ADVANCED COMPUTATIONAL TECHNIQUES FOR MATERIALS-BY-DESIGN

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Abstract

The objective of this work is to address a number of mathematical and computational issues critical to the development of a robust multi-length scale and multi-stage deformation process design simulator for the control of microstructure-sensitive properties in aircraft manufacturing applications. As part of the research effort, multiple technical developments are being accomplished. An efficient framework for accurately assessing the effect of uncertainty in process and material parameters, in initial conditions and in the microstructure has been developed. A spectral polynomial chaos framework as well as a novel support space method have been developed for analyzing uncertainty in metal forming problems. On the meso-scale, robust statistical learning techniques as well as gradient based methods have been formulated for process sequence selection and design of highly optimized synthetic microstructures. Maximum entropy concepts have been used to develop an algorithm for efficient reconstruction of microstructure classes using a limited number of microstructure realizations. It is strongly believed that these advanced techniques can drastically improve process and material predictions in critical components.

1 Status of effort

Substantial progress has been made in the achievement of the project objectives in the second year of this project. Particular contributions are briefly summarized below with more details given in the provided references.

1.1 Development of a novel probabilistic framework for analysis and design of metal forming processes [1]

This work introduces algorithms for quantifying uncertainty propagation in finite deformation problems. The first algorithm is based on the the Spectral Stochastic Finite Element Method (SSFEM). A spectral expansion of the current configuration of a deforming body is proposed using Legendre chaos expansions to compute the stochastic deformation gradient which is in turn used to compute the stochastic analogs of the various quantities which appear in large deformation analysis. A total Lagrangian approach to the stochastic large deformation is presented. The second algorithm is based on a finite element representation of the support space of the random variables. An example considering the effect of uncertainty in the state variable on the response of a heterogeneous tension specimen

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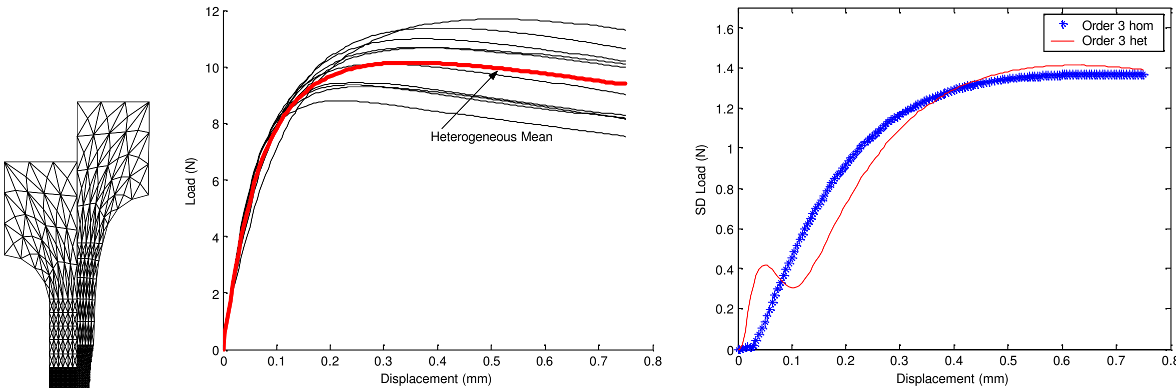

Figure 1: *Initial and final mean configuration for deterministic problem (left). Mean (center) and standard deviation (right) of load versus displacement. One simulation is able to provide complete probabilistic description of the propagation of uncertainty (here in the initial material state) during the deformation process.*

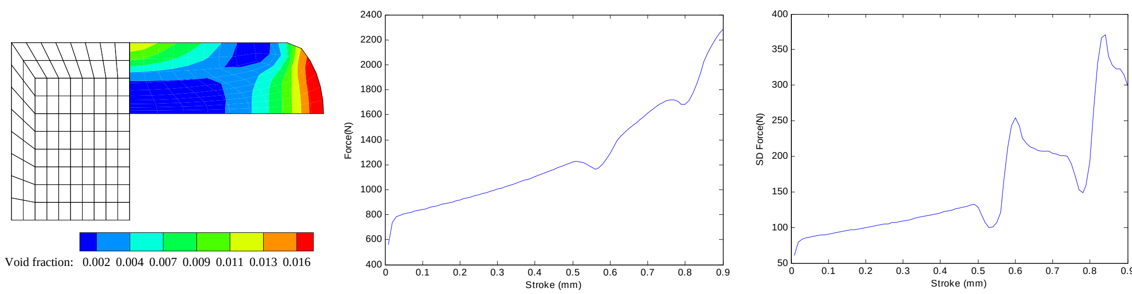

Figure 2: *Stochastic simulation of a cylinder upsetting process with randomness in the initial radius and the die workpiece friction. Initial and final mean configurations (left). Mean (center) and standard deviation (right) of the force versus stroke for the upsetting process. Initial and final mean configurations for the cylinder upsetting process (right).*

modeled using SSFEM is shown in Fig. 1. An example of open die forging under random preform shape and die-workpiece friction modeled using the support space method is shown in Fig. 2. Note that the support method provides the potential of full probabilistic analysis of complex deformation (and other continuum pde-based – see [2]) systems using legacy software for deterministic analysis of the underlying physical mechanisms (e.g. the deterministic 3D forming computational design simulator under development [3]).

1.2 Development of a multiscale microstructure design framework for polycrystalline materials

Many engineering materials are polycrystalline in nature and the presence of crystallographic characteristics like texture and misorientations affects several important physical properties. Deformation process design for control of microstructure sensitive properties involves development of a multi-scale tool where it would be possible to design required process sequence and macroscopic process parameters (die and preform shapes, forging velocities, etc.) [3]. In the second year of this project, we demonstrated innovative computational techniques including statistical learning, reduced order optimization [4], and multi-scale sensitivity analysis for designing deformation processes to tailor microstructures to achieve desired properties. Key recent developments are listed below:

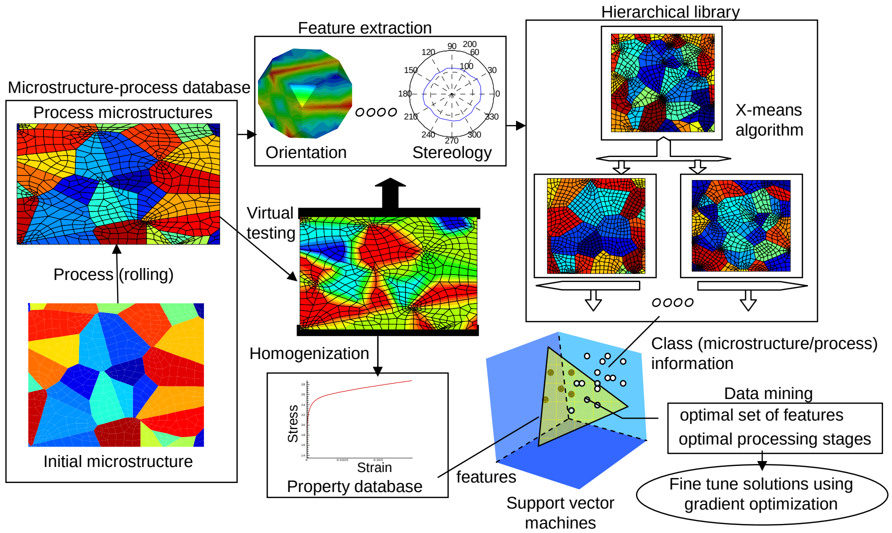

Figure 3: *A schematic of the statistical learning driven microstructure feature selection and design algorithm.*

- A toolbox for evaluating strength of polycrystalline microstructures based on image meshing and multi-scale homogenization techniques [5, 6]:

  We have recently developed tools for evaluating large strain mechanical response from 2D and 3D polycrystalline microstructures. Using microstructural images and the single crystal constitutive laws as input, the tool can be used by the forming industry to identify processing stages that would fine-tune the properties of microstructures. Statistical learning based methods have been developed to automate decision making. These design solutions can be used in conjunction with gradient optimization schemes for optimizing microstructure-sensitive properties. We have included meshing capabilities of the NIST software OOF-2 and parallel finite element processing tools. The method of multi-scale homogenization in the large strain regime is utilized to calculate the stress-strain response of microstructures consisting of aggregates of grains. The key goals of this tool is to provide engineers with a user-friendly yet powerful environment for conducting virtual tests with microstructural images with the goal of designing microstructures with desired strength.

- Optimal selection of textural and stereological features using statistical learning techniques [7, 8, 9, 10]:

  Since material behavior is determined by its microstructure, it is a problem of interest to evaluate the best microstructure that is suited for a particular application. A key problem is identification of the set of features suitable for a material used in a particular application and thus, also identify the processes that would lead to such features. We employ statistical learning tools for exploring the feature-property design space and thus, unearth the best microstructures for an application. Through microstructure interrogation schemes based on polycrystal plasticity theory, we create databases that explore a large range of anisotropic properties achievable in polycrystalline microstructures through thermo-mechanical processing. The schematic of the computational design scheme is presented in Fig. 3.

1.3 Information-theoretic microstructure reconstruction from available statistical information

Microstructures can be considered as realizations of a random process. The knowledge of this random process is limited since we are provided only with a set of features that the microstructure exhibits. Our task lies in reliably predicting the class of microstructures from this truncated description. Our interest also lies in obtaining property statistics of the microstructure of interest. In obtaining the samples generated using this random process, we use the principle of maximum entropy [11].

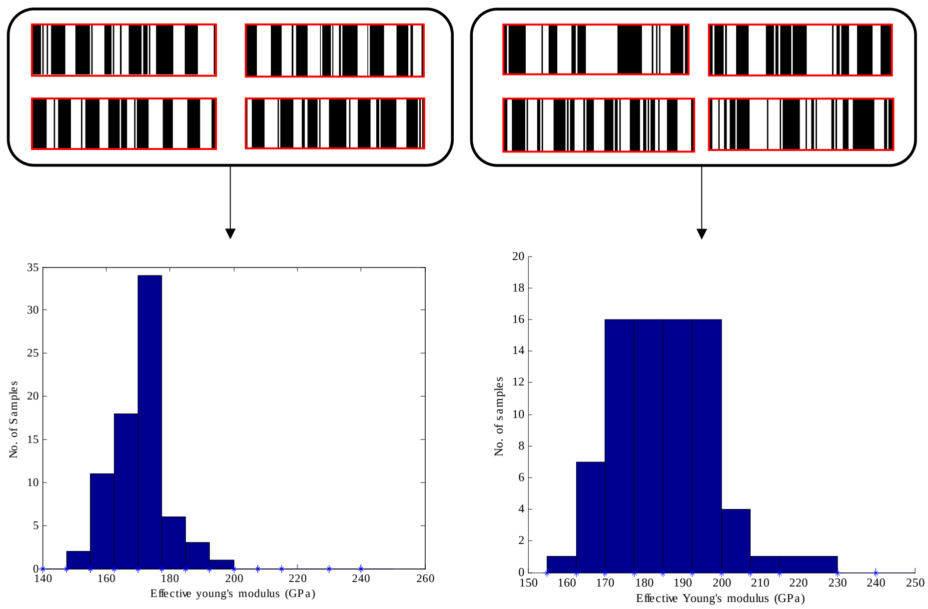

Figure 4: *(a) Samples of microstructure reconstructed using two-point correlation function as well as lineal path functions. The statistics of elastic properties that are obtained is shown (b) Samples of microstructure reconstructed using two-point correlation function. The statistics of elastic properties that are obtained is also shown.*

As a demonstration we show the reconstruction of one-dimensional hard-rods: Analytical expressions are available for two-point and lineal path correlation functions of 1d hard rod structures. Two means of reconstructions are considered in this section: (i) Reconstructing hard-rods from two-point correlation functions alone (ii) Reconstructing hard-rods from two-point and lineal path functions. Samples of 1d hard rods and their property statistics are shown in Figure 4. The statistics of properties clearly shows that in the case of incorporating more amount of information (connectivity information in the form of lineal path functions), the statistics are more sharp indicating the class of microstructures satisfying this condition is more profound.

A reconstruction of microstructure with short range correlations is shown in Fig. 5. Herein, we assume that the reconstructed microstructures are isotropic and homogeneous. Some examples of such materials include porous media, randomly polymerized plastics, and other. Our aim is to reconstruct these materials from their two-point correlation functions. Figure 5 shows some samples of porous materials with short range order that are reconstructed using the MAXENT scheme and the associated elastic property statistics.

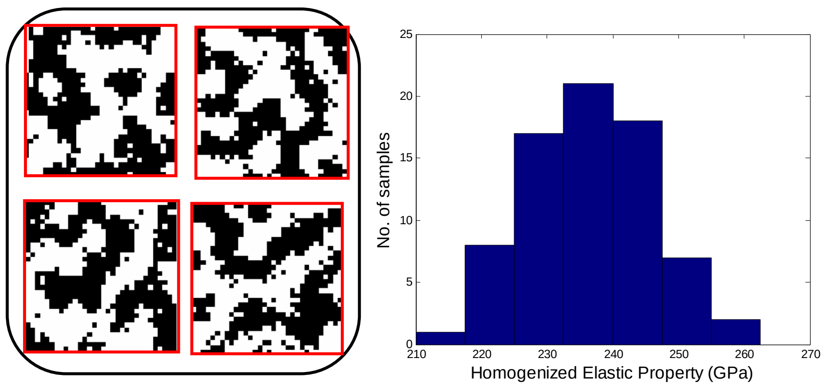

Figure 5: *Some samples of materials with short range order reconstructed in a* 32×32 *grid.*

We plan to explore the utility of this MAXENT-based reconstruction of microstructure classes in the context of a stochastic multiscale analysis and design. For example, the variability of the initial material state discussed in the example of Section 1.1 (refer to Fig. 1) can be obtained from a maximum entropy analysis using a finite number of experimental realizations of the polycrystal microstructure. Preliminary algorithms for such problems are discussed in [12].

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3 Honors & Awards Received

A number of key note and invited lectures were given based on this work. Complete details and power point presentations are given at http://mpdc.mae.cornell.edu/Publications/lectures.htm.

4 AFRL Point of Contact

This work is being communicated with the AFRL group of Dr. R. Dutton AFRL/MLLM.

5 Transitions

While no immediate commercialization plans are in place for the developed computational mathematics technologies, we strongly believe that their transition to immediate needs of AFRL and industrial partners is forthcoming.

6 New Discoveries

(a) Innovative statistical algorithms for exploring process/structure/property relations; (b) The first techniques reported for full-probabilistic modeling of deformation processes; (c) the first multiscale process design simulator being developed.