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Microstructure-based knowledge systems for capturing process-structure evolution linkages

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ABSTRACT

This paper reviews and advances a data science framework for capturing and communicating critical information regarding the evolution of material structure in spatiotemporal multiscale simulations. This approach is called the MKS (Materials Knowledge Systems) framework, and was previously applied successfully for capturing mainly the microstructure-property linkages in spatial multiscale simulations. This paper generalizes this framework by allowing the introduction of different basis functions, and explores their potential benefits in establishing the desired process-structure-property (PSP) linkages. These new developments are demonstrated using a Cahn-Hilliard simulation as an example case study, where structure evolution was predicted three orders of magnitude faster than an optimized numerical integration algorithm. This study suggests that the MKS localization framework provides an alternate method to learn the underlying embedded physics in a numerical model expressed through Green's function based influence kernels rather than differential equations, and potentially offers significant computational advantages in problems where numerical integration schemes are challenging to optimize. With this extension, we have now established a comprehensive framework for capturing PSP linkages for multiscale materials modeling and simulations in both space and time.

1. Introduction

Customized materials design (including the design of a manufacturing process route) resulting in the combination of properties desired for a specific application is a highly challenging inverse problem, owing mainly to the extremely large parameter space involved in defining the hierarchical internal structure of the material. However, this endeavor has great potential for impacting virtually all emerging technologies [1–11], with significant economic consequences. The central impediment comes from the need to consider the relevant details of the hierarchical internal structure (spanning a multitude of length scales) that control the properties of interest to a specific application. Additionally, a diverse range of coupled physical phenomena occur at different timescales at each of the different length scales. Therefore, one is generally daunted by the enormous difficulty involved in tailoring the material structure to yield desired combinations of properties or performance characteristics.

Historically, and mainly because of the difficulties mentioned above, materials development efforts have relied largely on experimentation. Consequently, many of the efforts aimed at designing and developing new/improved materials have incurred significant cost and time. Recent advances in physics-based modeling of multiscale materials phenomena [12–21] have raised the exciting possibility that the vast design space for experimentation can be constrained to a significant degree by embracing in silico simulations and explorations. In other words, there is a tremendous potential for significant reductions in cost and time incurred in materials development effort if one could judiciously utilize multiscale materials modeling and simulation tools in combination with a reduced number of experiments.

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The central impediments associated with the effective utilization of physics-based multiscale materials models in the materials development include: path dependent microstructure evolutions that depend on initial conditions, non-unique parameter selection for coupling multiscale models, approximations in microstructure representation, material property dependence on extreme values of microstructure distributions, large optimization space, metastablity of microstructure during use, and uncertainty in data, models and model parameters [18,22]. An important strategy in addressing these impediments involves the formulation and utilization of robust surrogate models (also called metamodels or emulators) for computationally efficient communication of critical information between well separated structure/length/time scales. Such low-dimensional, but sufficiently accurate, models present a computationally viable approach for exploring efficiently the extremely large materials design space.

In the context of hierarchical materials (with details of the material structure spanning multiple well-separated scales) surrogate models are needed to exchange high value information in both directions between the scales. Depending on the direction of information flow, the models can be classified as homogenization (information flowing from lower scales to higher scales) or localization (information flowing from higher scales to lower scales) relationships. It should be noted that localization linkages are significantly more difficult to establish compared to the homogenization linkages; indeed the latter are implicitly embedded within the former and can be recovered from them when needed.

2. Review of homogenization and localization approaches

Theories for predicting the properties of composite materials go as far back as 1873, with Maxwell predicting an effective conductivity for a region of a material with dilute inhomogeneities through a mean-field approximation [23–25]. The simplest, and most commonly used, homogenization methods for mechanical properties were developed by Voigt and Reuss [26,27], and provide "elementary" bounds for the estimates of the effective properties. These calculations typically involve simple volume-averaging of the properties at the microscale. The bounds obtained in this approach also correspond to the correct effective values for highly specialized microstructures. For example, the upper bounds obtained in these approaches typically correspond to microstructures where the microscale constituents have uniform shape, and are continuous and perfectly aligned along the loading direction (e.g., unidirectional, straight, and continuous fibers).

Hill and Hashin introduced the concept of a Representative Volume Element (RVE) [28,29] which can be defined as a statistically homogeneous subvolume where the length scale associated with the local perturbation in material properties is sufficiently small compared to the length scale of the subvolume (typically referred as "well-separated" length scales). With this definition, a mean-field approximation can be used to assign an effective property to a RVE. It can be shown that good estimates for a broad class of effective properties associated with an RVE can be expressed in the following generalized form [28]:

$$P_{eff} = \langle A(x)P(x) \rangle \tag{1}$$

where P_{eff} denotes the effective property, $\langle\rangle$ denotes ensemble average (also equal to volume average by virtue of the ergodic assumption), and $A(x)$ is a suitably defined tensor operator. The central challenge of this theory lies in the computation of the tensor operator.

While the theory described above emerged in the context of mechanical properties, it has also been successfully applied to material properties such as thermoelectric, piezoelectric, diffusion, and conductivity for composite materials [30]. A large variety of approaches have been built on this foundational framework, and have been employed successfully in addressing practical problems of interest in composite material systems. Hill developed the self-consistent method which employs Eshelby's solution to ellipsoidal inclusions in an infinite medium to find an approximate estimate of the effective properties [31,32]. An improved generalized self-consistent method emerged from the work of Hashin, Shtrikman, Christensen and Lo [29,33–36], which allows for more complex geometric shapes of the reinforcement phase. A good overall treatment of such approaches for homogenization theory or estimates can be found in the textbook by Qu and Cherkaoui [37] as well as the report by Bohm [24]. Further advanced theories of homogenization were established by Willis [38], and subsequently by Ponte-Castanada [39].

In a completely different approach, advanced composite theories were developed to specifically take into account the rich details of the material microstructure. These approaches utilized the formalism of n-point spatial correlations to quantify the details of the material microstructure together with the concept of Green's function to estimate the effective property of interest [40–46]. An overview of this more sophisticated approach for composite theories can be found in the book by Milton [30]. One of the earliest demonstration of this approach comes from Brown, who used a series expansions of a localization tensor to predict the electrical conductivity of a 2-phase material [47]. More rigorous applications of this approach can be found in the work of Torquato and co-workers [48,49].

The main limitation of the approach described above is that the Green's functions needed to implement the method are only available for cases involving highly idealized and simplified physics (i.e., material constitutive laws). The recently formulated Materials Knowledge Systems framework (MKS) addresses this critical gap by advancing a data-driven approach [20,50–53].

3. Homogenization and localization with MKS

MKS homogenization and localization linkages are created by merging concepts from the physics-based statistical continuum theories developed by Kroner [54,55], machine learning [56–58] and digital signal processing [59]. A generalized workflow for establishing the homogenization linkage (e.g., structure-property linkage) is shown in Fig. 1. Broadly, this workflow includes a calibration step and a validation step. More specifically, this data-driven approach captures the pertinent microstructure features through n-point spatial correlations and employs dimensionality reduction techniques to create low-dimensional microstructure descriptors [60–62]. Linkages between effective properties and these low dimensional descriptors are then created using regression techniques [63–65].

The MKS localization linkages are expressed as a series, where each term involves convolutions of physics-capturing kernels (based on Green's functions) with hierarchical microstructure descriptors. These kernels (referred to as influence functions) capture and organize the governing physics as convolution operators that are independent of the spatial arrangements of the local states in the material microstructure. Therefore, in the MKS localization approach, these kernels are calibrated with results produced using numerical tools (e.g., finite element models).

It is emphasized here that once the influence kernels in the MKS linkages are calibrated and validated, they can be used to predict the local responses for new microstructures at very minimal computational expense. Therefore, this approach is of particular value when one needs to explore a very large number of potential

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