Position Paper - Bruce Harmon - Iowa State University

First an brief introduction: I've written several documents and editorials on the promise of supercomputing, chaired review panels for supercomputer operations, and still serve on the advisory committee for the Swiss supercomputer program.

With the caveat that prediction in computing has been famously poor (often erring on the pessimistic side… e.g. "640k ought to be enough for anybody..." Bill Gates, 1981); the challenge for the NSF with their budget and the present state of hardware development suggests no clear path… but I don't believe that is the cause for pessimism. There was a recent period where the first slide everyone showed was of Moore's Law and how we would be obtaining Exascale computing by 2018 --- the danger of blind extrapolation! However the insight provided by David Gelernter is interesting: "In the technology world, <u>software</u>, not hardware, determines the state of the art and the pace of change."

While the future will certainly involve university research teams partnering with industry/government projects for testing and developing higher capacity computing facilities, I believe there is an opportunity for profitably promoting software development in a number of fields. New, compelling algorithms can be developed, tested and deployed with moderate size machines… breakthrough algorithms employed in various branches of science and engineering can be revolutionary.

New algorithms making use of the large scale computing now available is frontier science; or should be. Unfortunately there does not seem to be a coordinated and systematic vision on how to promote new or more efficient software; and perhaps more importantly how to make it available to a wider community (beyond the small group responsible for its creation). Serious software has grown well beyond a cottage industry. In some cases European agencies were the first to notice this and rather than compete on the hardware side, they adapted an emphasis on software. Teams in scientific specialty areas where algorithms and/or data bases are poised to make significant advances could well be the focus for new NSF initiatives.

Editorial submitted for the December 2010 issue of the Journal of Phase Equilibria and Diffusion by Bruce Harmon, Associate Editor.

CHANGE OR PERISH

The title of this editorial comes from the 2005 Pritzker Prize winner's speech. Thom Mayne is the principal at Morphosis, an architecture firm in Santa Monica California. With regard to computational advancement of ideas to reality he says: "The tools we now utilize simplify these potentialities and make them logical, allowing us to produce spaces that even ten years ago would have been difficult to conceive, much less build. Anything that is possible is realizable." Similar thoughts must surely permeate forefront design teams in automotive, aerospace, and other engineering industries. Some cutting edge entertainment and retail companies seem to have had related epiphanies.

In materials discovery there are also examples of computational adaptations needed for progress (or survival) and, similar to the industries listed above, commercial advantages are a strong driver. CALPHAD is an example well known to our community, while bio-tech companies represent a dynamic new example where ideas and drug design are developed *in silico* (an appropriate and common biology way of saying 'in computers').

There are certainly commercial pressures pushing for the development of new and better materials. For example, in the news this past year are articles calling for the development of stronger non-rare earth permanent magnets as China has gained a near monopoly in the mining and production of rare earth products. With their push for wind energy, China will soon be able to consume all their rare earth production for domestic wind turbine installations. There are calls for stronger materials, harder materials, higher temperature superconductors, materials that can better withstand nuclear reactor radiation, etc. But unlike some of the examples above, computer aided bulk material discovery is not yet a routine undertaking. The underlying quantum processes can be complex (beyond the purview of standard electronic structure algorithms), the number of possible combinatorial atomic configurations can be prohibitive to evaluate with precision, and the necessity of structural stability at elevated temperatures can hinder computational evaluations.

Government sponsored research in the early stages can nurture the development of computational methods, which in turn can lead to commercial development and promote greater applications. Recent statistics show that Europe has surpassed the US in the number of publications dealing with computational materials science and chemistry by 65%, and China's publications in this area are projected to surpass those of the US by 2012. Many software teams in Europe are centered around suites of codes, which are available for downloading or for sale, although the progenitors of most of the codes were developed in the US. A list of 24 such codes is presented in the recent publication "Numerical Methods for Electronic Structure Calculations of Materials" by Y. Saad, J. R. Chelikowsky, and S. M. Shontz (SIAM Review, v.52, No. 1, pp.3-54, 2010). There are a number of other codes that could have been listed, such as GAMESS (with 150,000 users). Bill Gates pioneered the concept that progress (and profit) is in the software, not the hardware. That may prove to be the case for advancing materials development as well.

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With computing capability continuing to dramatically increase (toward the exascale*), successful materials discovery *in silico* should be a success story accelerating for at least the next 50 years.

*See the author's previous editorial in the August 2009 issue of this journal.

So, while I greatly support the development of hardware (a vendor dependent task), I believe the science and engineering would benefit by a strong emphasis on the software.

Bruce Harmon