Editorial

In August I will be attending a high performance computing workshop intended to articulate visions driving the next generation of high performance supercomputers: computers three orders of magnitude more powerful than the petascale computers, which came online just within the last year. An exascale computer would be able to evaluate a million trillion floating-point operations per second. Imagine, if possible, every man, woman, and child on earth performing 170 million mathematical operations per second. If they all used advanced single processor desktop computers, then the problem would be to bring all that information together very quickly! But what could be learned? Global climate modeling at ever higher precision is of course one of the prime motivations, but there are also compelling opportunities in other disciplines such as astronomy, nuclear, and high energy physics. Chemistry and Engineering have their own favorites (e.g., combustion), but what about the materials community and, in particular, the topics often encountered in these pages?

Recent JPED editorials have taken note of the increasing number of thermodynamic and material property databases and the demand from commercial customers wanting to push beyond known regions of compositions, temperatures, and microstructures. Some of these editorials mention the progress in first principles calculations, but modern material explorations often entail so much complexity as to preclude a meaningful first principles approach. Indeed, it may be some time before quaternary, quinary, or higher order systems are routinely, let alone successfully, pursued ''in silico.'' There is therefore a healthy respect and admiration for the often heroic experimental efforts made to carefully map out and document phase regions and material properties, some far from equilibrium. Are we entering a period where we might expect more help from computations? The answer is, of course, 'yes,' but will it be incremental or transformative?

With exascale computing I believe there is an opportunity for a transformative period. For example, material searches for optimized radiation detection materials have systematically produced first principles databases of twenty to fifty thousand compounds, but have taken months to a year. In general, the work has been too slow to ignite the synergy arising from a close partnership between theory and experiment. Will that change when the time is reduced from six months to six hours? There has also been progress in the last year in developing and applying algorithms to search out stable structures and ''energy landscapes.'' See, for example, Nature **457**, 863-867 (2009), and J. Chem. Phys. **130**, 104504 (2009). Another development is a first principles approach to entropy driven stabilization (Phys. Rev. Lett. **100**, 095901 (2008)) without the need for molecular dynamics simulations. These and a number of other developments portend an increasingly relevant role for computational materials science. A transformative period may depend on whether the community can come together to collectively develop modern algorithms in a timely fashion for use on exascale computing platforms. I am optimistic.

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Journal of Phase Equilibria and Diffusion