

MULTISCALE DESIGN OF MATERIALS

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ABSTRACT

Current methods of materials development, relying mostly on experimental tests, are slow and expensive, often taking over a decade and costing many millions of dollars to develop and certify new materials for critical applications. Finding new approaches for materials development is essential. Moreover, it will be increasingly important for materials development to be integrated into overall product design and development. We discuss a program in which we are creating a framework to link multiscale materials information to do design across scales, based on an existing computational design platform, VE-Suite. We present the basic framework of our program and discuss progress to date. Since our goal is multiscale design, part of our efforts are focussed on creating new visualization tools and facilities to enhance the design process. We review progress in this area as well.

INTRODUCTION

A recent study¹ by the National Academy focused on the idea that computational materials engineering can be integrated with experimentation to accelerate materials development and lower cost. Referred to as *Integrated Computational Materials Engineering* (ICME), 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}

2011 saw the announcement of the *Materials Genome Initiative for Global Competitiveness* (MGI) by the Office of Science and Technology Policy. The MGI takes the idea of ICME one step further, arguing for a marriage of experiment, modeling/simulation, and information sciences to accelerate materials discovery as well as development.

The ideas behind both ICME and the MGI suggest 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. This approach is referred to as *concurrent*

design. The goal of the project described here 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 Figure 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.

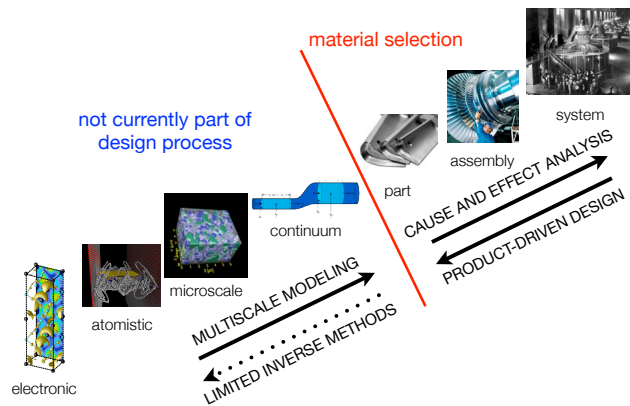


Figure 1: Concurrent design. The current design process, shown in the upper right, is coupled to materials design on the bottom left, as described in the text. Adapted from McDowell and Olson.⁵

APPROACH

There are three major questions that must be addressed when developing a multiscale design process: (1) What is the nature of multiscale design?; (2) How do we mathematically represent multiscale systems?; and How do we interact with multiscale systems? In this section we discuss our approach to answering all three questions.

The computational framework that will be employed to implement these ideas is VE-Suite, whose main purpose 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.⁶ 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.

NATURE OF MULTISCALE DESIGN

Design requires an interplay of a human (the designer) and information. The challenge for multiscale design arises from the complex nature of materials information and how that information is shared across scales. At each scale, the information may be quantitative, for example experimental measurements of elastic constants, or qualitative, as in a knowledge of the trends of how one materials parameter behaves in terms of another. Some of this knowledge may reside with “experts” who have an understanding of materials behavior that may not be easily represented for a computer system. How such information is gathered and incorporated into a multiscale information framework is a matter of current research. A promising approach is based on research on the use of *narrative structures*, in which the focus is on developing the overall information flow. It is much as in Aristotle’s famous quotation about writing:⁷ “Plot, then, is the first principle and, as it were soul of tragedy, while character is secondary”, in which he is saying that the most finely developed characters will not matter if the actions of the plot are weak. In the same way, managing multiscale information must focus first on the correct structure of the information.

An even bigger challenge for multiscale design is that it requires optimization across scales, which is complicated by the variables to be sampled having different accuracies and carrying different uncertainties (and costs) to the final predicted design. This type of problem is common, yet not well understood; a critical example is the use of climate simulators to predict climate change. There is a trade off in terms of the accuracies at each scale versus the cost of the simulations. Moreover, the statistical relationships between the simulations and the overall objective function used in the design process have not, in general, been determined.

Seeking the correct narrative structures and optimization strategies for a materials system is a formidable challenge, given the wide range of scales and the complexity of materials behavior. It is thus an advantage to seek a surrogate problem in which to develop a better understanding of information structures and flow. Indeed, we are seeking a *computational metaphor* that has many of the same essential attributes as the materials problem, but that is more tractable to implement and study. The hope is that such metaphors will lead to new approaches to this

complex problem, much in the same way that ideas from stigmergy have changed how one thinks of sensor arrays.⁸ To that end, we have examined a number of multiscale surrogate systems, including, among many others, the “PORS” problem⁹ and digital manufacturing.

MATHEMATICAL REPRESENTATION OF MULTISCALE SYSTEMS

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.

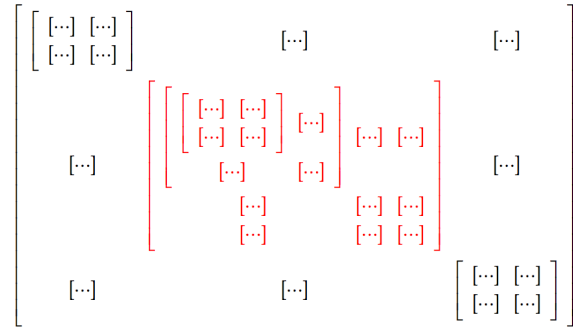


Figure 2: A schematic view of a set of objects linked into a unified structure, as described in the text.

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 to create a specific physical system. We show this schematically in Fig. 2, 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.

VISUALIZATION

As a first step in creating new tools for interacting with multiscale data, we developed a system for interactive visualization of large atomistic data sets using VE-Suite as the framework. Our goal was to address the visualization and interaction challenges that are roadblocks to performing true multiscale design. These datasets can come from either molecular dynamics or other simulations or from experimental techniques such as atom probe tomography (APT).

Traditional visualization tools cannot render large datasets at full fidelity. For example, when dealing with APT data it is common to only render 0.5 – 1% of the total atoms owing to the limitations of the visualization software used. To address this shortcoming, we implemented a technique that allows a much larger number of atoms to be drawn interactively. This technique is known as spherical impostor rendering and was first developed in the protein visualization community. To optimize this technique for the types of large datasets common in materials science we developed a way to minimize the number of operations required to draw each sphere. The result was that using a standard graphics processing unit (a Quadro FX 4800) we are able to produce a sphere rendering throughput rate of over 300 million spheres per second. Thus, we are able to render datasets of 10 million plus atoms *interactively* at full fidelity. In previous tools used to render APT data and molecular dynamics data, the practical upper limit was 10-50 thousand atoms and even this small number was restricted to exceptionally low framerates (3-5 frames per second) whereas our software can render 10 million plus spheres at 30 frames per

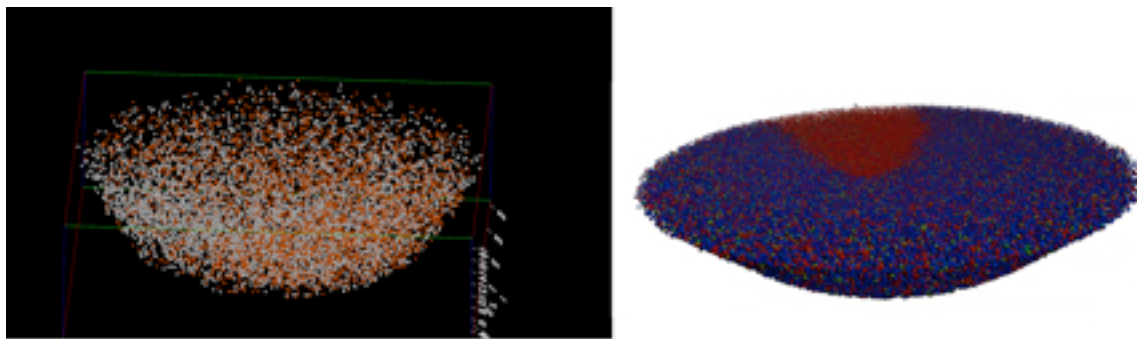


Figure 3. The difference between the standard technique for rendering APT data and our technique. A. Standard methods showing limited numbers of atoms. B. Our methods displaying the full dataset.

second, which represents an improvement to the overall sphere rendering throughput of over a factor of 100. Examples are shown in Figures 3 and 4.

From a practical standpoint, we can now interactively examine all the data in datasets for which we previously could not view more than 1% of the data at any give time. This increase in capability helps speed up the interpretation process and can help find new insights.

In addition to new rendering techniques we also designed and implemented a system for efficiently masking and filtering atoms in a dataset based on their properties. This allows the user to quickly select exactly the desired subset of atoms directly and see how a desired property is distributed across the desired subset of atoms. Figure 5 shows an example of how this capability is useful for identifying phases in APT data.

To improve the ease and effectiveness of exploring APT data, we implemented a tablet based user interface for manipulating the masking and colorization functions associated with the APT data. This user interface runs on an Apple iPad and communicates with VE-Suite over the wireless network allowing real-time interaction with the masking and colorization functions on the iPad while the results are displayed on either the desktop or immersive display running VE-Suite. This new display allows us to

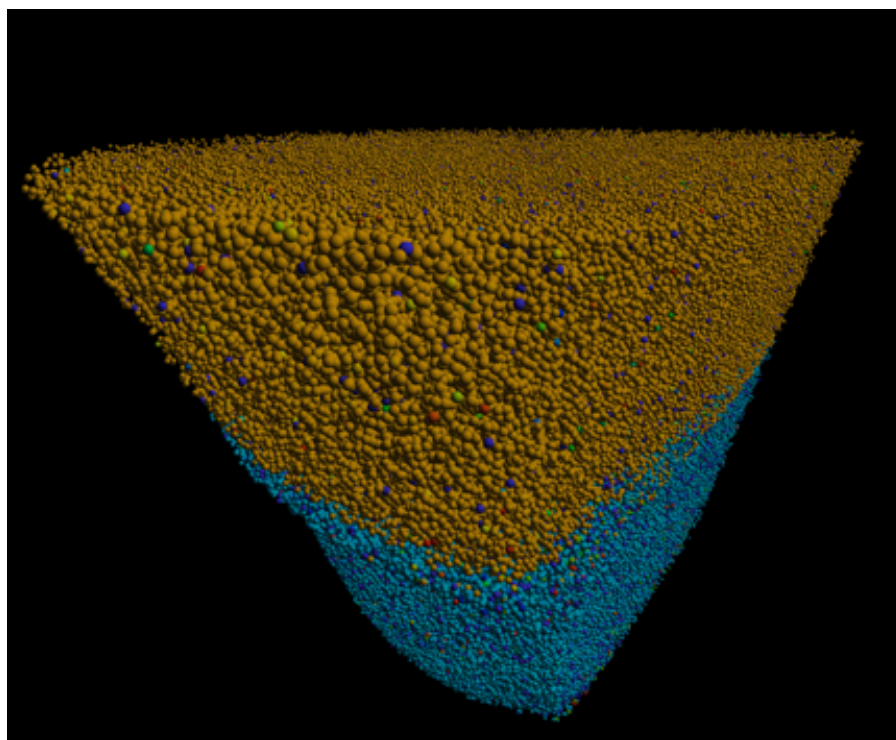


Figure 4. Slice away view of thin film copper deposited on a silicon tip. Using other software the full fidelity and density of the data would be inaccessible in the visualization process.

display the histogram data, which can be conveyed more effectively on a high resolution screen on a tablet while concurrently displaying the 3D atom positions and properties on a large 3D display, thus maximizing the effectiveness of each display device. Furthermore, this approach solves the problem of needing to perform complex interactions on the large display, which both frees up space and makes the interactions substantially easier. The result is that our system is easier to use and more aesthetically pleasing, allowing for quicker and more effective exploration of APT data. As we move forward with further explorations into multiscale design we plan to use the same tablet interface with large 3D screen model.

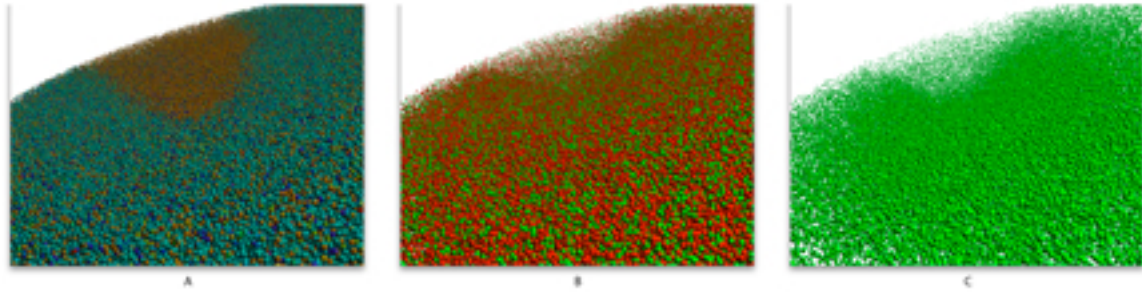


Figure 5. Images from APT analysis of Cu-Si system. (a) Teal atoms are Cu and orange atoms are Si. Two clear phases are identified: Si and Cu_3Si . (b) This plot only consists of atoms that evaporated as dimers. Each dimer is comprised of a red atom and a green atom, with the colorization used to identify pairs more easily. In the Cu_3Si phase, the density of dimer atoms is high, whereas in the Si phase very few dimers are present. The visualization ability to screen only dimer atoms allows us to track how atoms evaporate in different phases and structures, and to then relate the evaporation physics to the chemical bonding. (c) Only the dual hit half of each dimer is rendered to further accentuate the difference between the phases.

To effectively design across multiple scales it is necessary to represent and interact with systems that potentially bridge scales visually. In many cases this involves datasets that at one scale can contain a very large number of data points. This work represents our first attempt at designing a system that allows visualization and interaction with systems that cross potential design scales. The rendering, interaction, and filtering capabilities were all developed as part of the general VE-Suite tool chain in such a way that they can be used not only for atomistic data but other large datasets as well. We plan to use these capabilities when we tackle design problems that cross scales.

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.

Our initial test problem focusses on one of the most exciting new opportunities in materials today, additive, or digital, manufacturing, in which three-dimensional solid objects are created by

laying down successive layers of material based on a digital model. This problem will enable us to examine how tailored structures of materials, created by modifying the manufacturing process, affect overall properties of a designed part. This information will inform a design process, with the ultimate goal of creating a new design tool for additive manufacturing at the materials level.

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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