Title: “Pushing back the point of diminishing returns for parallel performance"
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Parallel application development is a major challenge requiring expertise in physical science, applied mathematics, computer science, and software engineering. Such complexity presents a challenge on current platforms, let alone exascale platforms. Exascale computing further complicates the programming environment by requiring extreme levels of parallelism (billions of threads) for efficient utilization. Another major concern is the reduction in mean time between failures expected for machines with so many components. Unfortunately, the existing MPI-centric approach to programming parallel machines has failed some application communities from its inception, and eventually MPI (or MPI + OpenMP, OpenCL, etc.) will be inadequate for all application communities as we move to exascale computing. This talk will discuss these issues and how they relate to a future exascale programming environment consisting of domain specific languages and high-level libraries, which together will hide architecture-specific complexity from domain scientists. Specific examples will be taken from the quantum chemistry domain, and these will illustrate not just the changes needed in the programming model, but also the changes needed in the way that application programmers and domain scientists must think about their problems.