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"What Have *We* Been Doing?"

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"What have we been doing with the 10^{12} increase in computational capability over the last 30 years?" That is the title of a talk I recently presented. Most everyone is familiar with Moore's Law, which tracks and predicts the density of components on computer chips resulting in the doubling of computing speed and capacity every 18 months. However, that only accounts for a factor of a million over 30 years. The other factor of a million arises from clever algorithm development and the advent of massively parallel computing, which itself often requires algorithm development. Along with these nearly unfathomable increases in computing capability have come concomitant increases in communication bandwidth. These new technologies are changing the economic and social commerce of the planet.

"What have we been doing?" We are impressed by the advances of graphical computer games, which now accommodate thousands of simultaneous on-line players. We all benefit from fast search algorithms with their data banks, and we all suffer with the flood of spam and viruses. In looking at other disciplines, we are sobered by the vast improvements in global climate modeling and its projections of warming and its consequences. In biology, computers are essential for mapping the genetic code. In design and manufacturing, we find six-sided 3-D "caves," where a building's walls, floors, and fixtures can be instantaneously modified and "tested," or human tourist guides can make us faint by having us jump off the Empire State Building or inspire our imagination by immersing us in the culture of ancient Rome. We might worry about invasion of privacy, as some beta-version surveillance algorithm scans through millions of phone calls per minute, or we can be thankful that such technology may prevent another 9/11. It is a new world.

But, "What have WE been doing?" As a community we can point to vast improvements in CALPHAD, first-principles density function theory (DFT), quantum Monte Carlo (QMC), and first-principles molecular dynamics (MD). Even classical MD has hit the milestone of simulating a system with 160 billion atoms. These are all exciting avenues, populated by dedicated and creative scientists pushing frontier issues. However, in my opinion, there has not been the progress that a trillion-fold increase in capability might portend. Are our systems too complex? Are we in need of novel algorithms and new approaches for taming complexity? Does Hilbert space expand too rapidly for quantum spin systems? (2^N grows rapidly) I am not sure of the answer. I think the low-hanging fruit is probably plucked as soon as computational capability reaches the necessary threshold. I believe paths such as "materials informatics" will be rapid and incremental, but not revolutionary. Therefore, I suspect the future revolutions in materials will continue to come via a combination of serendipity and human intellect (greatly aided by computers), neither of which is likely to increase by 10^{12} in the next 30 years. However, by all standards, the growth rate of computational materials science has been impressive in academia and in industry. We can certainly expect that to continue. We have been doing well!

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