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The use of discrete harmonics in direct multi-scale embedding of polycrystal plasticity

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Abstract

We describe an approach for directly embedding polycrystal plasticity models in component scale calculations, with an emphasis on computational tractability. Previously, we have employed adaptive sampling to mitigate the computational cost of direct embedding, achieving two or more orders of magnitude in wall-clock speedup compared to more traditional approaches. However, in our previous work the crystal orientation distribution function (crystallographic texture) was not allowed to evolve significantly. Here we discuss an approach that allows for evolving texture by employing discrete harmonics, effectively decoupling considerations related to accuracy of integrals in the homogenization from those related to adequate representation of the evolving texture. We discuss the basic behaviors and convergence of the new polycrystal plasticity framework. Specific applications focus on the deformation of titanium, including the effects of twinning. Overall, the discrete harmonic based framework offers an attractive path forward for computationally efficient multi-scale embedding of polycrystal plasticity.

Keywords: Multi-scale; Polycrystal; Crystal plasticity; Constitutive models; Finite element method; Adaptive sampling

1. Introduction

There is longstanding interest in models that are able to capture anisotropic plastic flow, for example in simulations of metal forming [1–3]. Preferred crystallographic orientation in polycrystals is a principal source of anisotropy. This preferred orientation is sometimes referred to as crystallographic texture, and it is characterized by an orientation distribution function (ODF) [4]. The ODF is an important touchstone between experiment and simulation as it is easily measured by diffraction methods, with various methods appropriate to probing different sample volumes [5,6]. Models parameterized from a fixed crystallographic texture have been used to capture aspects of anisotropic flow, for example [2,7]. For scenarios involving tighter coupling with fine-scale state or for which precomputation is unattractive,

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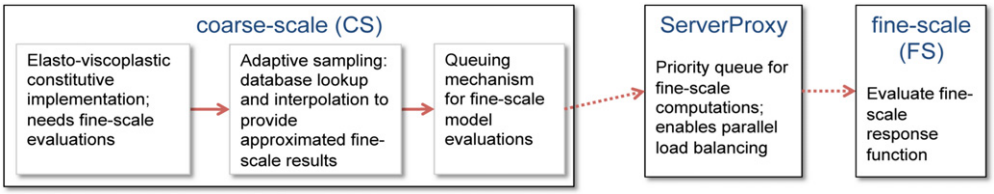

Fig. 1. Diagram outlining the call sequence by which the overall constitutive model obtains fine-scale model response information. Solid arrows indicate in-process function calls while dashed arrows indicate remote method invocation (RMI) [35]. In the case of the fine-scale (FS) evaluation itself, the remote method invocation is serviced using MPI-based parallel computing.

direct multi-scale embedding has been employed. However the computational cost of direct embedding of polycrystal plasticity is prohibitive, especially as one moves from relatively simple assumptions linking the deformation of the grains in the aggregate to models with higher fidelity and correspondingly higher computational expense [8–13].

To mitigate the cost of direct embedding, researchers have developed multi-scale embedding methodologies that employ adaptive sampling [14–19]. These techniques have some commonalities with *in situ* adaptive tabulation and similar schemes developed for modeling chemical kinetics [20–22]. Previous versions of the embedded polycrystal plasticity with adaptive sampling did not include texture evolution [17,23]. The primary thrust in the present work is to allow for texture evolution, including the effects of both crystallographic slip and deformation twinning, in a tractable multi-scale approach. Evolution of the texture, especially for materials that exhibit mechanical twinning, can significantly affect the evolution of flow stress at moderate levels of plastic deformation. It is worth noting that models to directly capture twin domain formation typically require fine computational grids and significant computational expense [24]. While there is utility in studies focused on details of twin formation, the focus here is on capturing the gross effects of texture evolution and twin formation on flow stress evolution.

The complexities of modeling texture evolution are well known [5]. For example, both spectral methods [25–29] and finite element based methods [30–32] have been employed to evolve the ODF. In spectral methods, the ODF is typically expressed in a Fourier series using symmetrized generalized spherical harmonics. Finite element schemes are often used over the Rodrigues parameter space. When accounting for mechanical twinning, the partial differential equation for ODF evolution becomes non-local, and such effects have been treated previously [8,33].

Here we use discrete harmonics based on a finite element discretization of Rodrigues space. This allows for independent control of the accuracy of ODF evolution and the accuracy of integrals over the orientation space. And, as shown below, we can capture salient features of texture evolution with many fewer parameters than are needed to track the orientations in a discrete aggregate based representation of a polycrystal. Nevertheless, the dimensionality of the polycrystal (fine-scale) response space remains relatively large—roughly 60 for the embedding in finite element calculations shown below. The input space includes the current state of the material and driving conditions such as stress state and temperature. The fine-scale model provides plastic deformation response and updated material state under these conditions. While the input dimension of the response space may be large, the portion of the response space probed in a given calculation tends to fall on a low-dimensional manifold [21,23]. The points on this manifold are not known ahead of time, motivating the use of an *in situ* adaptive sampling method that computes responses as needed.

Software modularity and multiple-program multiple-data (MPMD) parallelism are facilitated by the babel and co-op tools [34,35]. See [36,37] for a general discussion of advantages of MPMD parallelism for load balancing. Fig. 1 contains a diagram of the call sequence by which the overall constitutive model obtains fine-scale model response information. After development of the use of discrete harmonics in Section 2, we describe the constitutive model in Section 3. The fine-scale evaluations referenced in Fig. 1 amount to an evaluation or approximation of Eq. (24) as described below. In Section 4 we touch again on the decomposition of the workload onto computational resources, but we refer the interested reader to [23] for more details related to the use of computational resources. As described below, most of the calls to the adaptive sampling module result in an approximation of the fine-scale response based on previous evaluation data and do not require a new fine-scale model evaluation.

To demonstrate the convergence and efficacy of the discrete harmonic based approach, we show applications to the deformation of hexagonal α titanium, including mechanical twinning. This application is motivated by previously published work on this material [38]. Both Taylor (upper bound) and the more sophisticated but computationally intensive viscoplastic self-consistent (VPSC) type linking assumptions are used in the example calculations.