

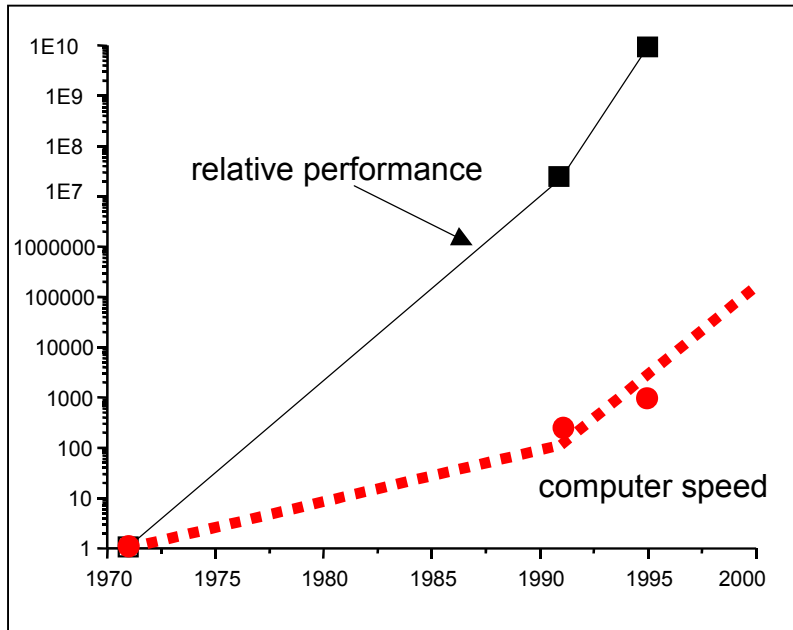
Computational Nanoscience on Earth Simulator Class Machines: A Revolution in Materials Science

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Since early times humanity has propelled itself forward through the development and exploitation of new materials – Bronze Age, Iron Age, etc. Advances in materials have driven economic, social, and scientific progress to the point that they profoundly shape our everyday lives. Advanced materials play a crucial, enabling role underlying virtually all technologies. Indeed, the current "Information Age" is built on the twin foundations of semiconductor processor and magnetic storage technologies developed over the last forty years. The exponential growth rate in both processing power and storage density has been made possible through control of materials properties at ever smaller length scales until they now approach a regime – the nanoscale – where advancing technology confronts fundamental physical limitations. While these barriers may limit further miniaturization of existing technologies, the nanoscale offers exciting possibilities for exploiting new classes of phenomena that only emerge at the nanometer scale and thereby produce revolutionary technological advances. Indeed, a number of nanoscale systems, including carbon nanotubes, fullerenes, molecular wires and switches, as well as nanoscale magnetic systems, have already demonstrated great potential for realizing new device paradigms. However, exploiting this potential poses the daunting task of obtaining unprecedented atomic-level control of materials properties and for describing the new – often quantum – phenomena. At the nanoscale materials properties differ radically from their bulk counterparts. Consequently, laboratory experimentation alone does not suffice. However, this is exactly the regime where modern predictive computational modeling coupled with Earth Simulator (ES) class computers can provide the scientific understanding and basis for systematic control of the phenomena and properties that are being exploited. Furthermore, progress in understanding of atomic and molecular properties at the nanoscale has the possibility for even broader impact. A sound microscopic understanding of molecules and their interactions will also lead to better understanding of biological systems, biological materials, and diseases. For example, better understanding of the microscopic interactions among genes (DNA), proteins, and the molecular signals that permeate the environment can be expected to lead to a revolution in biotechnology and “personalized” medicine.

For computational nanoscience to meet the challenge of understanding and controlling these systems, it must properly describe the physics of both short and long length and time scales. In addition, it must treat systems driven far from equilibrium and systems with many quantum degrees of freedom. To achieve these goals, fundamental changes in the way computation is done are needed. For example, since many of the paradigms upon which present computational methods of materials science are based fail at the nanoscale and in lower dimensions, many of these methods are of limited use. A significant shift in paradigms is needed. Recent progress in embedding quantum many-body techniques into *ab initio* electronic structure methods as well as new developments

in the treatment of electronic transport in the nonlinear response regime, indicate that such a paradigm shift is about to happen. But since most of these methods scale algebraically or even exponentially with materials complexity, investment in new hardware alone cannot meet the challenge in nanoscience – even a sudden increase in computer power by an order of magnitude will only lead to incremental changes in scientific output.



Relative performance increase of Ising model simulations (■) compared to the normalized speed of the computers (●) the simulations were executed on. The dashed line is a schematic of the increase in peak performance of the fastest supercomputers since 1972.

Fortunately, the experience in the field is that intellectual development, in the form of new algorithms, combinations of different methods, and new formalisms, greatly magnifies the raw performance increase of computers. This may be seen from the semi-log plot above, which shows the improvement in the simulation of Ising models used to study criticality. The lower curve shows the improvements of computer power since the early 1970s. The upper curve shows the increase in the number of effective spin flips simulated. If this increase were driven by the increase of computer power alone, these curves would be parallel. The slope of the relative performance increase is, however, much greater, indicating how the synergy between intellectual developments (theory and algorithms) and computer performance can magnify the increase in computer speed and make computations possible that would not be imaginable if only hardware improvements were made. Furthermore, the kink in both curves, which corresponds to the onset of massively parallel computing, shows how a change in architecture can drive intellectual development towards an even larger rate of increase of effective performance. Another example that illustrates this latter point is the development of the Locally Selfconsistent Multiple Scattering (LSMS) method. Challenged by the advent of massively parallel computer architectures, Stocks et al. managed to formally parse the physical problem into short and long length scales and were able to both parallelize and

achieve linear scaling for *ab initio* multiple scattering based electronic structure methods. Consequently, they were able to treat the first-principles spin dynamics of systems up to 2000 atoms. Since the algorithm scales almost ideally, an Earth Simulator class machine would allow the study of a system with 20,000 atoms, which corresponds to the *actual* size of experimentally interesting magnetic nano-particles. A simulation at this scale would open the door to new microscopic insights that are inaccessible experimentally. This would not be possible using previous algorithms, which scale like the cube of the number of atoms.

Given the opportunities and challenges presented by computational nanoscience and the ability of materials scientists, physicists, and chemists, to magnify any improvement in hardware architecture by several orders of magnitude, there is no doubt that a concomitant investment in a new generation of high performance computers and in computational materials science will lead to a revolutionary change in the kind of computational problems that can be addressed. The Earth Simulator class of high performance computers undoubtedly represents a similar challenge to computational scientists as did massively parallel computing. It is therefore reasonable to anticipate a million-fold increase in relative performance over the next five years if appropriate investments are made in computer hardware, algorithms, and methods development. While it is hard to predict exactly where the largest algorithmic improvements will happen, with such a scaling up one can be certain that computational nanoscience will:

- Allow first-principles simulations of the magnetic structure and magnetic moment dynamics of real magnetic nanostructures.
- Provide first-principles understanding of highly nonlinear electron and spin currents in nanoscale heterostructures and molecular devices to predict their properties.
- Allow a first-principles treatment of strongly correlated electron materials in nanostructures to predict the next generation of spintronics applications.
- Unlock the secrets of noncovalent interactions among DNA strands, proteins, and the molecular signals in living environment.