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Prediction of microscale plastic strain rate fields in two-phase composites subjected to an arbitrary macroscale strain rate using the materials knowledge system framework

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ABSTRACT

In this work, a data-driven reduced-order model is presented to predict the microscale spatial distribution of the plastic strain rate tensor in an isotropic two-phase composite subjected to an arbitrary macroscopically imposed strain rate tensor. This model was built using the framework of localization linkages called Material Knowledge Systems (MKS), which has been demonstrated to exhibit a remarkable combination of accuracy and low computational cost. In prior work, the MKS framework was successfully used to predict the local strain rate fields in multiphase composites subjected to a selected macroscale strain rate tensor. In this work, the MKS framework is extended to include the complete set of all macroscale strain rate tensors that could be applied. This is accomplished by developing novel representations that allow a parametrization of the localization kernel over the complete space of unit symmetric traceless second-rank tensors and implementing them with the required fast computational strategies. The MKS localization linkage produced in this work was calibrated and validated to results from microscale finite element models.

1. Introduction

Physics-based multiscale simulations that capture the relevant information arising from the inherent heterogeneity at a specific material length/structure scale, and propagate it both to higher and lower length/structure scales, are essential to the design, development, and deployment of new (or improved) structural materials in advanced technology applications [1–8]. These models aim to account more accurately for the effects of material heterogeneity at different length scales in predicting their macroscale properties or performance characteristics [7,9–11].

In multiscale approaches, salient information needs to be communicated effectively in both directions, from lower to higher scales (i.e., homogenization) as well as from higher to lower scales (i.e., localization). In general, localization demands significantly more effort and computational cost compared to homogenization. In fact, in many cases, one can show that homogenization relationships (or linkages) are automatically embedded in localization linkages (e.g., [12]). Localization linkages attempt to predict the spatial distribution of a response field at the lower length scale due to an imposed loading condition at a higher length scale. As a specific example, localization linkages can be developed to predict the microscale stress (or strain rate) field in a representative volume element (RVE) of the material microstructure for an imposed macroscale stress (or strain rate) [12–16]. Needless to say, these linkages are of vital importance to any practical multiscale modeling efforts.

Generalized composite theories that determine the effective response of heterogeneous materials form the theoretical foundation for localization linkages [17–25]. These theories employ the concept of a localization tensor that links the fields at a lower length scale to an imposed condition at a higher length scale. An example of such localization tensor is the fourth-rank elastic localization tensor, $\boldsymbol{a}(\boldsymbol{x})$, which relates the local elastic strain at any location of interest, $\boldsymbol{\varepsilon}(\boldsymbol{x})$, to the macroscopically imposed strain, $\boldsymbol{\varepsilon}(\boldsymbol{x})$, as [12].

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \boldsymbol{a}(\boldsymbol{x})\langle\boldsymbol{\varepsilon}(\boldsymbol{x})\rangle \tag{1}$$

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$$\boldsymbol{a}(\boldsymbol{x}) = \left(\boldsymbol{I} - \left\langle \boldsymbol{I}^{\boldsymbol{r}}(\boldsymbol{x},\boldsymbol{x}')\mathbf{C}'(\boldsymbol{x}')\right\rangle + \left\langle \boldsymbol{I}^{\boldsymbol{r}}(\boldsymbol{x},\boldsymbol{x}')\mathbf{C}'(\boldsymbol{x}')\boldsymbol{I}^{\boldsymbol{r}}(\boldsymbol{x},\boldsymbol{x}'')\mathbf{C}'(\boldsymbol{x}'')\right\rangle - \ldots\right) \tag{2}$$

where $\boldsymbol{I}$ is the fourth-rank identity tensor, $\mathbf{C}'(\boldsymbol{x})$ describes the perturbation in the local stiffness with respect to a selected reference medium, $\boldsymbol{x}$ is the spatial location of interest in the microstructure volume element, $\boldsymbol{I}^{\boldsymbol{r}}$ is a symmetrized derivative of the Green's function corresponding to the elastic properties of the selected reference medium, and $\langle\ldots\rangle$ brackets denote ensemble average over the RVE being studied (i.e., these brackets essentially represent volume averages over the RVE). Eq. (2) shows that the localization tensor can be obtained by evaluating the terms of an infinite series. In this series, one systematically adds the contribution from other spatial locations in the material microstructure to the localization tensor at the spatial location of interest. For example, the second term captures the contribution from spatial location $\boldsymbol{x}'$ on $\boldsymbol{a}(\boldsymbol{x})$, modulated through the kernel $\boldsymbol{I}^{\boldsymbol{r}}$ that decays sharply with $|\boldsymbol{x}' - \boldsymbol{x}|$. In a very similar manner, the next term captures the combined incremental contribution from spatial locations $\boldsymbol{x}'$ and $\boldsymbol{x}''$ on $\boldsymbol{a}(\boldsymbol{x})$ tensor, once again suitably modulated through Green's function based kernels. It is important to recognize that these terms capture systematically and hierarchically the spatial correlations in the material microstructure.

Although the physics-based models presented in Eqs. (1) and (2) are rigorously derived, their practical implementation in real-world applications has been hampered by the inability to establish the $\boldsymbol{I}^{\boldsymbol{r}}$ kernels for a broad range of materials phenomena of interest with sufficient accuracy [1,18,26–31]. In recent years, our research group has formulated and demonstrated a new data science framework called Material Knowledge System (MKS) for calibration of the $\boldsymbol{I}^{\boldsymbol{r}}$ kernels from numerical (e.g., finite element, phase-field) simulations performed on ensembles of digitally created microstructures [14–16,32–35]. Additionally, MKS casts the localization relationship (Eq. (2)) in a digital (discretized) form that allows one to exploit the properties of discrete Fourier transforms (DFTs). As a result, MKS linkages offer tremendous computational savings in rapid screening of a large number of candidate material microstructures in a multiscale materials design effort.

The MKS framework employs a digital representation of all the fields involved in Eqs. (1) and (2). The volumetric domain of the microstructure is binned into a uniform grid of voxels (spatial cells) that are enumerated by $\boldsymbol{s} \in \boldsymbol{S}$; this index can be treated as a vector index for multidimensional domains [12,34]. The potential material states, also called local states, allowed to occupy each spatial voxel are indexed by $h \in H$. The array $m_{\boldsymbol{s}}^{h}$ then reflects the volume fraction of spatial bin $\boldsymbol{s}$ occupied by local state h (cf. [17,36,37]). Employing this digitized description of microstructure allows casting the localization linkages as

$$\boldsymbol{p}_{\boldsymbol{s}} = \left(\sum_{h}^{H}\sum_{\boldsymbol{t}}^{\boldsymbol{S}} \alpha_{\boldsymbol{t}}^{h} m_{\boldsymbol{s}+\boldsymbol{t}}^{h} + \sum_{h}^{H}\sum_{h'}^{H}\sum_{\boldsymbol{t}}^{\boldsymbol{S}}\sum_{\boldsymbol{t}'}^{\boldsymbol{S}} \alpha_{\boldsymbol{t}\boldsymbol{t}'}^{hh'} m_{\boldsymbol{s}+\boldsymbol{t}}^{h} m_{\boldsymbol{s}+\boldsymbol{t}+\boldsymbol{t}'}^{h'} + \ldots\right)\langle \boldsymbol{p}\rangle \tag{3}$$

where $\boldsymbol{p}$ denotes the response field of interest (e.g., strain, strain rate) and $\boldsymbol{\alpha}$ is the microstructure-independent localization kernel (related to $\boldsymbol{I}^{\boldsymbol{r}}$). In this notation, $\boldsymbol{t}$ indexes the discretized vectors needed to identify the relative location of all the voxels in the RVE with respect to the voxel of interest (denoted by $\boldsymbol{s}$). For a uniformly tessellated periodic RVE, the set of values taken by $\boldsymbol{t}$ are identical to the values taken by $\boldsymbol{s}$ (i.e., $\boldsymbol{t} \in \boldsymbol{S}$). Prior work has established that the series in Eq. (3) can be truncated after the first term for composites with low to moderate contrast between the properties exhibited by the local states [13–16].

The viability and remarkable accuracy of the MKS localization linkage has been demonstrated on a broad range of multiscale materials phenomena [13–16,33,35,38,39]. These prior demonstrations have included rigid-plastic deformations in a composite material made of two isotropic phases. In such applications, the response field is selected as the strain rate tensor (i.e., $\boldsymbol{p} = \boldsymbol{D}$). The strain rate tensor is a second-rank tensor and the current MKS approach requires one to establish a different localization kernel for each $\boldsymbol{D}$ that can be applied at the macroscale (on the RVE of the microstructure). The number of distinct macroscopic strain rate tensors that could be imposed on a microstructure is infinite. Therefore, it is essential to seek a formalism for the efficient computation of $\boldsymbol{\alpha}$ as a function of $\boldsymbol{D}$. Indeed, the lack of such formalism is one of the main impediments in advancing the adoption of the MKS approach as a practical scale-bridging framework in fully-coupled multiscale modeling efforts. It is noted that prior MKS work on the elastic deformations in composites and polycrystalline materials circumvented this challenge by taking advantage of the superposition principle [14–16,39,40]. However, superposition principle is not applicable to the plastic deformations studied in this work.

It is also emphasized that our focus in this work will be on the localization of the imposed plastic stretching tensor at an instant in time. Therefore, if one is interested in simulating finite plastic strains in composite materials, one has to devise an additional strategy to integrate suitably the local plastic stretching tensors to finite strain levels, while accounting rigorously for the associated shape changes in the microstructure. This needs further development beyond the scope of the present study.

This work develops and demonstrates a novel approach that extends the MKS localization framework to rigid-plastic deformation in two-phase composite systems and enables the kernels to localize any arbitrary strain rate tensor imposed at the macroscale. For this extension, it has been assumed that the constituent phases exhibit rate-independent isotropic plasticity described by the commonly employed J_2 flow theory [41,42]. It should be noted that even though the selection of this simple material constitutive theory constrains the local plastic response to be isotropic, the overall behavior of the composite is allowed to be anisotropic. Our approach employs a clever parameterization of the complete space of traceless, symmetric, second-rank tensors of unit magnitude, and is inspired by certain prior applications in related problems [43–46]. Specifically, it is demonstrated that this new approach is viable for the present problem, and that it produces remarkably accurate predictions of the microscale plastic strain rate fields for plastic deformation in composites subjected to any arbitrary macroscopic strain rate tensor.

2. Extension of the MKS localization framework

The application of the MKS framework (Eq. (3)) to rigid-plastic deformations in a two-phase composite system can be expressed as

$$\boldsymbol{D}_{\boldsymbol{s}} = \left(\sum_{h}^{H}\sum_{\boldsymbol{t}}^{\boldsymbol{S}} \alpha_{\boldsymbol{t}}^{h}(\langle \boldsymbol{D}\rangle) m_{\boldsymbol{s}+\boldsymbol{t}}^{h} + \sum_{h}^{H}\sum_{h'}^{H}\sum_{\boldsymbol{t}}^{\boldsymbol{S}} \times \sum_{\boldsymbol{t}'}^{\boldsymbol{S}} \alpha_{\boldsymbol{t}\boldsymbol{t}'}^{hh'}(\langle \boldsymbol{D}\rangle) m_{\boldsymbol{s}+\boldsymbol{t}}^{h} m_{\boldsymbol{s}+\boldsymbol{t}+\boldsymbol{t}'}^{h'} + \ldots\right) \tag{4}$$

where $\boldsymbol{D}_{\boldsymbol{s}}$ denotes the spatially resolved strain rate tensor (i.e., stretching tensor) in the microstructure, and the dependence of the Green's function based kernel $\boldsymbol{\alpha}$ on the macroscopically imposed strain rate tensor is explicitly noted. As stated earlier, calibrating $\boldsymbol{\alpha}$