Simulation - Based Engineering Science

Revolutionizing Engineering Science through Simulation

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EXECUTIVE SUMMARY

S*imulation* refers to the application of computational models to the study and prediction of physical events or the behavior of engineered systems. The development of computer simulation has drawn from a deep pool of scientific, mathematical, computational, and engineering knowledge and methodologies. With the depth of its intellectual development and its wide range of applications, computer simulation has emerged as a powerful tool, one that promises to revolutionize the way engineering and science are conducted in the twenty-first century.

Computer simulation represents an extension of theoretical science in that it is based on mathematical models. Such models attempt to characterize the physical predictions or consequences of scientific theories. Simulation can be much more, however. For example, it can be used to explore new theories and to design new experiments to test these theories. Simulation also provides a powerful alternative to the techniques of experimental science and observation when phenomena are not observable or when measurements are impractical or too expensive.

Simulation-Based Engineering Science (SBES) is defined as the discipline that provides the scientific and mathematical basis for the simulation of engineered systems. Such systems range from microelectronic devices to automobiles, aircraft, and even the infrastructures of oilfields and cities. In a word, SBES fuses the knowledge and techniques of the traditional engineering fields—electrical, mechanical, civil, chemical, aerospace, nuclear, biomedical, and materials science—with the knowledge and techniques of fields like computer science, mathematics, and the physical and social sciences. As a result, finding costs. Better models of the subsurface would allow oil and gas companies to focus on prospects that offer the best return. As a result, they can allocate their capital much more efficiently.

The new SBES-related technologies have immediate application to other areas as well, including environmental remediation and storage of hazardous wastes. Again, these new application areas require an integrated and interactive simulation framework with multiscale capabilities. The development and use of such frameworks require the support of cross-disciplinary teams of researchers, including geoscientists, engineers, applied mathematicians, and computer scientists.

2.4 SBES in Materials

SBES-related technology may have its greatest societal impact where innovations in modeling and simulation methodologies intersect with innovations in materials. Multiscale modeling and simulation are transforming the science and technology of new-material development and the improvement of existing materials. This transformation is tantamount to a shift to a powerful new paradigm of engineering science. The new methods enable the unprecedented ability to manipulate metallic, ceramic, semiconductor, supramolecular, and polymeric materials. The results are material structures and devices that have remarkable physical, chemical, electronic, optical, and magnetic properties. We can now anticipate the molecular design of

With SBES, materials development becomes a unique opportunity for the integration of fundamental, interdisciplinary knowledge, with technological applications of obvious benefit to society.

composite materials with undreamed-of functionalities. Moreover, to reap the advantages that SBES technology brings to materials development, researchers from many disciplines would have to integrate their knowledge in the materials sciences. Such collaboration maximizes the possibilities for developing materials of great technological value.

The principle of materials design is rooted in the correlation of molecular structure with physical properties. From those correlations, models can be formulated that predict microstructural evolutions. Such models allow the researcher to investigate the mechanisms underlying the critical behaviors of materials and to systematically arrive at improved designs.

The use of simulations to uncover structure-property correlations can be superior to relying only on experimental data. The reason is that simulation provides detailed information regarding the evolved microstructure, as well as complete control over the initial and boundary conditions. Another significant aspect of SBES, one that makes future materials development more robust, is that it links simulation methods across different length and time scales. A great deal of progress is being made in the first principles calculations of electronic structure and in atomistic simulations. Now progress is also being made in connecting these two powerful techniques of probing physical phenomena in materials.

The benefits from new materials development are amply evident in the current progress in nanoscience and technology, a world-wide enterprise that can be compared to drug design. Because of the multiscale nature of materials modeling and simulation, SBES is destined to play a key role in nanoscience. SBES provides the capability of linking electronic-structure methods, which are necessary for dealing with novel nanostructures and functional properties, with atomistic and mesoscale techniques. That linkage ensures that the different phases of materials innovation—from design to testing to performance and lifetime evaluation—can all be simulated, examined, and optimized.

The power of multiscale computation can be seen in a number of high-profile applications involving the behavior of known materials in extreme environments. For example, a problem that has occupied the attention of a sizable community of researchers for several years is the characterization of the mechanical behavior of plastic deformation in metals at high pressure and high strain rate. The challenge, which is relevant to national security, is to conduct multiscale simulation that links all of the following: calculation of the core of a dislocation using electronic-structure methods; the modeling of dislocation mobility using molecular dynamics simulation; and the determination of constitutive relations for continuum-level codes. Multiscale simulation can also help solve problems in the development of the structural components of nuclear power reactors. Such materials must not only be radiation resistant, but they must have lifetimes of over 40 years.

Even for materials that do not have to stand up to the extreme conditions of high pressure and intense radiation, the field of materials innovation is rich with challenges to our understanding of the underlying microstructures of the materials. By meeting those challenges, we can reap enormous benefits. For example, we could generate a molecular model of cement, the most widely used substance made by humans. Such a model would help us develop a new cement with greater creep resistance and environmental durability. Similarly, models would help us improve the performance of catalysts for fuel-cell electric vehicles. We could also improve techniques in oilfield exploration, where instrumentation and digital management of hydrocarbon reservoirs are issues. In all these examples, improvements in materials performance would have great impact.

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Everywhere one looks there are problems important to society that require optimizing the functional properties of materials through the control of their microstructures. Clearly, SBES will have a long-term impact on materials innovation. Three attributes of SBES in particular lead to this conclusion.

- **Exceptional Bandwidth:** The conceptual basis of materials modeling and simulation encompasses all of the physical sciences. It makes no distinction between what belongs to physics versus chemistry versus engineering and so on. This universality of SBES technology represents a scientific bandwidth that is at least as broad as the entire range of multiscale applications in science and engineering. In materials modeling and simulation, as in SBES more generally, traditional disciplinary barriers vanish; all that matters is "the need to know."

- **Elimination of Empiricism:** A virtue of multiscale modeling is that the results from both modeling and simulation are conceptually and operationally quantifiable. Consequently, empirical assumptions can be systematically replaced by physically-based descriptions. Quantifiability allows researchers to scrutinize and upgrade any portion of a model and simulation in a controlled manner. They can thus probe a complex phenomenon detail by detail.

- **Visualization of Phenomena:** The numerical outputs from a simulation are generally data on the degrees of freedom characterizing the model. The availability of this kind of data lends itself not only to direct animation, but also to the visualization of the properties under analysis, properties that would not be accessible to experimental observation. In microscopy, for example, researchers can obtain structural information but usually without the energetics. Through simulation, however, they can have both. The same may be said of data on deformation mechanisms and reaction pathways.

These three attributes of SBES, of course, are not restricted to materials development; they apply equally well to the other areas of SBES application. In this section, however, the focus has been on the application of SBES to materials development. The point that emerges is that, aided by SBES technology, materials modeling and simulation, or computational materials, is becoming the sister science of computational physics and computational chemistry.

2.5 SBES in Industrial and Defense Applications

Simulation is ubiquitous in industry. It plays an essential role in the design of materials, manufacturing processes, and products. Increasingly, simulation is replacing physical tests to ensure product reliability and quality. Fewer tests mean fewer prototypes, and the result is a shorter design cycle. Steady reductions in design cycles, in turn, are crucial to U.S. efforts to remain competitive in a world where the pace at which new consumer products are being developed is increasing every day. The need for shorter design cycles also applies to our national defense and security. World events are often unpredictable; our defense industry must be able to design, modify, and manufacture equipment in quick response to military and police exigencies. A case in point is the unanticipated need to reinforce armored vehicles in Iraq after several such vehicles were destroyed by improvised explosive devices.

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The use of simulation has proved effective in some industrial applications. For example, in crashworthiness studies the few instances that simulations