

# Enabling Technologies for Innovative New Materials

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In the quest to develop innovative products, researchers are increasingly relying on computational technologies to help simulate the properties of new materials. Ultimately, scientists engaged in materials research aim to develop new compounds that can predictably be applied to a product development program. While there are many disciplines that contribute to the research of new materials, nanotechnology research offers the greatest opportunity to develop innovative compounds to significantly enhance products and quality of life for consumers.

Although researchers have recently developed the technology required to observe and manipulate atoms directly, the ability to manufacture commercial products from these models remains elusive. Further, most of the research thus far has been devoted to understanding the results of investigator-initiated exploratory research rather than from designing new materials to meet existing or newly identified needs. While a number of products on the market today have arisen from this ad hoc approach, a more rigorous scientific-based design and development process must be accomplished to achieve reliable returns from the technology. Rational nanomaterial design, a systematic approach that incorporates rigorous engineering design for commercialization, will be required to move the technology from a research problem to a viable tool used to predictably develop commercially successful products.

Successful rational design of nanomaterials can be achieved by understanding the fundamental atomic and molecular properties of the material at the nanoscale. Using advanced computational algorithms and high-performance

computers, models can be developed to predict and explore the fundamental relationships between a material's structure, properties, behavior, and composition. As a result, nanotechnology and its applications are currently a hot topic of discussion and debate in the computational science community.

## Computational materials science

The use of computational chemistry to understand the fundamental nature of materials can contribute to the efficient

materials, CMS has become one of the fastest growing areas in the field of materials research.

Still, today's R&D organizations face new productivity challenges that require optimized performance to maintain a competitive advantage. In today's global marketplace, with inexpensive personnel resources, efficient distributed manufacturing and distribution, and aggressive margin-depleting pricing, development groups are required to produce differentiated products more efficiently and more effectively. To survive in this environment, development teams must use production-oriented computational tools for materials research that allow for comprehensive product development pipelines that extend through rational design, identification, characterization, manufacturing, and testing of new materials.

Computational materials science comprises a number of research focus areas, each consisting of various theories for software solution development. Clearly, the fields that study the macroscopic properties of materials are well established. These include simulations of stiffness, flow, and viscosity, which are successfully accomplished through finite element analysis, computational fluid dynamics, and impact simulations. However, the techniques that examine a material's basic components, its electrons, atoms, molecules, and functional groups provide a more fundamental understanding of its basic components and properties. Knowledge of these factors can lead to a state of predictable and rational design and ultimately translate this knowledge into building a superior final product faster.

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development of new products. Significant advancements in software development, the ability to perform complex data analysis, and the capacity to predict the properties of new materials *in silico* before any laboratory effort have brought enormous efficiency to the materials research community. Clearly, the field of computational materials science (CMS) has become a key driver in materials innovation by facilitating effective modeling and analysis of both empirical and virtual chemical entities. Due to these advancements in understanding the physics and chemistry of

## Categories of molecular computational solutions

Simulations of these basic molecular components *in silico* are achieved through a number of techniques, each having unique capabilities to address a research question. The major focus areas can be summarized by the following categories:

1. *Quantum mechanics*. Quantum mechanics (QM) methods estimate molecular properties from the interactions of electrons and, because they are based on a fundamental equation of quantum physics, they are much more accurate than the models developed by molecular dynamics techniques. Additionally, QM methods are required if the processes under study involve the breaking and forming of chemical bonds. The breakage and creation of

analyses, a variety of molecular attributes can be estimated. For MD computations, larger groups of atoms can be modeled compared to QM, since it works at a lower level of complexity.

Recently, the advent of technologies have either mixed the QM and MD theory levels or expanded upon them. For instance, there are now QM/MM (quantum mechanics/molecular mechanics) methods that provide the benefits of both techniques by treating certain small but interesting regions of a model at the QM level and other regions at the MM level. The periodic boundary conditions (PBC) technique permits the modeling of extensive material regions that are based on the regular repetition of units. Historically, these techniques were only available with MM methods but are now also possible with QM approaches. There are various commercially avail-

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## Nanotechnology research is an evolving field focused on developing new materials composed of atomic-scale components.

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chemical bonds is a crucial step in the formation of every chemical compound. Due to the extremely complex analysis used in QM, the main disadvantage of this technique is that long computational times can be required to model a simple system. Significant computational resources should be accessible for meaningful calculations, and the size of the system that can be studied has typically been limited by this requirement.

2. *Molecular dynamics*. Molecular dynamics (MD) calculates the motions of atoms or molecules and, in these simulations, atoms and molecules are seen as compact entities without any substructure. Therefore, unlike in QM simulations, electrons are not “visible” or analyzed in MD. Based on these

able software solutions that combine QM and MD theory to study the properties of large molecules.

### *Mesoscale dynamics*

A broad term, mesoscale dynamics refers to the simulation of more than a few thousand atoms but less than billions. In mesoscale calculations, subunits that are larger than atoms, such as each monomer in a polymer, are used as the basis of calculation. Mesoscale dynamics simulations are often used to study chemical reactions, kinetics, interface dynamics, and crystal structures for solid materials, fluids, proteins, and gases. Because they use larger subunits than the molecular models, simulations can be developed over longer time intervals, thus allowing for the study of complex materials including liq-

uids and polymers on the nanometer to micron scale.

Appropriate application of these technologies into R&D efforts can dramatically improve product design efforts.

### **Productive and reliable computational materials research**

To build an infrastructure that effectively builds and supports the rational development of new materials, it is critical that a flexible and enabling high-performance computational platform be available. Beyond simply increasing the speed of data analysis, the infrastructure must offer scientists the ability to not only perform the tasks quickly and accurately, but also allow them to ask new questions of the data and, ultimately, bring their research forward into new, previously unimaginable areas. Ultimately, the type of questions researchers need to ask should not be limited by the infrastructure they depend upon. Today's reality is that computing solutions are typically restricted to systems based on high-volume microprocessors combined with the now-standard open-source Linux operating system. Within this area, there are numerous choices, and a careful assessment of various parameters should be considered before

making a computational system decision. These include:

- Size and nature of the problem
- Number of users working on the problem or on the research team
- Size of the data and how they are accessed (e.g., disk access vs resident in memory)
- Size of primary, intermediate, and final data (scratch data are often much larger than primary and final data)
- Available data management solutions for the platform
- Type of computational power needed to provide useful turnaround of workload: 1) type of math needed in calculations (e.g., integer vs floating point), 2) application performance on 32-bit vs 64-bit environment, and 3) speed of connection between components (e.g., processors, memory, visualization, and other peripherals)
- Requirement for and availability of scalable visualization for the platform
- Development environment to support custom algorithms where needed.

Based on the Intel® Itanium® 2 processor (Intel, Santa Clara, CA), the Altix® family of servers (SGI®, Mountain View, CA) offers key advantages for running computational materials research applications. It satisfies the requirements for a standard processor-based system running Linux, while offering the capabilities to support state-of-the-art R&D. Most of the popular applications used for the various materials research fields are ported to the Altix and many have been optimized for high performance on the system.

The Intel Itanium 2 processor is based on the Explicitly Parallel Instruction Computing (EPIC) architecture. Since the instruction set is explicitly parallel, the architecture attains high levels of parallelism inside the processor (so-called "instruction level parallelism"). Leveraging the EPIC architecture of the Intel Itanium 2 processors, the Altix adds parallel system architecture, a very large set of internal resources, and high bandwidth con-

nection to I/O and memory. This means that more jobs can be run and more users serviced in less time. With the large shared address space provided by the Altix NUMA architecture, programming is simplified significantly.

In addition to the raw processor performance offered by the Intel Itanium 2 processor, the 64-bit Altix offers scientists a virtually unlimited memory capability in a tightly coupled system. The ultrahigh-speed NUMALink™ communication environment (SGI) connects the Altix system's processors, memory, visualization, and other peripherals. With this capability, the shared-memory platform is able to perform complex simulations with turnaround times that accelerate, rather than stall, the R&D process. This is in stark contrast to the barriers presented by other cluster platforms in terms of job turnaround, ease of programming, and versatility.

### **Conclusion**

Nanotechnology research is an evolving field focused on developing new materials composed of atomic-scale components. To successfully develop these materials, significant computational chemistry research is required to simulate and model their properties. Depending on a model's complexity and composition, these computational simulations can require considerable computational performance and, to effectively develop new nanomaterials, a scientist must be able to assess multiple options. Therefore, a high-performance computing infrastructure is often required to allow scientists in this field to complete multiple "what-if" scenarios so that the best model or trends in the models can be identified.

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