Polycrystalline Superalloy Microstructures

- Two-phase polycrystalline microstructures are random fields in nature.
- The representation of the microstructure needs to combine both polycrystal and two-phase alloy features.
- The complete representation of two-phase polycrystalline microstructure is high-dimensional.



Optical micrographs of RR1000 superalloy: sub-solvus heat-treated for 4h at 1130C. (Courtesy of Rob Mitchell)

Uncertainties in Mesoscale Polycrystalline Microstructures

Topological Feature Space

- Grain size distribution
- Two-phase microstructure variation

Descriptor:

- Histogram of grain sizes (or "grain size vector")
- Correlation functions n-point correlation function

$$S^{ijk\dots t}(r_{ij}, r_{jk}, r_{ki}, \dots, r_{st}) = \frac{1}{V} \int_V I^i(x) I^j(x + r_{ij}) I^k(x + r_{ik}) \dots dx$$

Linear path function

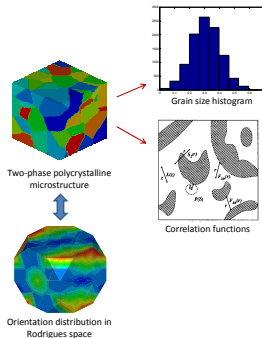
$$L^i(r) = \frac{1}{V} \int_V I^i(x) I^i(x + n) I^i(x + 2n) \dots I^i(x + r) dx$$

Orientational (texture) Feature Space

- Orientation distribution of grains

Descriptor:

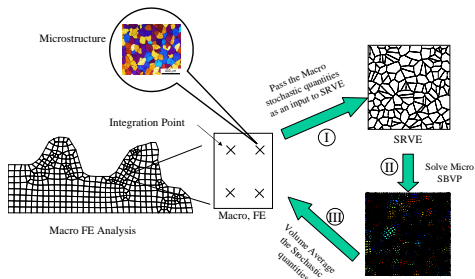
- Discrete representation: Vector of Rodrigues parameters $\mathbf{r}_i = \mathbf{n}_i \tan \phi_i/2$
- Continuum representation: Orientation distribution function (ODF)



Linking Between Mesoscale and Macroscale

Homogenization theory

- Deformation of a microstructure is controlled by the deformation gradient at the corresponding point on the macroscale. The response and properties of the microstructure are computed using crystal plasticity constitutive models. Their homogenized values are passed to the macroscale.
- Response/properties are random fields that are quantified by the microstructure uncertainties in lower scales.



Obtaining Homogenized Stochastic Quantities from Mesoscale

Goal: evaluating mechanical response/properties variability of microstructures (and further, of the entire turbine disk).

Steps:

- 1 Model Reduction: Given a set of microstructure snapshots, perform model reduction techniques to obtain low-dimensional representations to reduce the complexity of the stochastic input space.
- 2 Direct Computation: Interrogate each of the microstructures using direct models to obtain its mechanical response and properties.
- 3 Statistical Learning: Estimate mechanical response/properties variability of microstructures using stochastic methods.
- 4 Prediction: Given a new microstructure, first reduce its representation to low-dimensional space. Then, predict its response/properties with quantified uncertainties.

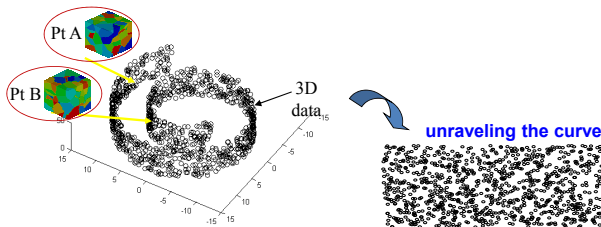
Model Reduction Techniques

Nonlinear model reduction (manifold Learning) on grain size

- Isometric mapping.
- The geometry of the manifold is reflected in the geodesic distance between point.

Algorithm

- Compute the low-dimensional representations of given high-dimensional points.



- Reconstruct high-dimensional representation of an arbitrary point in low-dimensional space.

Karhunen-Loève Expansion on texture

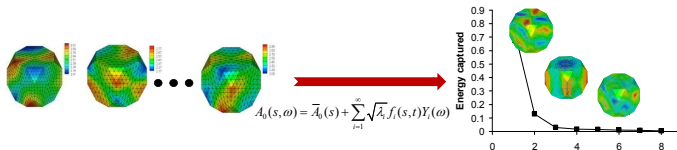
- Construct covariance matrix of given samples

$$\tilde{\mathbf{C}} = \frac{1}{N-1} \sum_{i=1}^N (\boldsymbol{\tau}_i - \bar{\boldsymbol{\tau}})^T (\boldsymbol{\tau}_i - \bar{\boldsymbol{\tau}}), \quad \bar{\boldsymbol{\tau}} = \frac{1}{N} \sum_{i=1}^N \boldsymbol{\tau}_i$$

- Solve eigenvalue problem and obtain eigenvalues ϕ_i and eigenfunctions λ_i of the matrix.
- The truncated K-L Expansion of the random vector $\boldsymbol{\tau}$ is then written as

$$\boldsymbol{\tau}(\mathbf{r}, \boldsymbol{\omega}) = \bar{\boldsymbol{\tau}}(\mathbf{r}, \boldsymbol{\omega}) + \sum_{i=1}^{d_2} \sqrt{\lambda_i} \phi_i(\mathbf{r}) \eta_i(\boldsymbol{\omega})$$

$\{\eta_i(\boldsymbol{\omega})\}$ is a set of uncorrelated random variables whose distribution can be estimated using the Maximum Entropy Principle.



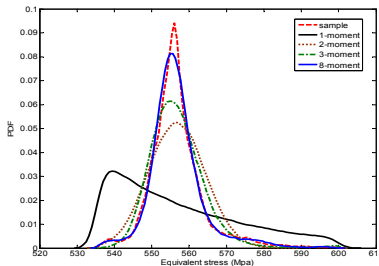
Uncertainty Quantification: Propagating microstructure uncertainty to material properties

Usually, a set of microstructure snapshots are given, whose properties can be computed beforehand (microstructure interrogation). We are interested to build a hypersurface of the material properties in the space of all allowable microstructures. The response/properties of a new microstructure (with complete probabilistic information, error bars) can then be estimated without any need to run the corresponding direct simulation.

- Maximum Entropy Principle
- Sparse Grid Collocation, HDMR
- Bayesian Regression

Method 1: Maximum Entropy Principle

- Sampling from low-dimensional representation space
- Performing a number of direct simulations and computing moments of response/properties using Monte Carlo simulation
- Using Maximum Entropy Principle to estimate response/properties distributions



Equivalent stress distribution of nickel microstructures under simple compression when $\epsilon = 0.2$.

Method 2: Adaptive Sparse Grid Collocation (ASGC)

- Mapping the low-dimensional stochastic (microstructure topology) input space to a unit hypercube
- Solving stochastic partial differential equations (SPDEs) using ASGC (based on sampling on the hypercube)

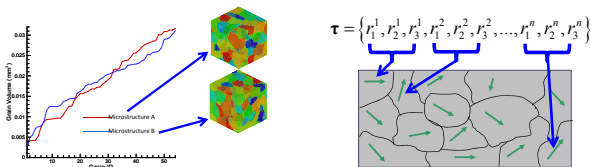
$$\hat{u}_{d,q}(t, \boldsymbol{\xi}) = \sum_{\|\mathbf{i}\| \leq d+q} \sum_{\mathbf{j} \in B_i} \omega_{\mathbf{j}}^{\mathbf{i}}(t) \cdot a_{\mathbf{j}}^{\mathbf{i}}(\boldsymbol{\xi})$$

- High dimension model representation (HDMR) integrated with ASGC can also be easily applied.

Example: Mechanical Response Variability of Nickel Due to Microstructural Uncertainties

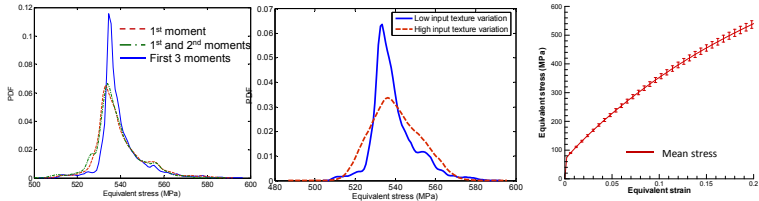
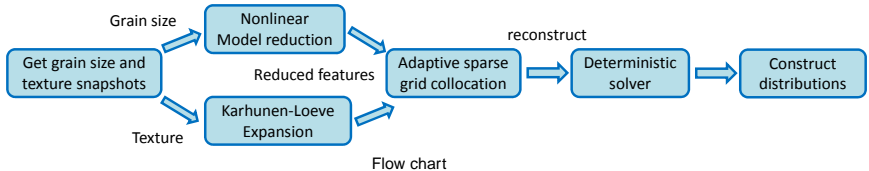
Discrete microstructure features representation:

- Grain size representation: "sorted grain size vector"
- Texture representation: vector of Rodrigues parameters



Microstructure snapshots satisfying certain constraints are provided

- Grain sizes of microstructure have the same mean size, standard deviation, and/or third order moment. Reconstruction techniques are used to produce microstructure realizations.
- Textures are generated by the same (deformation) process controlled by several random (process) variables (e.g. forging rate).

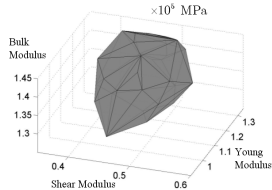
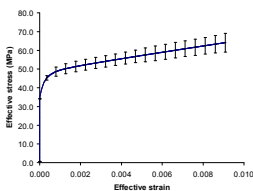
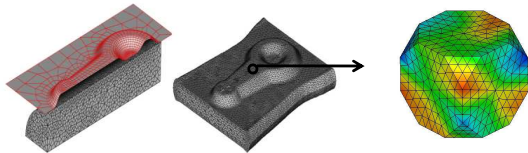


Effects of microstructural feature uncertainties on macroscopic effective stress distributions at $\epsilon = 0.2$ (N. Zabaras et al., 2010)

Example: Mechanical Property Variability of Copper due to Microstructural Uncertainties: Convex Hull of all Possible Properties and Affiliated Probabilities

Continuum microstructure features representation:

- Orientation distribution function (ODF) in Rodrigues fundamental zone.



Method 3: Bayesian Regression

- Build an adaptive and sparse Bayesian Regression Model (Relevance Kernel Machines, Sparse Representations)

$$y = \sum_{i=1}^M \beta_i \phi(\mathbf{x}_i) + \epsilon$$

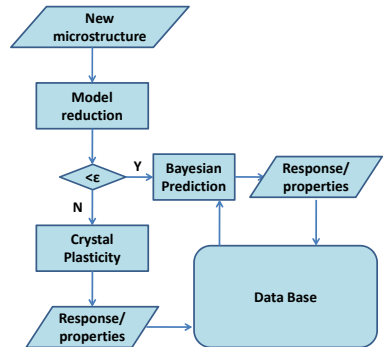
where $\phi(\mathbf{x}_i)$ denotes the basis functions (polynomial, Gaussian, radial, kernels, etc.) of the low-dimensional representation of the microstructures, and y denotes the corresponding response/property.

- Based on observed data, use SMC method to estimate the distribution of coefficients in the model
- Predict the property and error bars of new microstructures.

An Adaptive Bayesian Prediction Model

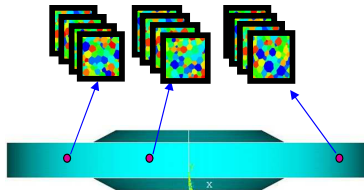
A dynamic method that combines direct simulation and Bayesian regression learning can be introduced.

- Perform model reduction of given microstructure snapshots and compute their response/properties using direct simulation.
- Construct a Bayesian regression model (sparse kernel interpolation) using the given data.
- Adaptivity is built to allow new data (microstructure and the corresponding properties) to be used for updating the response hypersurface. The variance predicted from the predictive distribution for a given input microstructure is used as an error criterion for adaptivity.
- Sequential Monte Carlo is used in building the hypersurface and predictive distribution.



Multiscale Model Reduction of Microstructure Random Field

- The microstructure varies at each point in the (forged) workpiece at different realizations of the forging process.
- The microstructure also varies from point to point within the same workpiece.
- One can construct a reduced-order stochastic model for each point. But how do you account for microstructure correlation to avoid the curse of dimensionality?
- Techniques to capture **the correlation** of microstructures in the continuum.
- Most of the computational methods are intractable unless we can find the correlation between all the microstructures and construct a reduced order model.
- Use a bi-orthogonal KLE decomposition



Turbine disk

Bi-Orthogonal Decomposition (for Texture Multiscale Reduction)

- Start from realizations of the texture random field varies in both meso (\mathbf{s}) and macroscale (\mathbf{x})

$$\mathbf{A}_i(\mathbf{x}, \mathbf{s}, \omega)$$

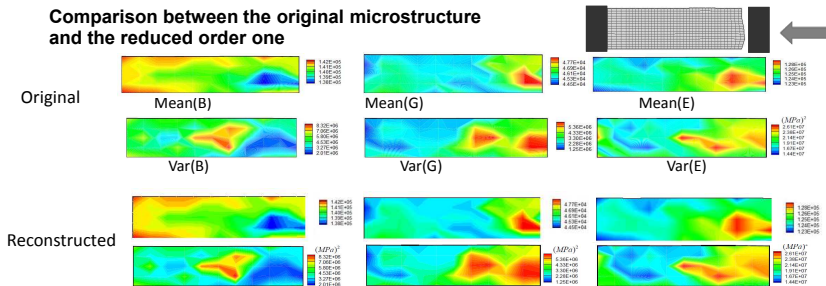
- Transform snapshots and construct covariance matrix at the meso-scale using all data in the macroscale.

$$\mathbf{C}(\mathbf{s}, \mathbf{s}') = \frac{1}{n_r} \sum_{j=1}^{n_r} \sum_{i_n=1}^{n_{elm}} \sum_{i_m=1}^{n_{int}} \hat{\mathbf{a}}_i(\mathbf{x}_{i_m}, \mathbf{s}, \xi_j) \hat{\mathbf{a}}_j^T(\mathbf{x}_{i_m}, \mathbf{s}', \xi_j) \hat{\eta}_{i_m} |J_{i_n}|$$

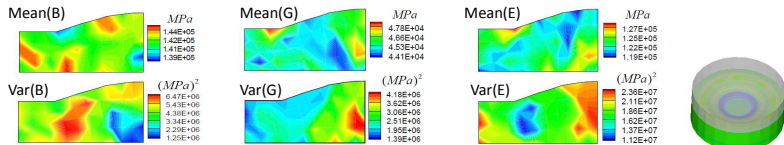
- Solve the eigenvalue problem to obtain the eigenvalues and eigenvectors:
 $\rho_i, \boldsymbol{\psi}_i(\mathbf{s})$
- The spatial modes are obtained by integrating over mesoscale variables

$$\boldsymbol{\Phi}_i(\mathbf{x}, \omega) = \frac{1}{\sqrt{(\rho_i)}} \int_{\mathcal{R}} \hat{\mathbf{a}}(\mathbf{x}, \mathbf{s}, \omega) d\mathbf{s}$$

Comparison between the original microstructure and the reduced order one



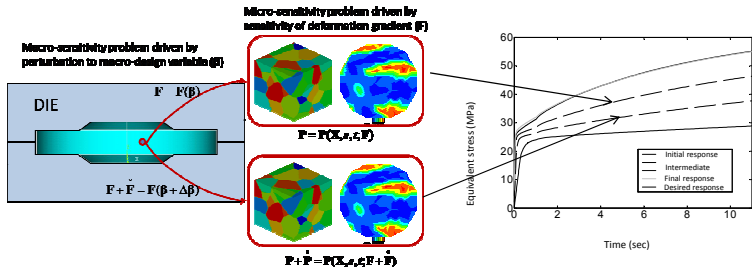
Effects of Uncertainty in Initial Texture



Computational design of deformation processes for desired microstructure-sensitive properties in the presence of uncertainty

Design Objectives:

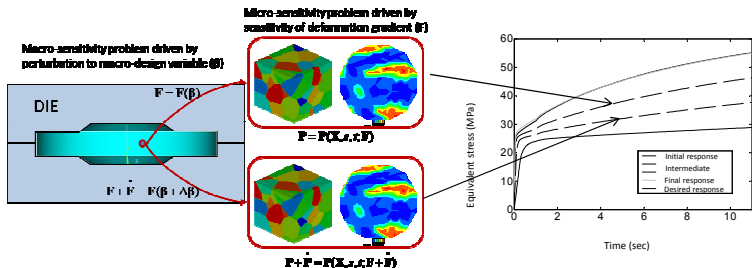
- Variability in disk properties (tensile and fatigue strength, stiffness, etc.)
- Geometric variability, Variability in obtained microstructures, etc.



Computational design of deformation processes for desired microstructure-sensitive properties in the presence of uncertainty

Design variables (random):

- Process sequence considered (multi-stage design)
- Process conditions (e.g. variabilities in preforms, dies, operating temperature, strain rates, etc.) and initial microstructures.



Challenges

- Complex multistage, multiscale and stochastic framework
- High dimensional random input/output
- Large variabilities require new thinking of modeling of SPDEs (e.g. Bayesian predictive modeling with sparse sampling vs sparse grids and HDMR). Sparse grids were shown recently to fail when used with data-driven non-linear stochastic input models (KPCA, IsoMap, etc.).
- Need for scalable exascale computing algorithms