Quantum Simulations in Materials Design, Nano Science and Technology

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Computational science is firmly established as a pillar of scientific discovery and technology promising unprecedented capability. NSF's ambitious petascale roadmap has dramatically accelerated the progress, but the competitive landscape is evolving, new architectures and capabilities are emerging, and the most compelling problems that could dramatically advance the human condition remain to be solved. It is thus critical for NSF to follow, and preferably lead, the “path to exascale”, while continuing to emphasize sustained rather than peak performance, as NSF has wisely done in the past. Furthermore, while the impact of the petascale roadmap on science is difficult to overestimate, the breakthroughs will not be realized without a new generation of computational tools that can provide truly reliable results for large systems. The emergence of computer hardware capable of reaching many sustained petaflops is only half of the solution. The other half is the development of a new generation of software tools that are capable of taking advantage of these architectures. Together, the rapid progress in hardware and software will enable a paradigm shift in how scientists use simulations because of the dramatic increase in the reliability of the computations and the size of the systems that may be studied.

These advances will enable accelerated design of materials and systems with radically new properties, relevant to virtually every sector of the economy, including energy, telecommunications and computers, medicine, and areas of national interest such as homeland security. The new “materials by design” paradigm has led to the creation of Materials Genome Initiative by the White House, in which NSF plays a major role. The promises of nanoscience and nanotechnology have also been amply recognized by NSF and other government agencies. Through NSF's leadership, the National Nanotechnology Initiative (NNI) has been established as a high-priority, multi-agency effort of funding long-term and high-risk R&D, through the corresponding efforts in other countries, and the creation of the various state, university and laboratory-based nanoscience centers. However, although the prospects for nanotechnology are very bright, its main current usage is either in niche applications, such as sunscreens, or in previously well-known areas, such as dispersed catalysts, where the use of nanoparticles has been established decades ago. This is because purposeful design and assembly of new materials or structures at the nanoscale is extremely difficult, preventing their rapid evaluation and limiting the potential for discovery. Confounding this difficulty, the *interesting* nanomaterials and structures are those whose properties *cannot* be simply predicted by scaling with size, because of emergent quantum phenomena and often also statistical fluctuations. Furthermore, while precise experimental control of the molecular assembly and nanoscale layout is still being developed, the fundamental understanding of the various nanoscale and molecular "building blocks" is often lacking. However, at the same time as the typical sizes of practical devices are shrinking, there is a dramatic expansion in the available computational resources, as well as important progress in theoretical methods. A confluence of the experimental and theoretical worlds is thus emerging in nanoscience, due to both experimental advances *and* the development of petascale hardware and new computational tools that enable simulations at unprecedented scale. The net effect is that we are approaching the point where the typical length scales of systems studied in nanoscience laboratories and the ones that can be modeled on petascale computers are finally meeting.

A major goal should be the development of multi-petaflops software tools to enable predictive simulations at unprecedented scale, which could impact several areas of science and engineering and become a source of new discoveries and economic growth. The simulation needs and their significance in several key areas are summarized in Table 1. While quantum simulations are often supplemented with simpler atomistic and continuum models, the quantum part is usually the bottleneck and requires the highest level of performance. Although the impact of petascale-level quantum simulation tools could be enormous, their development and adaptation to the petascale level is a highly non-trivial task. While some existing codes already reach a petaflop or more, additional development is needed to adapt them for a broad user community. Major algorithmic progress and optimization are also necessary, especially as we approach the 100's petaflops level through thousands of heterogeneous compute nodes. Additional issues include dealing with massive data generated by such simulations, validation of results with all their complexity, not only at a "single molecule" level, so that the predictions of simulations can be treated with confidence, and the ability of steering the simulations towards the most desirable outcome while dealing with exponentially increasing "design" landscape.

Table 1. Examples of Science and Technological Advances that become feasible with Quantum Nano-Simulation Tools and Petascale Computation.

Discipline	**Simulation Need**	**Significance**
Biochemistry and Molecular Biosciences	Structure/property relationships; mechanisms of enzymatic reactions.	Understanding of novel biochemical function and of essentials of life processes, enabling realistic, high-level models of biological systems. Tailoring antibiotics to fight new strains of bacteria.
Chemistry	Ab initio simulation of (nano) catalytic reactions in solution, charge-transfer reactions in solution, light-induced reactions.	Understanding and design of novel catalytic and bio-inspired reactions. Efficient conversion and trapping of pollutants, better routes to biofuels, simpler synthesis of new drugs.
Computer Science and Engineering	Simulation and design of photonic, molecular, nanoscale and spintronic devices.	Novel, ultrahigh-speed logic and memory with very low power requirements. Quantum computers.
Earth Science	Understanding of matter at extreme conditions.	Prediction of seismic shocks and volcano eruptions; understanding of planetary evolution.
Engineering	Simulation of chemical and biochemical processing; material stresses at extreme conditions	Cleaner manufacturing methods; novel and nanostructured materials; much reduced waste. Reduced-energy input engines and buildings.
Environmental Sciences	Formation, reactivity and transformation of pollutants; corrosion and breakdown processes.	Efficient conversion and trapping of pollutants, environmental sensors, new environmentally friendly cleanup processes.
Homeland Security	Development of chemical and biological sensors, design of impenetrable but breathable fabrics.	Sensors with nearly single-molecule detection limit, new protective clothing.
Materials Science	Multiscale modeling of complex and nanostructured materials/composites across many length and time scales. Design of new materials. Simulation of processes, including self-assembly.	"Virtual" design of materials with specified properties from first principles. Invention of nanostructured materials with novel properties. Understanding and prediction of material response, damage, and failure.