

MULTISCALE DESIGN OF MATERIALS

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ABSTRACT

Current methods of materials development, relying mostly on experimental tests, are slow and expensive. It often takes over a decade and costs many millions of dollars to develop and certify new materials for critical applications. With evolving constraints being placed on the use of materials arising from concerns with energy and materials resource sustainability, new approaches for materials development is essential. Moreover, it is increasingly important for materials development to be integrated into overall product design and development, allowing for optimal use of materials as well as enhancing our ability to recycle and reuse. In this paper, we discuss a new program in which we link methodologies developed over the past few decades in computational materials science to a modern computational design platform (VE-Suite) to enable the multiscale design of materials. Development of such multiscale design platforms is essential for the successful implementation of integrated computational materials engineering (ICME), an emerging discipline within materials development. We will present the basic framework of our program and discuss progress to date.

INTRODUCTION

Throughout history, humans have used materials effectively in products without knowing about the fundamental science that governs the material properties. For example, the smith that made swords out of Damascus steel knew the process that had to be followed, but not how the strength and toughness of the steel depended on its underlying microstructure. In many ways, the situation has not changed significantly when it comes to materials used in specific product development. The materials engineer is given a range of properties needed for the final product along with constraints such as cost and manufacturability and then typically uses standard sets of materials tables to define the options of materials that could be used in the product. New materials are rarely developed specifically for an application because of the cost and time to develop and certify them for use. Thus, in many ways materials engineering has become divorced from materials science.

A recent study¹ by the National Academy argues that there needs to be an improved way to develop new materials that speeds their development and lowers their costs. This report focused on the notion that computational materials engineering can be integrated with experimentation to

accelerate materials development and lower cost. This emphasis on computational materials design arises from increases in the availability of both computer hardware and advanced software. Many of the basic issues as well as the potential benefits were discussed by G. B. Olson over a decade ago.² Since that time, the basic tenants of ICME have begun to be adopted by industry as a means to decrease the cost and time of materials development.^{3,4}

The ICME report also suggests that there is a need for a new type of design in which the materials are designed and optimized concurrently with the product, which will enable better products and more effective use of materials. The goal of this work is to put in place a computational framework that will enable both of these goals.

CONCURRENT DESIGN

Figure 1 shows a schematic view of concurrent design based on a recent paper by McDowell and Olson.⁵ The top right shows the current approach to designing products in which information flows down from the assembled system level to provide constraints on the design of individual parts, and up from the parts to determine the properties of the system. As Fig. 1 indicates, the current approach typically stops above the diagonal line, with the parts selected from a known set of possibilities. In concurrent design, the materials themselves are included in the design process. The challenge is that the same type of information exchange that is available in our current design processes is not generally available for materials design. Materials modeling, in which we include modeling derived from experiment, may include a linkage of scales, a building up of details and accuracy from one scale to the next. We generally do not have, however, a way to inform the materials modeling of the overall design. This lack originates in the limited availability of inverse models in which one can describe properties at a finer scale based on information from a larger scale. This inability to exchange information between different scales is a major challenge for concurrent design.

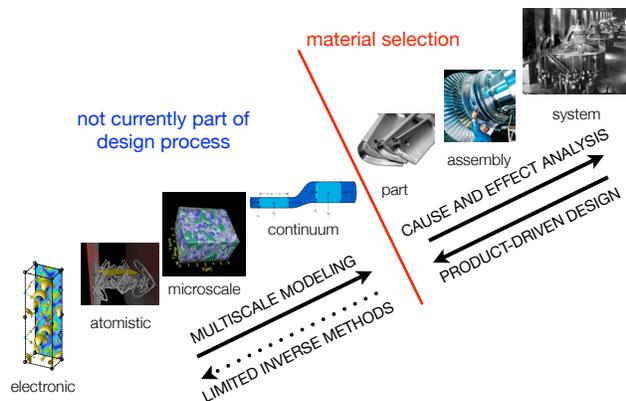


Figure 1: Concurrent design. The current design process, shown in the upper right, is coupled to materials design on the bottom left, as described in the text. Adapted from McDowell and Olson.⁵

APPROACH

The fundamental challenge of computational materials design is that the physical phenomena that determine materials behavior span many orders of magnitude in length and time scales. A further challenge is that these phenomena may be quite different depending on the materials properties under consideration. Thus, there is no single path for understanding and predicting materials behavior.⁶

Consider, as an example, the mechanical behavior of a metallic structure, as shown schematically in Fig. 2, adapted from a recent ICME study.^{3,7} The structure of interest is an engine block with a size on the order of a meter. Fundamentally, however, the properties are determined by the alloy from which the block was made. The properties of the alloy are atomic in nature with a length scale on the order of many Å (10^{-10} m). The mechanical properties of the engine block, however, are also affected by the microstructure of the material (i.e., the structure of the defect distributions, which may include grain boundaries, second-phase particles, and dislocations). These defects manifest themselves at a series of scales, so a complete description of the properties at a meter scale depends on a sequence of scales down to the Å level.

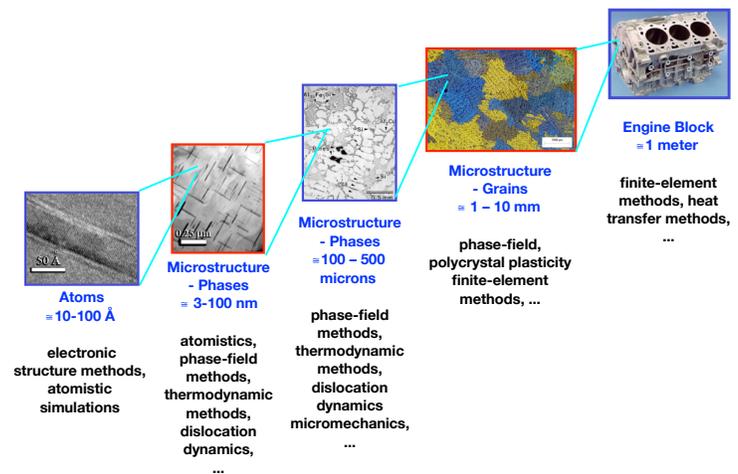


Figure 2: Scales of the mechanical properties and modeling approaches for an engine block. Adapted from Allison.⁷

Figure 2 also lists the various modeling methods that could be employed to describe the material properties at each scale. Much progress has been made in our ability to model phenomena at each of the scales listed. Many of the methods used in such modeling have been reviewed recently.⁸ We note that these methods are very different from each other in length and time scales, approach, algorithms, accuracy, and computational needs. Moreover, they are generally done by different research groups. We will not discuss any of these methods in this paper, but will focus instead on how the information is passed between the models, building a multiscale materials description which is the basis for much of this project.

The most common means of transferring information from one scale of length and time to another is through the use of reduced-order models based on the results of the finer scale. These models may be phenomenological in nature and could be based on experimental data rather than simulation, or they could be derived from a direct homogenization of finer-scale calculations.

Ultimately, however, calculations at a scale are done independently, based on some type of representation of finer-scale physics. This approach to passing information is often referred to as a “handshake” or as “message passing.” It reflects a loose coupling between scales in that what goes on at a finer scale is largely independent of the behavior at a larger scale.

There are a number of critical issues that arise in a message passing approach. For one, it is an inefficient use of information. The simulations at each scale typically involve a great number of variables, most of which have little or no informational value at a larger scale. For example, in describing plasticity, one focuses on the behavior of curvilinear lattice defects called dislocations. To calculate the properties of dislocations in an atomistic simulation, one typically includes many more atoms than are needed to describe the dislocations but that are needed to reduce simulation error. Thus, much of the computation time is “wasted” on the calculation of variables (e.g., positions and momenta of atoms) that are not specifically relevant to the dislocation process. Overcoming this issue is complicated because we do not know a priori which variables have critical information content. As a result, we typically determine more information than is needed. If we create a reduced-order model from that information, we cannot be sure that we have captured the appropriate critical information, which adds uncertainty to the models.

Another major complication of message passing is that it ignores non-linearities and overlaps between scales. For example, the blocks of phenomena in Fig.2 are artificial but reflect the types of models that we currently have available. If the physics cannot be separated into those blocks, then we cannot pass information in a sequential way and will have a tight, rather than a loose, coupling between scales. Another outcome of the loose coupling between scales is that there are few inverse models to enable predicting the behavior at a finer scale from the properties at a larger scale. The lack of inverse models was discussed above as a major challenge in concurrent design. These issues need further development, as will be discussed later in this paper.

If we are to use the type of modeling described in Figure 2 in a concurrent design process, we need to have a measure of uncertainty and, more importantly, risk. Uncertainty can arise from many factors, such as the use of models, a lack of experimental data, or computational approximations. Uncertainty only matters, however, if it adversely affects the final conclusions in a design process (i.e., if it creates the risk that the final design will be of poor quality). Thus, we need to reduce uncertainty only to the point that we reduce that risk.

MULTISCALE DESIGN

A number of developments are needed to create a multiscale concurrent design process.⁵ Advances in the materials models used to describe the response at each scale may be better physics or more computationally efficient algorithms or both. Better experimental data at each scale may be required to validate those models, especially experiments that better define the

microstructure-property relations. However, these developments are the standard focus of materials science and engineering and are not the specific thrust of this work.

Developments in information science—by which we mean the science of how we collect, classify, store, retrieve, and disseminate knowledge—are important in the development of multiscale design. Practical applications of information science in the form of creating efficient databases of information and the use of informatics to best extract the information needed for materials design⁹ is the primary focus of this work. An important task is to develop the means to manage information across scales, by which we mean the identification of critical information and the analysis of the uncertainty that arises from the use of incomplete information. Finally, we need a computational platform in which we can link materials design to the overall process design by performing multiscale optimization across scales. Fortunately, we have such a computational framework in VE-Suite, which will provide the basis of the computational platform needed to make concurrent materials design a reality.

VE-SUITE

The main purpose of VE-Suite is to create a space to enhance interactions between engineers and their design, with real-time interactions across a multitude of computational interfaces, by integrating modeling, analysis, and optimization with advanced visualization to create a design environment in which engineers can create and optimize products. To that end, it couples excellent physical-based modeling with information management and optimization. Numerous applications of VE-Suite have been made that show its capabilities.¹⁰

VE-Suite's visualization capabilities are unique through its ability to visualize over 100 million points from any data source across any visualization and computational platform. It allows for both two- and three-dimensional projection and real-time manipulation of the images.

Various aspects of VE-Suite have won numerous awards, including R&D 100 Awards in 2006, 2009, and 2010, as well as a National Excellence in Technology Transfer Award in 2009.

Using VE-Suite for Concurrent Design

One of the strengths of VE-Suite is its ability to integrate various computational codes within its framework. To date these codes include, but are not limited to FLUENT, STAR-CD, EnSight, ABAQUS, ANSYS, Pro/E, JT, MSC/PATRAN, ASPEN, DYNASIM, and MSC/NASTRAN. It is possible to add various, already existing computational materials models and simulation tools to the VE-Suite framework, which is vital to concurrent design.

VE-Suite is designed around the creation and linkage of objects that serve as a set of building blocks for a multiscale simulation. Each object represents a numerical representation of a physical process operating at some scale. It may, for example, represent the growth of grains in a metal. To define an object, one first needs to identify the physical process that it will represent and to create a physically based model to describe that process. For the grain growth example, the phase-field method might be sufficient. If there is more than one model in the object, the couplings between them will need to be defined and a common spatial frame established. Given the models that define the object, the information that is needed for that object—either from a global perspective (e.g., thermodynamic quantities) or specific information that may arise from a finer length or time scale (e.g., initial grain size, distribution of particles, etc.)—must be identified. Finally, the output of the model for serving as input for other objects needs to be defined. As noted above, a model may be phenomenological descriptions based on data. However, we also may employ a direct link to experiment by using the methods of materials informatics to extract critical information directly from the data, without the use of a model.

Once one has defined a set of objects, it is possible to create an object of objects to describe more complicated physical phenomena. For example, if one has an object to describe grain growth and another to model diffusion, creating a combined object enables a description of coupled growth and diffusion. Here, the first step will be to identify the set of objects needed to model a physical phenomena followed by determining the various inputs and outputs and the coupling them in a computationally efficient way.

The net result will be a set of computational building blocks that can be linked together to describe a specific physical system. Assembling blocks in this way is similar to how we can use actual building blocks (e.g., LEGO®) to create a specific physical system. We show this schematically in Fig. 3, in which we indicate objects as blocks along the diagonal and the couplings between them as off-diagonal elements. The center block represents an object of objects, in which a series of objects are linked into one. The linkages between blocks will be through the information that is passed from one block to another. In the message passing model, this could be an averaged quantity from one scale (e.g., mean grain size) passed to a phenomenological model of strength.

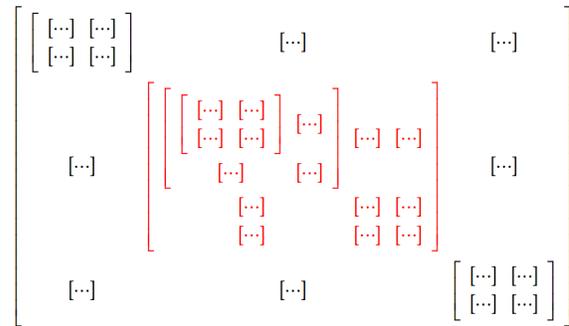


Figure 3: A schematic view of a set of objects linked into a unified structure, as described in the text.

While reduced-order models may be appropriate for some of the scales shown in Fig. 2, in many cases the physical phenomena are complicated and may require direct simulations and, thus, large-scale computations. VE-Suite is designed to work across platforms. Moreover, it has a hierarchical structure that enables computations to be farmed out to various platforms, including

high-performance computing, as needed. VE-Suite also includes a set of optimization tools that span across the objects and, hence, across scales. By directly coupling the scales in this way, we minimize, though not eliminate, the problem of the lack of inverse models.

PROGRESS AND PLANS

The implementation of materials modeling within VE-Suite is proceeding in steps. Step 1 involves the identification of the basic framework and an initial test problem. We are examining how to modify existing materials models to fit in the general structure of the VE-Suite objects discussed above. Step 2 will involve the creation of a series of materials objects designed to model a specific materials system, and which will be integrated within the VE-Suite framework. Step 3 will focus on predictions of materials response across scales, with no integration within the design process. Step 4 will couple a design of a simplified product with concurrent materials design, while in Step 5, we will move towards realistic products and materials.

A number of critical research efforts will be needed. Many of these are computational, such as the need to systematize the creation of objects and their linkages, while some are conceptual, for example the identification of critical variables. The ultimate goal of the project is to create a platform that makes concurrent design a reality. Along the way, the project is likely to change how we view multiscale materials behavior.

ACKNOWLEDGMENTS

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