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Seeking a sustainable approach for computational science[1]

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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, software, multidisciplinary physics, etc.)? Focusing on applications in chemistry and materials science, and motivated by the 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 under way. Radical changes in how we compute, going all the way back to the underlying numerical representation and algorithms used for the simulation, also promise great enhancements to both developer productivity and the accuracy of simulations.

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