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Uncertainty quantification for multiscale disk forging of polycrystal materials using probabilistic graphical model techniques

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ABSTRACT

The mechanical properties of a deformed workpiece are sensitive to the initial microstructure before processing commences. Generally, the initial microstructure is random in nature and location specific. The location-dependence of the microstructure dramatically increases the dimensionality of the stochastic input and thus leads to the "curse of dimensionality" in stochastic deformation problems. In this work, a graph-theoretic approach is used to address the stochastic multiscale deformation problem and compute the propagation of the initial microstructure uncertainty to the forged disk properties. Following the finite element representation of the multiscale deformation problem, a graphical representation is introduced with nodes in the graph representing the macro- and meso- scale random variables and links between nodes modeling the dependence relations between variables at each scale and across scales. Model reduction techniques are employed locally in the graph to represent the initial random microstructure. Then the conditional distribution of the multi-output mechanical responses on the low-dimensional representation of the initial microstructure is factorized into a product of local potential functions. An expectation-maximization algorithm is used to learn the non-parametric representation of these potentials using a set of training data. A non-parametric loopy belief propagation method is applied to perform uncertainty quantification tasks. The non-parametric nature of the model is able to capture non-Gaussian features of the responses. The developed framework can be used as a surrogate model to predict the mechanical response fields for any input microstructure realization as well as our confidence on such predictions. A multiscale disk forging example of FCC nickel is presented to demonstrate the accuracy and efficiency of the constructed framework for addressing uncertainty quantification problems in multiscale deformation processes.

1. Introduction

The macro-scale properties of polycrystalline materials (e.g. metals, alloys, etc.) are sensitive to the underlying microstructure. Microstructure uncertainty at a material point has been extensively studied using a variety of methods. For example, in [1,2], the principle of maximum entropy (MaxEnt) was used to describe the microstructure topology of two-phase and polycrystalline materials. A set of correlation functions or grain size moments were given as the prescribed constraints. Realizations of microstructures were then sampled from the MaxEnt distribution and interrogated using appropriate physical models, e.g., a crystal plasticity finite element method (CPFEM) [3]. The Monte Carlo (MC) method was adopted to compute the error-bars of the effective stress–strain response of face-centered-cubic (FCC) aluminum. In [4], the orientation distribution function (ODF) was adopted to describe the polycrystalline microstructure. A number of ODF samples were given as the input data. The Karhunen-Loève expansion (KLE) [5,6] was utilized to reduce the input complexity and facilitate the high-dimensional stochastic simulation. The stress–strain curve with error bars and the convex hull of elastic moduli of FCC aluminum after deformation were studied. Mechanical response variability due to both orientation and grain size uncertainties were studied in [7].

In this work, we are interested in modeling the variability of properties of the workpiece in a deformation process induced by variability in the initial microstructure. Therefore, we need to model the stochastic space of initial microstructures in the workpiece, not simply at a material point. To quantify the effect of microstructures on macro-properties and investigate uncertainty propagation through different length scales, a deterministic multiscale deformation simulator needs to be adopted. Each point of the workpiece is associated with a microstructure in the meso-scale (Fig. 1), the

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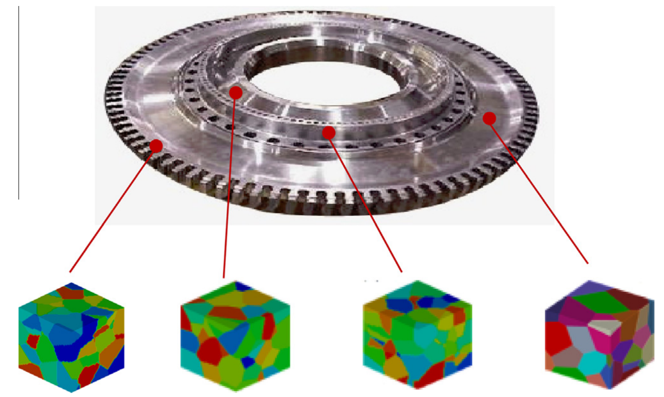

Fig. 1. The microstructure (meso-scale) features vary with location and across different realizations of the disk. Exploring these correlations is important in addressing the high-dimensionality of the random microstructure field.

deformation of which is controlled by the local deformation gradient estimated in the macro-scale. Mechanical properties/responses of the material point are evaluated via proper (e.g. crystal plasticity) constitutive models applied on the deformed microstructure. In general, microstructures are location-specific (meaning that microstructures associated with different spatial points have different distributions) [8]. As a result, the stochastic input to a multiscale deformation simulator is extremely high-dimensional, which prevents one from efficiently quantifying the variability of properties of interest. This problem is usually referred to as the "curse of dimensionality". In [9], the authors introduced a novel data-driven bi-orthogonal Karhunen-Loève Expansion (KLE) strategy, which decomposed the multiscale random microstructure into a few modes in both the macro- and meso-scales. The macro modes were further expanded through a second-level KLE to separate the random and spatial coordinates. A high-dimensional multiscale disk forging example of FCC nickel was provided to show the merit of this methodology.

Recently in [10,11], two distinct probabilistic graphical model based uncertainty quantification frameworks were presented and applied to flows in random heterogeneous media. Here we extend the approach in [10] to study uncertainty quantification in multiscale disk forging problems. The adopted probabilistic graphical model includes the following features: (1) a spatially localized model reduction technique is applied to reduce the dimensionality of the microstructure input; (2) the high-dimensional probabilistic relationship between the random microstructure input and the random response (mechanical properties) is addressed by decomposing the global problem into spatially local low-dimensional problems defined in the graph; (3) a non-parametric nature of the framework is adopted that is able to capture non-Gaussian features; and (4) a sampling based non-parametric belief propagation algorithm [12,13] is utilized to carry out the inference problems related to uncertainty propagation and surrogate prediction problems.

The paper is organized as follows. First, the stochastic multiscale disk forging problem is introduced in Section 2. Then the procedure of constructing an appropriate probabilistic graphical model and associated algorithms are presented in Sections 3 and 4. Various examples are given in Section 5 demonstrating the efficiency of the developed framework. Brief discussion and conclusions are provided in Section 6.

2. Stochastic multiscale disk forging problem

We next provide the representation of the microstructure (Section 2.1). The multiscale deterministic solver for the forging process is then briefly introduced in Section 2.2. The deterministic solver is used to solve an axisymmetric disk forging problem as illustrated in Fig. 2. Finally, in Section 2.3, we discuss the construction of a stochastic input microstructure model.

2.1. Microstructure representation

The location specific random microstructure is defined as a random field $\mathbf{A} = \{\mathbf{A}_\mathbf{x} : \mathbf{x} \in D\}$, where $D \subset \mathbb{R}^d, d = 1, 2, 3$ is the spatial domain of interest (physical space). For numerical simulation, a discrete form of $\mathbf{A}$ is needed. We discretize the macro-scale workpiece using finite elements, and employ an array of orientational features of constitutive grains to represent the microstructure at each integration point of the finite element discretization. Note that the crystal plasticity constitutive model adopted here (discussed next) only updates grain orientations while keeping the grain sizes fixed, i.e., only the orientation information is considered. Therefore, the source of uncertainty in the stochastic simulation is the texture of the microstructure in the workpiece before processing. Texture has been proven to have a great effect on the mechanical properties of polycrystals [9]. For a microstructure (e.g. FCC nickel) composed of N_{gr} grains, the orientations are described by Rodrigues parameters [14], an axis-angle representation that consists of three components defined as:

$$\mathbf{r} = \mathbf{w} \ \tan\frac{\theta}{2}, \tag{1}$$

where $\mathbf{r} = \{r_1, r_2, r_3\}$ are the three Rodrigues components, $\mathbf{w} = \{w_1, w_2, w_3\}$ gives the direction cosines of the rotation axis with respect to microstructure coordinates, and θ is the rotation angle. As a result, the location dependent random microstructure field $\mathbf{A}$ can be written as

$$\mathbf{A} = (\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_{N_\mathcal{I}}), \tag{2}$$

where $N_\mathcal{I}$ denotes the number of integration points on the finite element mesh, $\mathbf{A}_i$ describes the microstructure at the ith integration point, which contains $3 \times N_{gr}$ random variables. The resultant polycrystalline microstructure representation is thus high-dimensional. For example, for a 2D workpiece dicretized by n_{el} quadrilateral elements, each of which has n_{int} integration points (thus with $N_I = n_{el} \times n_{int}$), the total dimensionality of the microstructure is $3 \times N_{gr} \times n_{el} \times n_{int}$.

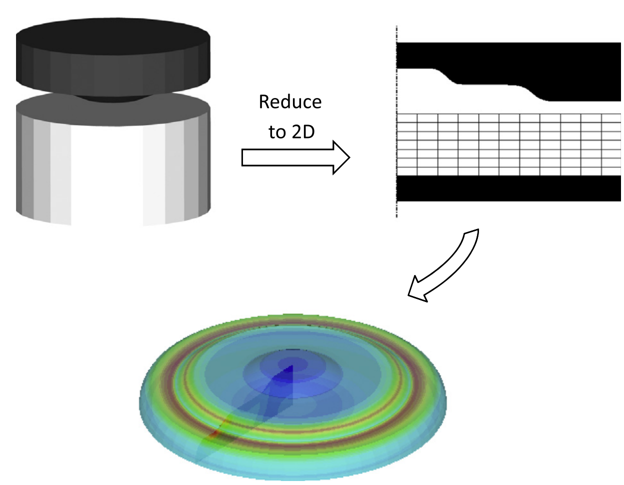

Fig. 2. Schematic view of the workpiece and die in a disk forging process. The bottom figure shows the disk shape by rotating the final 2D plane obtained from the multiscale forging solver around the central axis.