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Representation and calibration of elastic localization kernels for a broad class of cubic polycrystals

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Abstract—Localization kernels play an important role in the study of hierarchical material systems with well separated length scales. They allow for a computationally efficient communication of critical information between the constituent length scales. They are particularly well suited for capturing how an imposed variable (e.g., stress or strain) at the higher length scale is spatially distributed at the lower length scale (i.e., localization linkages). In recent work, our research group has presented a novel framework called Materials Knowledge Systems (MKS) for the representation and calibration of the localization kernels, and demonstrated the viability of this approach on selected individual material systems. In this work, we present and demonstrate an important extension to the MKS framework that allows representation and calibration of the localization kernels for an entire class of materials (e.g., a selected class of single phase cubic polycrystalline materials).
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1. Introduction

Most advanced material systems of interest to emerging technologies exhibit rich hierarchical internal structures with well separated length scales. The mechanical response of such material systems has been addressed rigorously in prior literature using generalized composite theories [1–12]. Inherent to these theories is the concept of a scale-bridging localization tensor that relates the local fields of interest at the microscale to the macroscale (typically averaged) fields. For example, the fourth-rank localization tensor for elastic deformation, $\boldsymbol{a}$, can be defined to relate the local elastic strain at any location of interest in the microstructure to the macroscale strain imposed on the composite material system as:

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

$$\boldsymbol{a}(x) = (\boldsymbol{I} - \boldsymbol{\Gamma}(x,x')\boldsymbol{C}'(x') + \boldsymbol{\Gamma}(x,x')\boldsymbol{C}'(x')\boldsymbol{\Gamma}(x',x'')\boldsymbol{C}'(x'') - \cdots) \tag{2}$$

In Eq. (2), $\boldsymbol{I}$ is the fourth-rank identity tensor, $\boldsymbol{C}'(x)$ is the deviation in the local elastic stiffness at spatial location x with respect to that of a selected reference medium, $\boldsymbol{\Gamma}$ is a symmetrized derivative of the Green's function defined using the elastic properties of a selected reference medium [1,10,13], and $\langle\,\rangle$ brackets denote an ensemble average over a representative volume element (RVE) of the material microstructure.

Eq. (2) can be transformed into a more computationally useful form by taking advantage of the concept of spatially resolved microstructure function $m(x,n)$ [14] that reflects the probability density associated with finding the local state n (to within an invariant measure dn) at the spatial location x (note that $m(x,n)dn$ reflects the corresponding probability). The local state identifies the specific combination of local features (including phase identifiers, elemental compositions, crystal lattice orientations, etc.) needed to uniquely define the relevant local physical properties at the spatial location x. Furthermore, the complete set of all distinct local states that are possible in a given material system is referred to as the local state space, denoted by H (i.e., $n \in H$). Introducing this concept, invoking the ergodic hypothesis, and substituting $r = x - x'$, one can recast Eq. (1) as [15,16]:

$$\begin{aligned}\boldsymbol{\varepsilon}(x) = \Bigg(\boldsymbol{I} - \int_R \int_H \boldsymbol{\alpha}(r,n)m(x+r,n)dndr \\ + \int_R \int_R \int_H \int_H \tilde{\boldsymbol{\alpha}}(r,r',n,n')m(x+r,n) \\ m(x+r+r',n')dndn'drdr' - \cdots\Bigg)\langle\boldsymbol{\varepsilon}(x)\rangle\end{aligned} \tag{3}$$

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The structure of Eq. (3) offers many computational advantages. First, the terms $\boldsymbol{\alpha}(r,n)$ and $\tilde{\boldsymbol{\alpha}}(r,r',n,n')$ are independent of the microstructure function. In other words, they capture the microstructure-independent physics governing the local elastic response of a composite material. Second, the terms in Eq. (3) can be efficiently computed using discrete Fourier transforms (DFTs). Consequently, the terms $\boldsymbol{\alpha}(r,n)$ and $\tilde{\boldsymbol{\alpha}}(r,r',n,n')$ are referred to as first-order and second-order localization kernels (or influence functions), respectively. Note that Eq. (3) represents an infinite series expansion of a highly nonlinear function, where each term of the series captures a linearized contribution from a specific topological feature in the microstructure.

There have been essentially two main difficulties in the computation of the localization kernels defined in Eq. (3). The first difficulty stems from the fact that $\boldsymbol{\Gamma}(r)$ (embedded in the localization kernels; see Eq. (2)) exhibits a singularity at $r=0$. The second difficulty is that the convergence of the series is quite sensitive to the selection of the reference medium (e.g., [17]). In an effort to overcome these impediments, our research group has developed a novel data-driven framework called Materials Knowledge System (MKS) [18–24]. In the MKS approach, localization kernels are obtained by a calibration procedure that involves matching the predictions of Eq. (3) to the corresponding predictions from previously validated numerical models (e.g., finite element models) for a broad range of exemplar microstructures. The central advantage of the MKS methodology lies in its computational efficiency. Once the localization kernels are calibrated, they can be applied to new microstructures with very little computational cost, often orders of magnitude lower than what is needed to execute the previously established numerical model. The viability and the computational advantages of the MKS approach have been successfully demonstrated for thermo-elastic deformation fields in composites [19], rigid-viscoplastic deformation fields in composites [18], the evolution of the composition fields in spinodal decomposition of binary alloys [21], and the elastic deformation fields in single-phase polycrystalline aggregates [24].

It is noted here that all of the prior case studies in MKS have utilized a single descriptor of the local state (usually the phase identifier or the crystal lattice orientation or the local chemical composition). It is anticipated that most advanced materials explored in emerging technologies will demand the use of complex descriptors for the local state. In this paper, we present a generalized framework that allows the combined use of multiple descriptors for the local state. More specifically, building on our earlier work [9,24–30], we demonstrate the tremendous advantages of Fourier representations of the localization kernels in arriving at compact representations that facilitate easy calibration over extremely large domains of interest (covering a very broad range of material systems). Since the calibration process needs to be performed only once, the extended MKS framework presented here opens a completely new and practical approach for addressing multiscale hierarchical modeling and simulations [31–39]. More importantly, the extensible approach presented here allows community-wide sharing and curation of the core materials knowledge through the potential establishment of an e-library of localization kernels. This is mainly facilitated by the fact that the localization kernels in the MKS framework are designed to be independent of the microstructure function.

2. The generalized MKS framework

We seek a computationally efficient form of Eq. (3) using spectral representations. Specifically, we seek representations of the following type for the various functions in Eq. (3) (only the functions in the first term are shown below; the representations can be extended in future to higher-order terms in the series):

$$m(x,n) = \sum_L \sum_s M_s^L Q_L(n)\chi_s(x),$$
$$\boldsymbol{\alpha}(r,n) = \sum_L \sum_t \boldsymbol{A}_t^L(n) Q_L(n)\chi_t(r) \tag{4}$$

In Eq. (4), $Q_L(n)$ is a suitably selected Fourier basis for functions defined on the local state space (examples will be provided later) with the following orthonormal properties:

$$\int_H Q_L(n)Q_{L'}^*(n)dn = \frac{\delta_{LL'}}{N_L} \tag{5}$$

where the superscript * denotes a complex conjugate, $\delta_{LL'}$ is the Kronecker delta, and N_L is a constant that might depend on L. $\chi_s(x)$ in Eq. (4) defines an indicator basis which essentially tessellates the spatial domain into a uniform grid [14]. This function is defined such that its value is one for all points belonging to spatial bin s, and zero for all points outside. The choice of the indicator basis for the spatial variables in Eq. (4) is primarily motivated by the fact that it allows for the use of discrete Fourier transforms (DFTs) in carrying out the integrals in Eq. (3). Using the orthogonal properties of both bases, we can show

$$M_s^L = \frac{N_L}{\Delta}\int_{H,V} m(x,n)Q_L^*(n)\chi_s(x)dndx$$
$$\boldsymbol{A}_t^L = \frac{N_L}{\Delta}\int_{H,R} \boldsymbol{\alpha}(r,n)Q_L^*(n)\chi_t(r)dndr \tag{6}$$

where Δ is the volume of the spatial bin.

Introducing these spectral representations into Eq. (3), we derive here a generalized form of the MKS:

$$\boldsymbol{p}_s = \left(\sum_L\sum_t \frac{\Delta}{N_L}\boldsymbol{A}_t^L M_{s+t}^L + \sum_L\sum_{L'}\sum_t\sum_{t'}\frac{\Delta^2}{N_L N_{L'}}\boldsymbol{A}_t^{LL'}M_{s+t}^L M_{s+t+t'}^{L'} + \cdots\right)\langle \boldsymbol{p}\rangle \tag{7}$$

It is pointed that if the $Q_L(n)$ were selected to be the indicator functions (i.e., a simple binning of the local state space), we would recover the simpler MKS formulation utilized in our prior studies involving multiphase composites [18–20,22,39]. Likewise, if the local state was selected to the crystal lattice orientation and the Fourier basis was selected to the generalized spherical harmonics (GSHs) [40], we would recover the MKS formulation we have recently demonstrated for elastic deformations in single phase polycrystalline microstructures [24]. We believe that the formulation presented above is the most general and practical MKS formulation that will be applicable for a very broad range of advanced material systems.

The similarity of the generalized MKS formulation presented here to the versions in our prior work [19–23] suggests the use of the same overall strategy (from our prior work) for calibrating the influence coefficients (such as $\boldsymbol{A}_t^L$) in Eq. (7). The overall workflow involved in building the MKS databases is shown in Fig. 1 as a broadly usable template. This procedure involves four different main tasks (color coded in Fig. 1) with several subtasks. Although this

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