Stochastic Multiscale/Multistage Modeling of Engine Disks

Proposal#: N10A-028-0433

STTR - Phase I Kick Off Meeting – Monday June 28, 2010
Probabilistic Prediction of Location-Specific Microstructure in Turbine Disks

The Office of Naval Research

Cornell University
Advanced Dynamics Inc.
Team Members

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Advanced Dynamics Inc. (ADI) is a high-tech firm. The Company was incorporated in 2005 in Salt Lake City, and moved to Lexington, KY in 2006. The company resides at University of Kentucky (UK) research campus, and have access to all UK resources.

- Total 15 employees: 9 full time and 6 part time

- Extensive Collaborations with US. Top Universities including Cornell University, Duke University, Georgia Tech, University of California at Berkeley, University of Oklahoma, Utah State University, University of Kentucky, University of Utah

- Extensive Collaboration and Partner with Leading Aerospace Industries: Including Boeing Company, Bell Helicopter Sikorsky Aircraft, and AeroVironment, Inc.

- ADI currently is preparing to Launch a Comprehensive and Integrated Variable-fidelity Modeling and Simulation Software Package ASTE-P for Aerospace Vehicles from Subsonic to Hypersonic Flights

- ADI Has Been Awarded nearly 20 DoD/NASA SBIR/STTR Projects
ASTE-P Main Panel Screenshots
A unified solver for both fluid and structure dynamics: Enhanced Material Point Method (MPM) and Pure Particle Method (PPM) have been developed by Advanced Dynamics for such solvers. In such solvers, the fluid and structure dynamics are simultaneously solved using the same numerical procedure with the exception of different constitutive laws followed by different type of materials.

MPI and OpenMP Massively Parallel Solvers
**MD Nanotube Simulation**

**Constant flux simulation**
- Pour the heat to the tube and remove from the liquid
- Monitor the temperature profile

**Relaxation Simulation**
- Heat the nanotube instantaneously
- Monitor the system relaxation

- PCFF force field - all atom model
- Carbon nanotube in octane liquid
(1) Bar element

(2) Beam element

(3) Plain element

(4) Plate element

(5) Shell element

(6) Solid element
FE Modeling of Surface Crack Growth in Ti Tubes

FE Modeling

FE Meshing

FE Stress

K-a Curve

Fatigue Loading

da/dN – Delta K

a – N curve

a0 – curve

Verification
Crack Growth in X-FEM
Probabilistic Fatigue Crack Initiation and Growth in Spot Welded Joints

Figure 1: Minivan FE model
Figure 2: T joint FE model
Figure 3: Spot weld FE model
Figure 4: FE stress result
Figure 5: Loading spectrum
Figure 6: Moment spectrum
Figure 7: Median $\varepsilon - \overline{N}$ curve
Figure 8: Median fatigue life $\bar{N}$
Figure 9: Probability density of $N_a$
Material Process Design & Control Laboratory: Overview

The Materials Process Design and Control (MPDC) Laboratory performs applied & basic research in the interface of computational mathematics and materials.

Research emphasis:

- Computational design and control of materials processes (solidification, crystal growth, deformation processes)
- Materials design, control of microstructure-sensitive properties
- Understanding and controlling the effects of microstructure evolution in material properties
- Stochastic multiscale materials modeling
- Uncertainty Quantification and propagation in complex systems
Sample of Computational Methods/Software Developed

- Level set methods for modeling and controlling dendritic solidification in the presence of melt flow.
- Multiscale methods for casting processes.
- Continuum sensitivity methods for the design of multiscale deformation processes.
- Statistical methods for the exploration of process/structure/property relations of polycrystals
- Data-driven model reduction and representation of random microstructures
- Predicting property variability in random heterogeneous media
- Bayesian inference methods & inverse problems
**MPDC: Sponsors, Collaborators, Facilities**

**Sponsors:** Support of our work has been provided by Federal sources and private corporations. Current projects are funded by:

- Air Force Office of Scientific Research – Comp. Mathematics Program
- MURI-09 OSD/AFOSR on Uncertainty Quantification
- National Science Foundation (Materials and Mathematics programs)
- Army Research Office (Materials Science Program)
- Department of Energy, Office of Science
- Office of Naval Research (STTR-Phase I)

**Personnel:** 9 PhD students

**Facilities:** 64 node supercomputing cluster, access to TeraGrid resources and to the fastest petascale (DoE) supercomputer within U.S.
Collaboration Plans

A dynamic collaboration between MPDC at Cornell and Advanced Dynamics Inc. will be implemented. Step to foster collaboration and technology transfer include but not limited to:

- Weekly teleconferencing for coordinating algorithmic developments, share data and discuss milestones
- Exchange of regular visits of the PI and Co-PI
- Longer term visits of Advanced Dynamics Inc. to Cornell University
- Longer term visits of Cornell Graduate Assistants to Advanced Dynamics (e.g. during the summer months)
- Continuous evaluation of software developed for immediate technology transfer
- Common visits and presentations of work to industrial manufacturers of engine disks as well as to engine users (Boeing, GE, UTRC, etc.)
**STTR-Phase I Tasks**

**Requirement:** Establish a primary probabilistic modeling and simulation approach that enables prediction of location-specific microstructure, life-limiting features and bulk residual stresses due to processing and fabrication. Validate the model using published data for titanium or superalloy components with dual microstructure.

**Proposed Plan of Activity:**

Developing numerical tools for microstructure evolution (from solidification to grain growth).

Developing **predictive model** for estimating nickel-based superalloy microstructure properties.

Establish stochastic multiscale framework to predict variability in mechanical properties and residual stresses due to the uncertainties of microstructures and process parameters.
Source of Uncertainties

The microstructure of nickel-based superalloy is a random field. The randomness of the microstructure comes from:

- Grain structure topology (grain size, grain shape)
- Grain orientation
- Gamma prime phase statistics (shape, size, volume fraction, distribution, etc.)

These features along with process parameters such as temperature, forging rate, etc., form the source of uncertainties in the turbine disk design. The properties of a disk are largely dependent on these factors.

To study the variability of the turbines disk, it is important to study the uncertainties of the microstructures and their effect on the material properties. Our goal of proposed work in Phase I is to explore the uncertainties in the nickel-based superalloy turbine disks and to predict variability of their properties. This will give significant guidance in industrial process design.

The main tasks for Phase I of this STTR project are summarized next followed by discussion of each task (prior related work and proposed work).
# Proposed Tasks, Timeline and Milestones

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Task 1: Solidification and Grain Growth Simulation
Nickel-based Superalloy Microstructures

Develop numerical tools to generate FCC nickel-based superalloy microstructures.

Grain structures of a nickel-based superalloy turbine disk having dual-microstructures.

Gamma prime morphology nickel-based superalloy turbine disk having dual-microstructures.

(J. Gayda, T. P. Gabb, and P. T. Kantzos, 2004)

The γ’ precipitates are coherently embedded in the γ matrix (γ- γ’ grain). The grain structure can be approximated as a polycrystalline microstructure of a single phase FCC nickel in solidification and grain growth simulation. Each grain is a γ-γ’ composite. The details of γ- γ’ grain is not explicitly described in microstructure generation but will be modeled in dislocation dynamics simulation.
Nickel-based Superalloy Microstructures

A polycrystalline microstructure of superalloy is an aggregate of grains having different orientations. Depending on the heat treatment, the precipitates will comprise of a mixture of primary, secondary and tertiary types. The primary $\gamma'$ is typically between grains of ($\gamma$-$\gamma'$), while the secondary and tertiary are precipitates within the $\gamma$-$\gamma'$ grains.

In the proposed work of Phase I, we put our focus on the microstructures only containing the secondary and tertiary precipitates (the microstructures consist of $\gamma$ - $\gamma'$ grains). Since $\gamma'$ precipitates are coherently embedded in $\gamma$ matrix, they have the same or very similar crystal structures. It is reasonable to model the mesoscale superalloy microstructure realizations as a single-phase polycrystal. Each grain of the microstructure is composed of $\gamma$ matrix and $\gamma'$ precipitates. The properties of the grain take the combination (mixture) of both $\gamma$ and $\gamma'$ features.
Gamma Prime Phase Modeling

- A single γ- γ’ grain is a two-phase structure. The accurate descriptions of a two-phase microstructure morphology are microstructural correlation functions such as n-point probability functions, surface correlation functions, lineal-path function, etc. (e.g. see Torquato, 2002).

- Since γ’ precipitates are regular distributed in roughly cuboidal shapes, the exact configuration of the grain structure (γ’ shape, location, etc.) do not affect the properties in a significant manner. The really important factors are the volume fraction, size, and anti-phase boundary (APB) energy of the precipitates.

- Therefore, in Phase I, we are going to simplify the representation of a γ- γ’ grain using volume fraction and the particle size information of γ’ precipitates. A realization of the γ- γ’ grain can be modeled as a cell in which γ’ particles are uniformly distributed. The number of the precipitates are controlled by the volume fraction and the size distribution. This model is an adequate approximation to real γ- γ’ grains and also can be conveniently adopted in dislocation dynamics simulations.

- In Phase II, we will adopt more sophisticated statistical models to provide more realistic representation of γ- γ’ two-phase structure.
In prior work, a solidification framework of modeling multiphase polycrystalline microstructures was established (L. Tan & N. Zabaras, 2006, 2007a,b,c).

Methodologies and features:
- Level set method for tracking liquid-solid interface (more physical than cellular automata (CA) method).
  \[
  \phi(x, t) = \begin{cases} 
  +d(x, t) & x \not\in \Omega \\
  0 & x \in \Gamma \\
  -d(x, t) & x \in \Omega 
  \end{cases}
  \]
- Assume solidification occurs in a finite width interface to allow proper treatment of energy conservation (\(w \to 0\) is also admissible).
- Energy conservation leads to mesh-Independent growth conditions
- Allow multiple interfaces for modeling multiphase alloy systems

1. A signed distance function for each phase
2. Markers (orientations of the grains) to identify different solid regions.
Large Scale Solidification Process Simulation
High Performance Parallel Computation

Adaptive mesh and Domain Decomposition (using Petsc)
**Multi-scale Solidification Framework**

At each grid node $x$, want to know:

$T(x,t), f^x, \Lambda^x$

**Step 1**

Model $M$

At each grid node $x$, obtain solution and extract features at $x$

$F_M^x$

**Step 2**

At each grid node $x$, find a sample problem $P$ satisfying $F_M^x = F_M^P$

**Step 3**

$T(x,t)$

$\rho c \frac{\partial T}{\partial t} = k \nabla^2 T - \rho L \dot{f}$

$\dot{f}^{x}, \Lambda^x$

$T(x,t)$

$\dot{f}^{P}, \Lambda^P$

Assume $=$
Multiscale Solidification: Predicted Microstructure Features

Results in rectangle: predicted microstructure
Results in the middle: fully-resolved model results
Black solid line: predicted CET transition location
Nickel Superalloy Microstructure Modeling: Task 1

Producing realizations of microstructures
- Generate initial (solidification) microstructures by extending the current framework.
- Phase field /Monte Carlo methods will be employed to model the grain growth process during heat treatment based on the initial microstructures obtained from solidification. Control the temperature and aging time to generate microstructures with different grain sizes (Dual Microstructure Heat Treatment, DMHT).
- The microstructures after heat treatment will be the input to the crystal plasticity constitutive model, which analyzes their mechanical properties.

![Diagram of disk rim and disk bore with microstructure images](image-url)
Nickel Superalloy Microstructure Modeling: Task 1

To be specific, we separate the microstructure generation into the following steps (solidification and grain growth)

1. Generate the initial microstructure using level set solidification method (This step simulates solidification during vacuum arc remelting (VAR))
2. Starting with the initial microstructure generated from solidification, we adopt phase field/Monte Carlo model to control the grain growth of the microstructure (This is the step simulating heat treatment). In this step, different conditions (e.g. temperature, aging time, etc.) will be applied so that microstructures with various grain sizes can be obtained. The large grain microstructures correspond to the ones at the rim of the disk, while small size grains correspond to core structures. This is to mimic the DMHT process.

The final microstructures will be the input model to crystal plasticity simulator, which will estimate the mechanical properties of the superalloy microstructures.

Challenge: Controlling the temperature to obtain desired microstructures.
Microstructure description (grain size, orientation, etc.).
Task 2: Mechanical Properties of Polycrystalline Microstructures

Crystal plasticity constitutive model
Constitutive Model for Nickel-based Superalloys

Develop constitutive model for nickel-based superalloys based on crystal plasticity theory. The constitutive model will be the deterministic simulator in stochastic simulations for quantifying microstructural property variability and the point simulator in multiscale disk forging process.

- Evaluating mechanical properties of realizations of nickel-based superalloy microstructures.
- Predicting mechanical response and texture evolution of microstructures subjected to deformation.

Since in Phase I, $\gamma'$ phase precipitates are coherently embedded in $\gamma$ matrix, we will treat a $\gamma$-$\gamma'$ grain as a single crystal. The crystal plasticity constitutive model adopts the effective properties for the composite of $\gamma$-$\gamma'$ grain.

Methodologies:

- Lagrangian FEM method (allows computing residual stresses)
- Rate-independent crystal plasticity (rate-dependent also available)
- Continuum slip theory
- Homogenization of discrete aggregates
Continuum vs Discrete Microstructure Modeling

Microstructure representation:
Polycrystalline microstructures can be modeled in two ways: Continuum field or discrete grain structure.

Continuum representation:
No microstructure topology. The macroscopic properties are integrated based on ODF over texture space.

Discrete representation:
Microstructure is modeled realistically as grain aggregates. The macroscopic properties are averaged over the microstructure domain.

\[ \langle X \rangle = \int_X X(s,t)A(s,t)\,dv \]

\[ \langle X \rangle = \frac{1}{V} \int_V X\,dV \]
The gain structure topology is not considered. The mechanical property of a microstructure is computed by integrating the microscopic properties over the Rodrigues fundamental zone.

Orientation Distribution Function (ODF) – $A(s, t)$

- Determines the volume fraction of crystals within a region $R'$ of the RF fundamental region $R$
- Probability of finding a crystal orientation within a region $R'$ of the fundamental region
- Characterizes texture evolution

ODF evolution equation (continuum representation) – Lagrangian Description

$$
\frac{\partial A(s, t)}{\partial t} + A(s, t) \nabla \cdot v(s, t) = 0
$$

(S. Ganapathysubramanian and N. Zabaras, 2005)
Discrete Microstructure

A realistic polycrystalline microstructure is modeled as an aggregate of grains. Both topological (grain size, grain shape) and orientational (texture) features are considered.

Grain orientation evolution is controlled by elastic deformation

\[ m_t^\alpha = F^e(t)m_0^\alpha \]
\[ n_t^\alpha = F^{e-T}(t)n_0^\alpha \]

The property of the microstructure is the volume average over all the grains containing in the microstructure

\[ \langle X \rangle = \frac{1}{V} \int_V X dV = \frac{1}{V} \sum_i X_i V_i \]

(W. Li and N. Zabaras, 2009)
Microscale Constitutive Model

Crystal plasticity theory

\[ F = F^e F^p \]
\[ \bar{E}_{\text{trial}} = \frac{1}{2} \left( C_{\text{trial}} - I \right) \]
\[ F_{\text{trial}} = F \left( F_n^p \right)^{-1} \]
\[ C_{\text{trial}} = \left( F_{\text{trial}} \right)^T F_{\text{trial}} \]
\[ \tau_{\text{trial}} = \bar{T}_{\text{trial}} \cdot S_0^\alpha \]

Determine active slip system

\[ PA = \{ \alpha \mid \left| \tau_{\text{trial}} \right| > s^\alpha (t) \} \]
\[ 1 - m : \text{active slip systems} \quad \text{where} \quad b^\alpha = \left| \tau_{\text{trial}} \right| - s^\alpha (t) \]

Hardening law

\[ s^\alpha (t) = s^\alpha (t) + \sum_{\beta \in \text{Active}} h^\alpha \Delta \gamma^\beta, \text{for all } \alpha \]

No grain size effect

\[ \dot{s}(t) = \dot{s}(t) + \frac{k_0 \alpha^2 \mu^2 b}{2 \left( \dot{s}(t) - \dot{s}_0 \right)} \sum_{\beta \in \text{Active}} \lambda^\beta \Delta \gamma^\beta + \theta_0 \left( \dot{s}_s - \dot{s}(t) \right) \sum_{\beta \in \text{Active}} \Delta \gamma^\beta \]

Grain size effect

Update plastic and elastic deformation gradient, Cauchy stress, and PK-I stress, etc.

\[ F^p = \left( I + \sum_{\alpha \text{are active}} \Delta \gamma^\alpha S_0^\alpha \text{sgn}(\tau_{\text{trial}}) \right) F_n^p \]
\[ F^e = F \left( F^p \right)^{-1} \]
\[ \bar{E}^e = \frac{1}{2} \left( (F^e)^T F^e - I \right) \]

(L. Anand and M. Kothari, 1996)
Point simulator
Extend current crystal plasticity constitutive model to two-phase superalloys. The properties of the microstructure will be obtained by homogenization throughout the whole microstructure.

Method 1: Assign different material parameters to grains representing different phases (general two-phase alloys).

Material Parameters of each phase: initial slip resistance $\hat{s}_0$, saturation strength $\hat{s}_s$, shear modulus $\mu$, elastic constants $C_{11}, C_{12}, C_{44}$, material constants $k_0, k_1$, etc.

Optical micrographs of RR1000 superalloy: (a) sub-solvus heat-treated for 4 h at 1130 °C. (Courtesy of Rob Mitchell)
**Planned Constitutive Work – Task 2**

Method 2: In nickel-based superalloys, we plan to assign effective material parameters that describe the properties of the composite of the two-phase, since γ’ phase precipitates are coherently embedded in the γ grains and we model the microstructure as a single phase polycrystal.

The effective parameters will be extracted from the discrete dislocation dynamics model using regression techniques.

![Dark-field transmission electron micrograph of γ' precipitates in a Ni–13.4 at%Al alloy, aged at 640 °C for 1000 h (S. V. Prikhodko and A. J. Ardell, 2003).](image_url)

**Challenge**: How to determine material parameters used in crystal plasticity including the effects of microstructure features (grain size, texture, γ’ volume fraction, γ’ distribution, etc.).
Linking Strategy Between Scales

Dislocation dynamics → Crystal plasticity → Stress strain curve

microscale → mesoscale → macroscale

- Phenomenological model through regression technique. Passing model parameters ($\hat{s}_0$, $\hat{s}_s$, and $\theta_0$).
- Crystal plasticity constitutive model: $\hat{s} = \hat{s}_0 + \theta_0 \left( \frac{\hat{s}_s - \hat{s}}{\hat{s}_s - \hat{s}_0} \right) \sum_{\beta \in \text{Active}} |\Delta y^\beta|$

Homogenization theory. Obtain macroscopic properties or response through volume average.

Uncertainties in microstructure that induce property variability:
Grain size, texture, process parameters, $\gamma'$ volume fraction, size and APB energy.
Task 3: Dislocation Dynamics Simulation of Precipitation Hardened Superalloys
Discrete Dislocation Simulation

The plastic deformation and hardening mechanism of crystalline materials are determined by dislocation motion and interactions. The properties of the high performance superalloys are controlled by the γ’ precipitates coherently embedded in the γ matrix. The hardening effect of γ’ precipitate mainly comes from their resistance to the dislocation motion. Micro-scale discrete dislocation (DD) simulation can give physical insight to the γ’ precipitate hardening and provide basic parameters to the crystal plasticity model.

Tool: ParaDiS  (http://paradis.stanford.edu/)

Virtual experimental procedure:
Force (elasticity theory) -> Velocity (mobility law) -> Topology change -> Properties

Goal: Implement precipitation hardening model and extract parameters used in crystal plasticity.

Discrete Dislocation Dynamics

Dislocation Dynamics (DD) is a numerical method to simulate dislocation motion and interaction behavior in a crystal cell. Since dislocations define plastic yield and flow behavior, the direct simulation of dislocations can provide physical insight to microstructure properties. DD simulation is also referred to as ‘virtual experiment of dislocation behavior’.

Algorithms in ParaDiS:

- Segment-node representation of dislocations.
- Non-singular elasticity theory for estimating stress field.

\[
\sigma_{\alpha\beta}(x) = \frac{\mu}{8\pi} \oint_J \partial_i \partial_p \partial_p R_a \left( b_m \epsilon_{im\alpha} dx'_{\alpha} + b_m \epsilon_{im\beta} dx'_{\beta} \right) \\
+ \frac{\mu}{4\pi(1-\nu)} \oint_J b_m \epsilon_{imk} \left( \partial_i \partial_\alpha \partial_\beta R_a - \delta_{\alpha\beta} \partial_i \partial_p \partial_p R_a \right) dx'_{k}
\]

- Line mobility law to describe the velocity-force relationship.

\[
v_i = \frac{M}{\sum l_{ij}/2} f_i
\]

- Trapezoid integration for computing new positions of nodes.
- Topology changes (split, merge, etc.).
- Fast multipole method to account for long distance interactions.
- Domain decomposition method for high performance parallel computation.

(V.V. Bulatov and W. Cai, 2006)
Benchmark Example: Frank-Read Source (FCC Ni)

\[ M = 51 \text{ GPa}, \quad \nu = 0.37, \quad b = 0.251 \text{ nm}, \quad \text{Mobility} = 10^4 \text{ Ns/m}^2 \]
Massive Dislocation Dynamics Simulation

Core radius = 6b  
Poisson ratio = 3.0e-01  
Temperature = 3.000000e+02  
Edge Mobility = 2.000000e+04  
Core Energy = 0  
Strain Rate = 1.0e+03

Shear Modulus = 28.8 GPa  
Magnitude of Burgers Vector = 0.238000e nm  
Screw Mobility = 2.000000e+04  
Enable Cross Slip  
Strain rate direction = [1 -2 1]
Precipitation Hardening

Ni-based superalloys possess a characteristic microstructure in which cuboidal γ’ phases are precipitated in the γ matrix. The degree of lattice mismatch between the γ and γ’ phases is small and form coherent interfaces. Therefore, dislocations can cut through the particles and a force is exerted on a dislocation when it is creating or recovering an anti-phase boundary (APB).

Consider a straight segment of length $L$ that travels in its normal direction at a distance $n$. The APB energy of the swept area is

$$E_{\text{APB}} = \gamma_{\text{APB}} Ln$$

where $\gamma_{\text{APB}}$ is the inherent APB energy per unit area. Assume that the back force on dislocation is constant inside the precipitate. Then the work performed by the dislocation is

$$W = F_b Ln$$

where $F_b$ is the back force per unit length on the dislocation. From the last two equations, we obtain

$$F_b = \gamma_{\text{APB}}$$

When the next position of a dislocation node $i$ is in the area of γ’ precipitate, or the dislocation expands the APB, the node receives a repulsive force of $F_b$. 
**Precipitation Hardening**

The back force on the dislocation segment is within the slip plane

\[ \mathbf{n} = \frac{\mathbf{b} \times \xi}{\|\mathbf{b} \times \xi\|} \]

The force on the segment \( i \) is perpendicular to the segment

\[ \mathbf{f}_i = \frac{\mathbf{n}_i \times \xi_i}{\|\mathbf{n}_i \times \xi_i\|} \cdot \chi_{APB} \cdot L_i \]

Assume the segment force is uniformly carried by the two nodes (A, B) at its ends

\[ \mathbf{f}_{A,i} = \mathbf{f}_{B,i} = \frac{\mathbf{n}_i \times \xi_i}{\|\mathbf{n}_i \times \xi_i\|} \cdot \chi_{APB} \cdot \frac{L_i}{2} \]

The total nodal force is modified as the sum of segment-segment interactions, external applied stress field induced PK force and the local back force from cutting the precipitate.

\[ \mathbf{f}_i = \mathbf{f}_{i}^{el} + \mathbf{f}_i^{ext} + \mathbf{f}_i^{precip} \]
Precipitate Obstruction of Dislocation Motion

No precipitate

A precipitate at (0, -4000, 10500)b
Radius = 500b
APB = 500000 mJ/(m²)
Frank-Read Source in Precipitation Hardened Superalloy
Precipitation Hardening Effect

APB energy density = 200 mJ/m², radius ~ N(100b, (10b)^2)
The precipitates are uniformly distributed in the simulation cell.

(B. Wen and N. Zabaras, 2010)
**DD Simulations of Precipitation Hardening: Task 3**

Complete current precipitation hardening model and extract material parameters that can be used in the crystal plasticity model. Probing the precipitate effect on superalloy properties. Conduct simulations with massive dislocations and multiple precipitates in 3D simulation cell. The cuboidal precipitates are uniformly distributed in the simulation cell with size following the WLS distribution theory (A.L. Kulkarni and K. Krishnamurthy, 2004).

![Proposed initial configuration of DD simulation.](image)

**New:** Three dimensional massive dislocation dynamics in precipitation hardened superalloys.

**Challenge:** How to model the precipitation hardening; Computational efficiency.
Linking Dislocation Dynamics and Crystal Plasticity: Task 3

In crystal plasticity, we can write the hardening law as

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

where \( \hat{s} \) is the critical resolved shear stress (CRSS) of a slip system, \( \hat{s}_0 \) is the initial slip resistance, \( \hat{s}_s \) is the saturation slip strength, \( \theta_0 \) is the initial hardening rate. In this equation, \( \hat{s}_0 \), \( \hat{s}_s \), and \( \theta_0 \) are not known beforehand. We can further modify the hardening equation to the form when a constant strain rate is applied

\[
\hat{s} = \hat{s}_s - (\hat{s}_s - \hat{s}_0) \exp\left(-\frac{\theta_0}{\hat{s}_s - \hat{s}_0} C t\right)
\]

Extracting CRSS relationship with time from DD simulation, we can curve fit those parameters and use them in the crystal plasticity model.

In this way, the DD simulation is linked to crystal plasticity.
Source of Uncertainties in DD Simulation

- The topology of the simulation cell, the configuration and APB energy of γ' precipitates, and the input parameters to DD determine the mechanical response of the simulation. Since precipitate information is provided by volume fraction and size distribution, many realizations of precipitate configuration can be generated given the same information, and each of them will result in a specific mechanical response. Therefore, the material parameters ($\hat{s}_0$, $\hat{s}_r$, and $\theta_0$) fitted from each simulation will vary. This results in uncertainties.

- Multiple simulations will be performed to obtain a statistical description of these parameters (distributions). The uncertainty about the parameters will be a source to the following probabilistic studies of turbine disk properties (to be undertaken in Phase II).
Task 4: Variability of Mechanical Properties Due to Uncertainties in Microstructures and Process Parameters

Probabilistic Learning of Polycrystal Properties
Problem definition

- Employing appropriate mathematical representation of random fields (microstructures, process parameters, etc.).
- Reducing high-dimensional random fields.
- Exploring variability in material properties/response due to microstructure and process uncertainties.
- Predicting material properties/response given microstructure statistic information or/and process parameters.
Variability of Macroscopic Response Due to Microscopic Feature Uncertainties.

Texture, grain size effects
Variability of Material Properties

Problem definition

Given:
- Grain size snapshots constrained by moments (mean size, standard deviation, higher-order moments).
- Texture snapshots from random process.

Goal:
- The variability in material properties and response

Methodologies

- Model reduction to reduce the complexity of stochastic input
  - Nonlinear Model Reduction (manifold learning) to reduce grain size space
  - Karhunen-Loeve Expansion to reduce texture space

- Adaptive sparse grid collocation to solve stochastic partial differential equations (modeling of deformation, thermal, etc. in random microstructures)

(Z. Li, B. Wen and N. Zabaras, 2010)
Simulation Procedure

Get grain size and texture snapshots

Grain size: Nonlinear Model reduction
Texture: Karhunen-Loeve Expansion

Reduced features

Adaptive sparse grid collocation
reconstruct

Deterministic solver

Construct property distributions
Microstructure Representation

Microstructures obtained from certain processes satisfy some specific experimentally determined statistics of grain size distribution.

Each microstructure that satisfies the given statistics of the grain size distribution is a point that lies on a manifold embedded in a high-dimensional space.

Grain size descriptor: “sorted grain size vector”

Euclidean distance: different of two microstructures

\[ D(A, B) = \left( \sum_{i=1}^{n} (GS_i^A - GS_i^B)^2 \right)^{1/2} \]
Nonlinear Model Reduction on Grain Size Feature

Given a set of \( N \) unordered points belonging to a manifold \( \mathcal{M} \) embedded in a high-dimensional space \( \mathbb{R}^n \), find a low-dimensional region \( \mathcal{A} \subset \mathbb{R}^d \) that parameterizes \( \mathcal{M} \), where \( d << n \).

(B. Ganapathysubramanian and N. Zabaras, 2008)
Texture Modeling

The properties of a polycrystalline microstructure are highly dependent on its texture: orientation distribution of grains.

Orientation representation: Rodrigues parameters

$$r_1 = w_1 \tan \frac{\phi}{2}, \quad r_2 = w_2 \tan \frac{\phi}{2}, \quad r_3 = w_3 \tan \frac{\phi}{2}$$

Texture representation: Orientation Distribution Function (ODF)

A discrete form: $$\tau(r) = \left\{ r_1^1, r_2^1, r_3^1, \ldots, r_1^n, r_2^n, r_3^n \right\}$$

12 slip systems in FCC

$$m^\alpha_{\text{local}} : \langle 111 \rangle$$

$$n^\alpha_{\text{local}} : [110]$$

Orientation dependence of slip system (anisotropy in crystalline materials)

$$m^{j,\alpha} = R^j m^\alpha_{\text{local}}$$

$$n^{j,\alpha} = R^j n^\alpha_{\text{local}}$$

where

$$R^j = \frac{1}{1 + r^j \cdot r^j} \left( I (1 - r^j \cdot r^j) + 2 \left( r^j \otimes r^j - I \times r^j \right) \right)$$
Generation of Initial Texture Samples

Initial texture samples can be obtained by a sequence of random processing simulations with various deformation rate

\[
L = \omega_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & -0.5 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_3 \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \omega_4 \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \omega_5 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \omega_6 \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \omega_7 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} + \omega_8 \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\]

\[\omega_1, \omega_2, \ldots, \omega_8\] are random coefficients corresponding to tension/compression, plain strain compression, shear and rotation.

The slip systems are updated during deformation as

\[
m^\alpha_t = F^e(t)m^\alpha_0
\]
\[
n^\alpha_t = F^{e-T}(t)n^\alpha_0
\]

Therefore the new orientations can be recovered from the rotation part of the elastic deformation gradient.

\[
F^e(t) = R^e(t)U^e(t)
\]
Karhunen-Loeve Expansion on Texture Samples

Deterministic texture $\tau_0$ → Random process controlled by $\{\omega_1, \omega_2, \ldots, \omega_8\}$ → Initial texture samples $\tau_1, \tau_2, \ldots, \tau_N$

Given $N$ texture examples, construct covariance matrix of these samples

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

The truncated Karhunen-Loeve Expansion of a random vector $\tau$ is

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

where $\phi_i, \lambda_i$ are the $i$th eigenvector and eigenvalue of $\tilde{C}$, respectively. $\{\eta_i(\omega)\}$ are a set of uncorrelated random variables satisfying

$$E(\eta_i(\omega)) = 0, \quad E(\eta_i(\omega) \eta_j(\omega)) = \delta_{ij}, \quad i, j = 1, \ldots, d$$

Texture random field thus transformed to low-dimensional space $\eta \in \mathbb{R}^d$
Maximum Entropy Estimation of the Distribution of $\eta$

To sample new texture, we can sample $\eta$ instead, and then transform it back to the texture space. The distribution of $\eta$ is needed.

**Maximum Entropy Estimation (MaxEnt):** amongst the probability distributions that satisfy our incomplete information about the system, the probability distribution that maximizes entropy is the least-biased estimate that can be made. In agrees with everything that is known but carefully avoids anything that is unknown.

The form of MaxEnt distribution is

$$p^*(x) = \frac{e^{-\sum_{n=1}^{N} \lambda_n f(x)}}{Z}, \quad Z = \int e^{-\sum_{n=1}^{N} \lambda_n f(x)} \, dx$$

which maximize the entropy

$$H(p) = -\sum_{i=1}^{M} p(x_i) \log(p(x_i))$$

and satisfies constraints

$$E(f_n(x)) = M_n, \quad n = 1, 2, ...$$

When the uncorrelated constraints are satisfied, the MaxEnt distribution is a standard Gaussian distribution

$$\eta \sim N(0, I)$$
Inverse CDF Transformation

Uncorrelated Gaussian random variables are independent in current case. To employ Sparse Grid Collocation method, Gaussian distribution needs to be transformed to a uniform hypercube $[0,1]^d$.

The cumulative distribution function (CDF) for standard Gaussian is

$$\Phi_{\eta_i}(\eta_i) = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{\eta_i}{\sqrt{2}} \right) \right]$$

which is uniformly distributed in $[0,1]$. Given a point in the hypercube $\zeta \in [0,1]^d$, we can also find a corresponding point in the original distribution by

$$\eta_i = \Phi^{-1}(\eta_i), \quad i = 1,\ldots,d$$

This process transforms a node in sparse grid back to a point in Gaussian distribution, and it can be further recovered to a texture realization.
Adaptive Sparse Grid Collocation

Sparse grid collocation is an effective method (more efficient than Monte Carlo Method) to solve SPDEs with controlled error. It approximates the multi-dimensional stochastic space using interpolating functions on a set of collocation points.

The interested function can be approximated by

$$u(x, \xi(\omega)) = \sum_{|i| \leq q} \sum_{j} \omega_j^i(x) a_j^i(\xi(\omega))$$

Hierarchical surplus

Interpolating function

The mean of the random solution is evaluated as

$$E(u(t)) = \sum_{|i| \leq q} \sum_{j} \omega_j^i(x) \cdot \int_L a_j^i(\xi) d\xi$$

In the context of adaptivity, new support nodes are added to the hypercube only if the error indicator is larger than a threshold $\varepsilon$:

$$\gamma_j^i = \frac{\| \omega_j^i(x) \cdot \int_L a_j^i(\xi) d\xi \|_{L_2}}{\| E_{|i|-d-1} \|_{L_2}} > \varepsilon$$

Ma and Zabaras, JCP, 2008, 2010
Variability of Mechanical Response (Discrete Representation)

Grain size effect

Effective stress distribution at strain 0.2

Grain size sample constraints:

1. Mean volume 0.0185 mm³
2. 2nd moment 3.704x10⁻⁴ mm⁶
3. 3rd moment 8.637x10⁻⁶ mm⁹

Initial texture generated by

\[
L = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_3 \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}
\]

Initial texture generated by

\[
L = \omega_1 \begin{bmatrix} 0.5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \omega_2 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \omega_3 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{bmatrix}
\]
Variability of Macroscale Properties (Continuum Representation)

- Uncertainty in underlying micro-structure (continuum Texture)

Approach

- Karhunen-Loeve expansion
- Maximum Entropy Principle

\[ A_0(s, \omega) = \hat{A}_0(s) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} f_i(s, t) Y_i(\omega) \]

Continuum representation of texture in Rodrigues space

Variation of stress-strain response

(K. Kouchmeshky and N. Zabaras, 2009) Property convex hull
Modeling the Effects of Microstructural Uncertainty: Task 4

- Develop reduced-order stochastic representations of Ni superalloy microstructures – this is a data-driven approach (using either simulated from Task 1 microstructures or experimental snapshots).

- Use this stochastic input models together with adaptive sparse grid collocation methods to produce complete probabilistic description of homogenized properties of superalloy microstructures.

- Compute the convex hull of mechanical properties of Ni-superalloy microstructures induced by uncertainty in the description of the microstructures. Compute the affiliated probabilities for these properties.

- These developments will be critical in Phase II of the project towards a materials design approach.
Task 5:
Variation of Macro-scale Properties Due to Multi-scale Sources of Uncertainties

A model reduction of the multiscale input for uncertainty quantification in multiscale deformation processes
In the one way coupling, the uncertainty is localized, i.e. the random microstructures are not the same (from the same distribution) at different locations.

In this case, the random support space is the tensor product of all the support of the random variables. It will result in thousands of random variables on the macroscale.

Most of the computational methods are intractable unless we can find the correlation between all the microstructures and construct a reduced order model.
At each macro scale point, due to the randomness of the microstructure, we will have a set of (microstructure) samples (realizations).

One can construct a reduced order stochastic model for each point (e.g. linear or non-linear POD). However, in this case, the reduced-order model cannot see the correlation between the set of random variables at different macro points.

This will result in a huge dimension of the random space and thus the problem becomes computationally intractable.
**Construct the Reduced Order Representation of Texture**

Step 1: Start from realizations of the texture

\[ A_i(x, s, \omega) \]

Step 2: Transform the realization using

\[ \tilde{a}_i(x, s, \omega) = \log(A_i(x, s, \omega) - A_{\text{min}}) \]

\[ \tilde{a}_i(x, s, \omega) = \bar{a}(x, s, \omega) + \tilde{a}_i(x, s, \omega) \]

Step 3: Construct the Covariance using the snapshots

\[ C(s, s') = \frac{1}{n_r} \sum_{j=1}^{n_r} \sum_{i_n=1}^{n_r} \sum_{i_m=1}^{n_r} \tilde{a}_j(x_{i_n}, s, \xi_j) \tilde{a}_j^T(x_{i_m}, s', \xi_j) \hat{\eta}_{i_n} \left| J_{i_m} \right| \]

Step 4: Obtain the eigenvalues and eigenvectors: \( \rho_i, \psi_i(s) \)

Step 5: Obtain the spatial modes

\[ \Phi_i(x, \omega) = \frac{1}{\sqrt{\rho_i}} \int_{\Omega} \tilde{a}(x, s, \omega) \psi_i(s) ds \]

Step 6: Decompose the spatial modes using the polynomial Chaos:

\[ \Phi_i(x, \omega) := \Phi_i(x, \zeta_1(\omega), ..., \zeta_n(\omega)) = \sum_j \phi_{ij}(x) \eta_j(\omega) \]

\[ \phi_{ij}(x) = \frac{\langle \Phi_i(x, \zeta) \eta_j \rangle}{\langle \eta_j^2 \rangle} \]

\( \eta_i(\omega) \) are in a one to one correspondent to the Hermite polynomials.
Mechanical Properties of Forging Workpiece

Comparison between the original microstructure and the reduced order one

Original

Mean(B)

Var(B)

Reconstructed

Mean(G)

Var(G)

Mean(E)

Var(E)

Effects of Uncertainty in Initial Texture

Mean(B)

Var(B)

Mean(G)

Var(G)

Mean(E)

Var(E)

(B. Kouchmeshky and N. Zabaras, 2010)
**Property Variability of Ni Superalloys: Task 5**

**Computing variability in properties induced by microstructure uncertainty**
- Embedding new point simulator in stochastic framework. Predicting variability in microstructures and mechanical properties (including residual stresses) in a forged product.

- To be specific, the variability of the property of a microstructure comes from both the polycrystal features and the γ’ precipitate character. The uncertainties in polycrystal features such as grain size and texture effect can be analyzed as demonstrated earlier. Moreover, in nickel-based superalloy, the precipitate distribution, volume fraction, size, and APB energy affect the properties significantly.

- These characters are also random fields. In our model in Phase I, the effects of precipitates are evaluated using DD simulation and accounted through the parameters in the crystal plasticity model. For different initial configuration of dislocations and precipitates, the results will provide distinct properties. Therefore, in the proposed work for superalloy, material parameters such as the initial slip resistance, the saturation slip strength, and the initial hardening rate are also treated as random inputs. The statistics of these parameters are about to be obtained through multiple DD simulations (Monte Carlo Sampling).
Furthermore, due to the location dependence of the microstructure, the random fields of microstructure features and parameters are in general high dimensional. Bi-orthogonal decomposition is required for the multi-scale microstructure model reduction (this decomposition captures the correlation of microstructures from point to point).

Process parameters are also the source of uncertainties. Since different parameters result in distinct microstructures, their effect on the properties are accounted by the uncertainties in microstructures.
**Summary: Tasks 4 and 5**

**New**: Model reduction on multi scales, stochastic analysis, and multiscale deterministic solver will be integrated to facilitate the probabilistic prediction.

**Challenge**: Finding appropriate (sufficient and limited) features of superalloys that affect the mechanical properties. The metric of representing superalloy microstructures. Effective model reduction technique to reduce high-dimensional spatial dependent random fields. Reconstruction of the microstructure.

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<td>Grain size distribution</td>
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<td>In Phase II, bi-orthogonal decomposition will be developed and employed to address the curse of dimensionality in stochastic multiscale forging simulations</td>
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<td>Process parameters</td>
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Probabilistic prediction of mechanical properties of superalloy turbine disks.

In Phase II, bi-orthogonal decomposition will be developed and employed to address the curse of dimensionality in stochastic multiscale forging simulations.
Task 6: Initiate Multiscale Framework
**Initializing Multiscale framework: Task 6**

In the optional phase, we plan to initialize the multiscale framework of modeling a turbine disk. The crystal plasticity constitutive model will be coupled with the disk forging simulation. Each macro point on the disk will be associated with an underlying microstructure obtained from phase field model. The deformation of the microstructure is controlled by the forging process in the macroscale, while the mechanical properties and texture evolution will be captured, more precisely, based on the crystal plasticity constitutive model, whose parameters are extracted from microscale DD simulation. The linking between macroscale and mesoscale is based on homogenization theory.

![Multiscale framework of turbine disk forging](image)
Work Tasks
Work Tasks

Task 1: Producing realizations of microstructures
Extend current microstructure evolution tool to model dual microstructures (various grain size at different location).

Task 2: Point simulator
Extend current crystal plasticity constitutive model to two-phase alloys.

Task 3: Dislocation dynamics simulations of precipitation hardening
Complete current precipitation hardening model and extract material parameters that can be used in crystal plasticity model. Probing the precipitate effect on superalloy properties. Conduct a simulation with massive dislocations and multiple precipitates in 3D simulation cell, so that the complex interactions are accounted.

Task 4: Computing variability in properties induced by microstructure uncertainty
Embedding new point simulator in stochastic framework. Predicting variability in microstructures and mechanical properties.

Task 5: Forming of turbine disk
Modify current forging program to model turbine disk forming process.

Task 6: Preliminary developments towards a multiscale framework (Option)
# Proposed Tasks, Timeline and Milestones

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<th>Task Name and Team Player</th>
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<td>Producing realizations of microstructures (ADI, CU)</td>
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<td>2</td>
<td>Point simulator (ADI, CU)</td>
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<td>3</td>
<td>Dislocation dynamics simulation with precipitation hardening (ADI, CU)</td>
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<td>Showing variability in properties induced by variations in microstructures (ADI, CU)</td>
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## Milestones

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<td>6</td>
<td>Phase I Final Report (ADI, CU) X</td>
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Design of microstructure-sensitive properties in elasto-viscoplastic polycrystals

Related Work for Phase II
Problem definition

- Developing a Multi-scale, multi-stage design platform in the presence of microstructure and process uncertainties.

- Turbine disk forging simulator.

- Optimizing the probabilistic distribution of disk process parameters and microstructures for desired properties.
Prior Work

Continuum sensitivity method for microstructure design

1. Discretize infinite dimensional design space into a finite dimensional space
2. Differentiate the continuum governing equations with respect to the design variables
3. Discretize the equations using finite elements
4. Solve and compute the gradients
5. Gradient optimization

(V. Sundararaghavan and N. Zabaras, 2008)
Definition of homogenized velocity gradient

\[ \overline{L} = \overline{FF}^{-1} \]

Decomposition of homogenized velocity gradient into basic 2D modes – Plane Strain Compression, Shear and Rotation

\[ \overline{L} = \alpha_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \alpha_2 \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \alpha_3 \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

Design objective – to minimize mean square error from discretized desired property (\( \Omega \))

\[
\min_{\alpha} F(\alpha) = \frac{1}{N_s} \sum_{i=1}^{N_s} \left( \Omega^i \left( B(\alpha) \right) - \Omega^i_{\text{desired}} \right)^2
\]
Multi-scale Sensitivity Analysis

- Perturbed homogenized deformation gradient
  \[
  \overset{o}{\bar{F}}_{n+1} = \left( \overset{o}{\bar{F}}_n + \overset{o}{\bar{L}}_{n+1} \Delta t \right) \left( I + \bar{I}_{n+1} \Delta t \right)
  \]

- **Sensitivity linking assumption:**
  The sensitivity of the averaged deformation gradient at a material point is taken to be the same as the sensitivity of the deformation gradient on the boundary of the underlying microstructure, in the reference frame.

- Sensitivity equilibrium equation (Total Lagrangian)
  \[
  \nabla_o \cdot \bar{P} = 0
  \]
Sensitivity equations for the crystal constitutive problem

- Sensitivity hardening law

\[ \frac{\partial s^\alpha}{\partial t} = \sum_\beta \left[ h^{\alpha\beta} \gamma^\beta + h^{\alpha\beta} \hat{\gamma}^\beta \right] \]

- Sensitivity flow rule

\[ \mathbf{L} = \sum \left[ \frac{\partial \dot{\gamma}^\alpha}{\partial \tau^\alpha} \tau^\alpha + \frac{\partial \dot{\gamma}^\alpha}{\partial s^\alpha} s^\alpha + \frac{\partial \dot{\gamma}^\alpha}{\partial \theta^\alpha} \theta^\alpha \right] s^0 \]

\[ \frac{\partial \dot{\mathbf{F}}^\rho}{\partial t} = \mathbf{L} \dot{\mathbf{F}}^\rho + \dot{\mathbf{L}} \mathbf{F}^\rho \]

- Sensitivity constitutive law for stress

\[ \ddot{\mathbf{T}} = \left( \frac{\partial \mathbf{C}^e}{\partial \theta} \right) \dot{\mathbf{E}}^e + \mathbf{C}^e \left[ \text{sym} \left( \mathbf{F}^{eT} \dot{\mathbf{F}}^e \right) \right] \]

- From this derive sensitivity of PK 1 stress

\[ \dot{\mathbf{P}} = \mathbf{B} \dot{\mathbf{F}} + \mathbf{A} \dot{\theta} + \mathbf{B} \]

(V. Sundararaghavan and N. Zabaras, 2006)
Example: Design of process modes for a desired response

Desired response

Final microstructure of the design solution

Misorientation map

Change in Neo-Eulerian angle (deg)

Cost function

Iterations

(a) Desired response
(b) Equivalent stress (MPa) vs. Time (sec)
(c) Misorientation map
(d) Cost function vs. Iterations
Design for response in the second stage after unloading

At the end of stage 1

After unloading

During stage 2
Proposed Work: Phase II

- Applying continuum sensitivity method (CSM) to turbine disk design in a multiscale, multistage stochastic framework.
- Computational design of deformation process for desired microstructure-sensitive properties in the presence of uncertainty.

New: Multiscale, multistage optimization framework.
Challenge: Reduction of random fields so that the optimization is feasible.
Merit: Design and optimize the distribution of mechanical properties of turbine disk product.