

Amgen Seminar Series in Chemical Engineering
in
Cherry Auditorium, Kirk Hall, 1 PM

Presents on October 22, 2009

From Solar Cells to Exascale Computing

By

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Beginning with a brief overview of a boundary integral problem that led from an intractable computational problem to model an efficient solar cell but through a novel mathematical formulation became tractable, I will lay the foundation of the importance of mathematics in computation. This problem led to my career in High Performance Computing (HPC). Today, as we move from the Petascale era to Exascale era, HPC is a tool frequently used to understand complex problems in numerous areas such as aerospace, biology, climate modeling and energy. Scientists and engineers working on problems in these and other areas demand ever increasing compute power for their problems. In order to satisfy the demand for increase performance to achieve breakthrough science and engineering, we turn to parallelism through large systems with multi-core chips. For these systems to be useful massive parallelism at the chip level is not sufficient. I will describe some of the challenges that will need to be considered in designing Petascale and eventually Exascale systems. Through the combination of HPC hardware coupled with novel mathematical and algorithmic approaches, such as those described in the initial problem of this talk, some efforts toward breakthroughs in science and engineering are described. While progress is being made, there remain many challenges for the computational science and engineering community to apply ultra-scale, multi-core systems to “Big” science problems with impact on society. In conclusion, some discussion not only on the most obvious way to use ultra-scale, multi-core HPC systems will be given but also some thoughts on how one might use such systems to tackle previously intractable problems.

This series at the University of Rhode Island is made possible through the generosity of Amgen, West Greenwich, R.I.