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Editorial

Computer-aided multi-scale materials and product design

The success of computer-aided design (CAD) tools in engineering design has been witnessed in the past four decades. Advanced CAD tools have become a critical enabling technology in product design since they help build virtual prototypes of complex products (e.g. automobiles, airplanes, and electronic appliances). In today's CAD-enabled design processes, design engineers *select* available materials from databases to realize desired product functionality. Material databases are constructed by materials scientists and engineers based on the experimentally tested physical properties of existing materials. Therefore, the available 'degrees of freedom' for design engineers to control and optimize the performance of products are restricted to geometry and topology only. To offer design engineers more degrees of freedom, the additional dimension of material properties in the design solution space is highly valuable. Customizable materials can provide extra flexibility to realize the increasingly intricate product functionality. In other words, materials selection should be replaced by *materials design* to better meet stakeholders' requirements in modern product realization.

It can be envisioned that design engineers will perform product and materials design aided by multi-scale CAD software tools in the near future. They can not only perform the traditional geometry construction and structural analysis in such a multi-scale CAD environment, but also customize the material properties for some local region of the design by simply zooming into the specific region to specify material compositions or crystalline configurations. Design occurs concurrently at multiple length scales, including nano-, meso-, micro-, and macro-scales. Extensive problem-specific materials customization is thus achievable. Design decisions made at the microscopic levels determine the physical properties of new materials and the behavior of products. Materials design is integrated with geometry and topology design at the macroscopic level. Multi-scale CAD software tools help engineers to set functional objectives at different scales, construct material-inclusive product models, simulate and optimize design, and guide laboratory efforts to implement materials and target behaviors of final products.

The value of a multi-scale CAD environment lies in its seamless knowledge integration across disciplinary boundaries. The conventional material selection approach that design engineers usually take is based on the isolated databases that were built without the input of problem-specific needs. Such a one-directional bottom-up approach to discover, devise, and deploy new materials has a long development cycle and is not cost-effective. Even the materials science and engineering community has realized that the 'lack of design' limits the rapid advancement of engineering materials. Therefore, a systems engineering approach to integrate processing, structure, property, and performance for materials design has been adopted (see: Olson, G. B., "*Computational design of hierarchically structured materials*", Science, 1997, Vol. 277, No. 5330, pp. 1237–1242). A new term of Integrated Computational Materials Engineering (ICME) was coined to capture the top-down and target-oriented design process for materials that employs modern computational power to represent fine-grained microstructures, to simulate multi-level properties, and to devise fabrication processes of new materials. Most recently a new Materials Genome Initiative was kicked off in the U.S.A. to develop a new materials innovation infrastructure of computational and experimental tools along with digital data to accelerate materials development.

Various technical challenges to realize the new computational infrastructure for materials design also provide research opportunities, such as (i) how to rigorously quantify microstructure-property-processing relationships and establish high-level abstraction of materials knowledge, (ii) how to effectively extract useful information and knowledge out of abundant characterization data, (iii) how to integrate information and knowledge gained from simulation at individual scales for multi-scale systems design, (iv) how to improve efficiency and accuracy in such multi-scale simulation schemes, (v) how to extend available design methodologies such as data mining, analysis, and optimization in materials design, and (vi) how to quantify uncertainties in the design process, specifically variability caused by inherent randomness and incertitude due to the lack of perfect knowledge, in order to improve the robustness of design. In this special issue, the paper entitled "*Key computational modeling issues in Integrated Computational Materials Engineering*", authored by Panchal, J.H., Kalidindi, S.R., and McDowell, D.L. provides an extended overview of the major ongoing research elements in ICME, including materials databases for information collected from characterization, microstructure knowledge systems that represent and visualize high-level knowledge about materials, multi-scale modeling for materials design, uncertainty quantification and management.

Similar to the conventional CAD at bulk scale as the first tool for virtual prototyping, the primary function of multi-scale CAD is to allow for the efficient construction and interactive modification of geometric models for microstructures at small scales. Existing boundary-representation based parametric modeling approaches have become inefficient in model construction at nano- and meso-scales where geometry and topology are highly complex, because a great number of control points are required. New modeling and representation techniques are thus needed. For example, an implicit modeling approach can efficiently represent super-porous microstructures with intricate topology. To design material properties, the local control of shapes in microstructures is no longer important. It is more critical to allow design engineers to modify the overall structure globally in a representative volume

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element with easily controllable parameters and relate the values of parameters to the overall physical properties so that structure-property relationships can be established. The implicit modeling approach can serve this purpose well.

The geometric modeling of microstructures is still in its infancy. More research efforts are still needed. The efficiency and controllability of complex and porous shapes are the most important research topics for the interactive modeling of microstructures. The research problems tackled by the paper of Fryazinov, O., Vilbrandt, T., and Pasko, A. entitled "*Multi-scale space-variant FRep cellular structures*", are fairly representative. The authors present an implicit surface (or functional) representation that models volumetric cellular structures. By combining periodic sawtooth and triangular wave functions with R-functions, complex cellular structures can be built efficiently. The geometry of the unit cell can be extended to domains of different sizes easily. The flexibility and controllability of shapes are also demonstrated, where users can introduce variations by applying parameterization of functions, and compose geometries by operations such as metamorphosis, Boolean, and offset.

Boundary surface based representation is commonly used in modeling three-dimensional (3D) objects at the macroscopic level. As the modeling domain is zoomed into the atomistic level, precisely-defined and clear-cut boundaries of physical objects are no longer available. The shape and profile of atoms and molecules have to be measured indirectly, e.g. via the interacting force or electrical tunneling current between the molecule and an atomic scanning probe. The boundaries of molecules are vague, and molecular structures always change dynamically at non-zero temperatures. Even the shapes of a molecule before and after the measurement by a scanning probe are likely to be different because the observation procedure has changed the system itself as a result of physical interaction between the probe and the molecule.

There are various interesting research issues of computational geometry in the modeling and visualization of microscopic structures. For instance, distance geometry is a constraint satisfaction problem of finding the coordinates of a set of points given their pair-wise distances, which is used to determine atomic positions in biomolecular structure reconstruction from Nuclear Magnetic Resonance spectroscopy data. 3D Voronoi tessellation is widely applied in modeling polycrystalline microstructures, where Voronoi cells naturally represent polyhedral grains. The paper entitled "*Anomalies in quasi-triangulations and beta-complexes of spherical atoms in molecules*" and authored by Kim, D.-S., Cho, Y., Ryu, J., Kim, J.-K., and Kim, D. generalizes the conventional Voronoi diagram to the Voronoi diagram of spheres. The scheme is used to capture geometry and proximity of atoms. Geometric properties of biomolecules such as volume and pocket regions can be computed efficiently from the corresponding so-called beta-complexes in analysis (e.g. protein-ligand docking for drug design). Some anomaly cases of the diagram are also sensitive to the topology of particles so that they can effectively detect the proximity changes of atoms.

Beyond the traditional engineering domain, various modeling and simulation techniques at multiple scales have been developed and are becoming mature and prevalent in computational physics, chemistry, and materials sciences. These tools naturally become part of the solution for the computational design of materials and products. Fig. 1 shows the most used simulation approaches at different length scales, including quantum Monte Carlo, Hartree–Fock self-consistent field, and density functional theory (DFT), which are considered to be first-principles, as well as tight binding, molecular dynamics (MD), kinetic Monte Carlo (KMC), dislocation dynamics, and others that are typically semi-empirical or empirical. These first-principles approaches are numerical methods to solve the time-dependent or time-independent Schrödinger equations, which are regarded as the

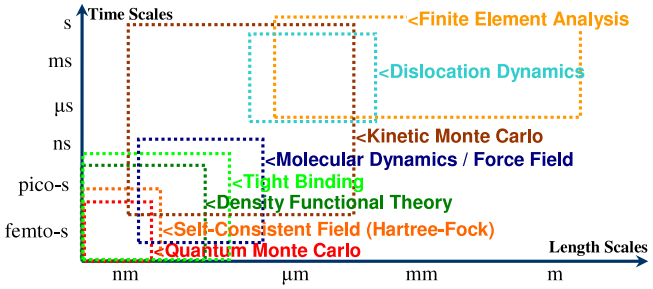

Fig. 1. Various simulation methods at different length and time scales.

fundamental description of our physical world from the level of electrons. Unfortunately, the exact solution of the equation beyond the one-electron system is not available. Hence, various approximation methods have been developed in these first-principles approaches. The central idea is to estimate the system's energy known as potential energy surface (PES) as a result of electron distributions such that ions can relax and redistribute towards stable or meta-stable configurations with local minimum energy levels. One major goal of materials design is to find such configurations that possess desirable physical properties. In other words, geometries at the atomistic level can be mapped to physical properties directly. For the empirical or semi-empirical approaches, usually approximated potential functions fitted from experimental data are used to simulate the behaviors of systems. It is important to note that different simulation methods have their own applicable spatial and temporal scales, as outlined by the boxes in Fig. 1. Simulation methods for small scales will become too computationally expensive to be applicable for large systems. Among the first-principles quantum-level simulation methods, DFT is the most efficient one for systems that are large enough and meaningful for engineering.

Optimization methods are extensively used in searching optimal geometries of stable atomistic structures during materials design. In addition, searching saddle points of PES is also important to simulate and predict phase transitions in designing phase change materials. Phase transition is a geometric and topological transformation process of materials from one phase (corresponding to a stable structure) to another, each of which has a unique and homogeneous physical property. Modern product design heavily depends on such phase change materials, e.g. hard-disk, CD-ROM, memory for information storage and battery, shape memory alloy for energy storage. Entitled "*Geometry guided crystal phase transition pathway search*", the paper authored by Crnkic, E., He, L., and Wang, Y. presents an approach of computer-aided transition pathway design for phase change materials which uses integrated information of geometry and physics. The crystal structures are constructed by an implicit model, called periodic surface. The metamorphosis of the periodic surface model provides predictions of geometry changes, which in turn serves as a good initial guess of a phase transition path that guides the detailed searching of saddle points on PES generated by DFT. This geometry guided approach improves the accuracy and effectiveness of a first-principles phase transition pathway search, which is demonstrated by several examples of crystals.

As our study reaches the scales of microstructures, uncertainty becomes a significant component in the modeling, simulation, or experiment. At the very fundamental level, quantum uncertainty is inherent in the properties of all wave-like systems, and electron's stochastic behavior is prominent. The famous Heisenberg uncertainty principle also shows the lower bound of correlated standard deviations between position and momentum. At the atomic level, defects and dislocations appear randomly in crystalline structures. At the mesoscale, material distributions exhibit stochasticity and

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irregularity of phase compositions, locations, and orientations. Uncertainties universally appear in the characterization, measurement, modeling, and simulation of imperfect materials. Lack of knowledge, systematic error, approximation and numerical errors are the major sources of epistemic uncertainty. The need for separating aleatory and epistemic uncertainties is more evident in multi-scale system analysis than in traditional analysis. Measurement data for unconventionally small or large systems are typically scarce, vary greatly in terms of forms and quality, or are even impossible to measure.

The accumulation of engineering design knowledge is through better understanding our targeted system via computational predictions, physical experiments, or both. As experimental techniques, particularly micro-imaging methods, advance in recent years, data from materials characterization are being accumulated quickly. The data-driven approach has become a valuable way to define the structure-property relationship of microstructures. Given the randomness of the microstructure distributions, the challenge is how to extract useful knowledge out of seemingly disorganized materials information for the purpose of design. The paper, "*Computational microstructure characterization and reconstruction for stochastic multi-scale material design*", authored by Liu, Y., Greene, M.S., Chen, W., Dikin, D.A., and Liu, W.K. illustrates an image-based characterization and stochastic materials model reconstruction for microscopic design. Statistical descriptions of two-point correlation in multi-phase materials can be extracted by analyzing images. The further abstraction of the statistical distributions can be achieved by regression based on several key materials characteristic parameters, which is used to establish a quantitative structure–property–process relation. Not only can these types of relation be used to facilitate the realization of desirable physical properties by designing compositions of heterogeneous materials, but also they can guide and control the fabrication of random microstructures.

As mentioned previously, different simulation methods are applicable for specific spatial and temporal scales. In order to provide overall structure properties with fine-grained and detailed information, multi-scale simulation approaches are thus needed in order to strike a balance between prediction fidelity and computational efficiency. Various multi-scale simulation methods have been developed for different application domains. The well-known first-principles approaches include first-principles MD with the quantum-atomistic coupling, and on-the-fly KMC as the DFT-KMC coupling. For engineering applications particularly in mechanics, various approaches have been developed, such as quasi-continuum, coarse-grained molecular dynamics, the variational multi-scale method, concurrent coupling, coupled atomistic/discrete-dislocation, adaptive multi-scale modeling, mathematical homogenization, the heterogeneous multi-scale method, multi-scale finite-element method, bridging scale method, bridging domain method, etc. Similarly, the paper authored by Hatami-Marbini, H., Shahsavari, A., and Picu, R.C. entitled "*Multi-scale modeling of semiflexible random fibrous structures*", demonstrates a stochastic homogenization approach for the mechanics of cross-linked fiber networks, which connects properties of individual fibers in a representative volume element to the continuum regime. It is observed that the consideration of correlation between elements becomes important when the size of elements is below some threshold with respect to fiber geometry. The Young's modulus correlation function for the stochastic finite element method at the continuum regime can be effectively derived from the fiber level mechanics. Such an analysis and simulation approach is crucial in information exchange between scales in a multi-scale CAD environment.

Computer-aided materials design has started bringing benefits to manufacturing industries for designing various products, such as microelectronic and optical materials in the semiconductor industry, drugs and biomimetric materials in the pharmaceutical and biotech industries, catalysis and coatings in the chemical industry, batteries in the automotive industry, and sensors in the aerospace industry, to name but a few. It is envisioned that multi-scale CAD systems will become an indispensable enabling technology of product design and virtual prototyping in the future, although much more work is needed to bring this paradigm into full practice. We hope that the papers included in this special issue will shed some light on the state-of-the-art and future research directions, thus encouraging new contributions from more researchers to this exciting area of computer-aided design.

We think our authors contributed valuable ideas to this special issue. We would like to thank all of them for their contributions as well as for their considerate cooperation in the review process. We are also in debt towards our reviewers who carefully studied all submissions throughout many cycles of the review process, provided constructive feedback for the authors on the original and the revised submissions, and provided helpful recommendations for us. Their rigorous review reports triggered active discussions and largely helped improve the quality of the included papers.

List of papers (only for production purposes)

J.H. Panchal, S.R. Kalidindi, D.L. McDowell (2012) Key computational modeling issues in Integrated Computational Materials Engineering.
O. Fryazinov, T. Vilbrandt, A. Pasko (2012) Multi-scale space-variant FRep cellular structures.
D.-K. Kim, Y. Cho, J. Ryun, J.-K. Kim, and D. Kim (2012) Anomalies in quasi-triangulations and beta-complexes of spherical atoms in molecules.
E. Crnkic, L. He, Y. Wang (2012) Geometry guided crystal phase transition pathway search.
Y. Liu, M.S. Greene, W. Chen, D.A. Dikin, W.K. Liu (2012) Computational microstructure characterization and reconstruction for stochastic multi-scale material design.
H. Hatami-Marbini, A. Shahsavari, R.C. Picu (2012) Multi-scale modeling of semiflexible random fibrous structures.

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