# Foreword to Special Issue on Linking Discrete and Continuum Models

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As the field of computational materials science expands, an increasing agreement is developing in the engineering and scientific community that modeling should be an integral part of materials research and design. Modeling is being used as an analysis tool in industry to support the development of new products and processes. The trend is driven by the fact that modeling helps reduce prototyping costs, reduces the time to market and assists product optimization.

In some fields of engineering, modeling plays a more important role than in the others. For example, heavy use of modeling is made in circuit design and fluid flow applications. Applications that require modeling the response of solid materials benefit less. The fundamental reason for this situation is the comparatively lower accuracy and higher complexity of the available models describing solids. Material behavior is controlled by multiple physical phenomena that take place on various scales and by the interactions of these phenomena across scales. Current development of material modeling does not permit the full integration of the relevant physics. Most current models address a single physical process (deformation, heat transport, diffusion, etc) or, at most, two such as in thermo-mechanics, and are defined on a single spatial scale. They include constitutive equations which are supposed to reflect the coarse-grained behavior of the underlying scales. The constitutive laws are inherently imperfect, being experimentally validated on a restricted domain of variation of their parameters. The uncertainty incorporated in the model by their use is often difficult to estimate. An alternative to the use of constitutive equations is provided by multiscale modeling, in which the relevant physics is explicitly captured on multiple spatial and temporal scales. The development of such unitary modeling capability is the objective of the emerging field of computational materials science.

A large variety of single-scale models has been developed over the years. At the smallest scale, that of the electronic structure, ab-initio calculations are performed. On the scale of the lattice in crystalline materials or the molecular scale in polymeric systems, the method of choice is atomistic modeling. In these models, each atom in the system is explicitly represented and its trajectory is traced. Discrete coarse grained models are used on larger scales. Examples from this category are discrete dislocation dynamics (DDD) models that capture the behavior of large populations of dislocations and coarse-grained polymer models, in which a group of atoms belonging to a macromolecule are coarse grained into an equivalent object of physical properties defined based on separate atomistic simulations. Continuum models are used to represent the system behavior on larger scales. In these models, one identifies the physics of interest and integrates the relevant partial differential equations. The various physical phenomena are typically decoupled in the continuum and in some coarse grained models, while the physics is intrinsically coupled in the atomistics. The scale at which the transition from discrete to continuum is made is largely problem dependent. For example, continuum elasticity may be used down to the atomic scale, while classical plasticity breaks down on the micrometer scale, the scale on which dislocation self-organization takes place.

Multiscale models are based on the hierarchy formed by the techniques discussed above and their linkages. Linking the electronic structure and atomistics (discrete-to-discrete linkage) is usually performed by the derivation of a semi-empirical interatomic potential description of atomic scale energetics. In this approach, the electronic degrees of freedom are represented schematically through an effective potential. The potentials may be adjusted to fit a database of experimental and quantum mechanically-derived material properties. Linkages between continuum scales (continuum-to-continuum linkages) can be performed by a variety of methods. These may be grouped in two categories: sequential and embedded schemes. Embedded techniques include domain decomposition and the multigrid method. Sequential schemes are of the variational multiscale type or are based on asymptotic expansions in space and time.

Arguably the most challenging scale linking problem

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is that of coupling discrete and continuum models. In this Special Issue of the Journal of Multiscale Computational Engineering, a collection of articles that exemplify the state of the art in this field is being brought together.

Two main classes of methods have been proposed to address linking discrete and continuum systems. The first class includes methods that are sequential in nature. In these procedures, the input to a scale is provided by the statistical behavior of the underlying scale. A typical example is the calibration of constitutive equations to be used on continuum scales, based on the response of discrete models. The article by Grijicic, Guoxin and Joseph demonstrates such a procedure. These authors perform atomistic simulations to calibrate constitutive equations describing the response of particular types of interfaces subjected to opening and shear. These laws are then used to describe the response of interlamellar interfaces and colony boundaries represented as cohesive zones in a continuum finite element model of a complex Ti alloy. The continuum model is used to investigate the mechanisms controlling the fracture toughness of the material. Another example from this category is provided in the article by Picu, in which a higher order, non-local continuum constitutive model for rubber elasticity is developed based on molecular considerations. The classical, local constitutive model of rubber elasticity is applicable to the situations, in which the deformation fields do not vary significantly on a length scale comparable with the size of a macromolecule. In this case, homogenization over molecular-size volume elements is possible. In some modern nanostructured polymers, however, the fields vary on the sub-molecular scale, and the classical molecular scale theory is not applicable. The new formulation proposed in the article provides an "atomistically-informed" alternative to the classical molecular scale theory of rubbers.

An interesting example of coupling physical phenomena across the discrete-continuum demarcation line is discussed in the article by Johnson, Bose, Goldberg and Robinson. These authors present a procedure by which linear elasticity is coupled with electronic structure calculations in order to analyze the effect of strain on the optical and electronic properties of the material. The results of this model are successfully compared with experimental spectral data.

Another sequential scheme, presented by Fish and Schwob, is obtained by extending the formalism of the mathematical homogenization theory developed for continuum systems. The main distinctions between the conventional mathematical homogenization theory and this generalized approach are that the asymptotic expansion contains multiple time scales, the continuum model possessing internal spatial and temporal scales, and that the multiple space-time asymptotic expansion is combined with equations describing the motion of atoms, rather than with continuum PDEs.

The second class of methods aimed at coupling discrete and continuum systems includes techniques that embed several types of models into a unique framework. Typical examples are explicitly coupled atomistic-continuum and discrete dislocation dynamics-continuum models. An excellent review of the state of the art in coupling atomistic and continuum models is presented in the article by Miller. In these models, the domain of interest is divided into regions of high and low deformation gradients. The highly deformed regions are represented atomistically, while the rest of the model is continuum. The two regions are coupled by suitable "handshaking" procedures. The article also reviews techniques used to couple atomistics, discrete dislocation dynamics and continuum models. Another example of linking discrete dislocation dynamics and continuum elasticity is discussed in the review by Zbib, Shehadeh, Khan and Karami. The authors present an overview of the modeling and simulation methods used in DDD and a procedure to couple DDD with continuum elasto-viscoplastic finite elements. A variety of applications of the coupled method is presented, ranging from modeling nanoindentation to understanding the interaction of dislocations with shock waves. Two other embedded schemes in which the domain of interest is decomposed into continuum and discrete regions linked by appropriate operators are discussed in the article by Belytschko and Xiao. The article by Shen and Wang presents a summary of recent advances along the line of modeling large populations of dislocations and the linkage with continuum crystal plasticity models. Shen and Wang pioneered the use of the concept, developed in phase field modeling of phase transformations, to represent dislocation dynamics. Here, the field variables denote the amount of dissregistry in the glide plane corresponding to a dislocation core, a generalization to 3D of the idea embedded in the Peierls-Nabarro model of a dislocation. The model is applied to the study of several fundamental mechanisms of plastic deformation. Finally, the article by Harik presents a purely continuum analysis of a problem defined on the discrete-continuum transition scale.

Spatial and temporal scale linking is a challenging task. Despite the important advances made to date, the capabilities of current modeling methods are too limited to warrant their incorporation in commercial packages. These procedures are still in their embryonic development stage and their use outside the community of developers is rather limited. The future of the field depends on the close collaboration of experimentalists, theorists and computational scientists. We hope that this volume will stimulate interest in these methods and foster their future development.