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Developing scientific communities that can drive the exascale computing roadmap

Abstract

Supercomputing facilities have become large (and expensive) research infrastructures. The dramatic increase in power consumption – from a 100 kW in the past to a few MW today and tens of MW by the time performance reaches exascale – is putting pressure on computational scientists to articulate the needs of such infrastructures. In analogy to common practice in the physical sciences, where user communities drive the design and construction of instruments, a concept of computational end-stations was introduced and experimented with several years ago at ORNL. In this presentation, I will show how the concept was further developed in the Swiss High-Performance Computing and Networking (HPCN) initiative, where particular attention was given to developing HPCN expertise in the teams that develop large community codes that are usually not affiliated with supercomputing centers. The model is being developed within the European PRACE project as well. I will discuss how we are using these community efforts to drive the development supercomputing systems that will be installed in the coming years at the Swiss National Supercomputing Center (CSCS) in Lugano.

Biosketch

Thomas Schulthess received his PhD in physics in 1994 from ETH Zurich. After a postdoctoral fellowship at Lawrence Livermore National Laboratory, he moved to Oak Ridge National Laboratory (ORNL) in 1997. In 2002 he became group leader of the Computational Materials Sciences Group in ORNL's Computer Science and Mathematics Division, and in 2005 he received a second appointment to lead the Nanomaterials Theory Institute of ORNL's Center for Nanophase Materials Sciences (CNMS). Since October 2008, Thomas holds a chair in Computational Physics at ETH Zurich and directs the Swiss National Supercomputing Center (CSCS) in Lugano. He currently holds a visiting distinguished professor appointment at ORNL. Thomas' research interests are in condensed matter physics. He led the teams that were awarded the 2008 and 2009 ACM Gordon Bell Prizes, and that were the first to sustain petaflop/s performance in productive simulations.