Planning for Change: Designing Large-Scale Software Systems for Emerging HPC Environments

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ABSTRACT

Computational chemistry is a leading consumer of resources many of the largest high-performance computer (HPC) systems around the world. For the last several decades, the architectures of these systems has been quite stable. But due to a number of drivers, we are entering a period that will see much greater levels of flux and diversity in HPC architectures, to which computational chemists will have to adapt.

In this talk, I will provide some background on why this is happening and how computer vendors, computing facilities, and funding agencies are responding to the situation (focusing on the U.S. Dept. of Energy). I will also discuss the next-generation DOE leadership-class computer systems, as well as the drive to exascale systems in the following generation.

I will then discuss some of the considerations and strategies available to help developers create large-scale, complex software systems that can more easily adapt to changes not only in computer architectures, but also to the rapid progress and changing needs of the science. These strategies range from high-level considerations of software architecture and design to much more implementation-specific details such as choice of language and programming model.

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