Paths for computational chemistry to the exascale

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Many are now questioning whether our current approaches to developing software for science and engineering are sustainable. In particular, can we deliver to society and the nation the full benefits expected from high-performance simulation at the peta and exascales? Or is innovative science being stifled by the increasing complexities of all aspects of our problem space (rapidly changing hardware including GPGPU and other accelerator technologies, software design, parallel programming models, multidisciplinary physics, etc.)?

Focusing on applications in chemistry and materials science, and motivated co-design of exascale hardware and software, I will discuss many of these issues including how chemistry has already been forced to adopt solutions that differ quite sharply to those in the mainstream, and how these solutions position us well for the technology transitions now underway.

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