LECTURES on Numerical Mathematics and Applications

27 - 28 August 2014, Würzburg, Germany
Julius-Maximilians-Universität Würzburg, Germany

Ulrich Ruede
Universität Erlangen-Nürnberg

Challenges and Opportunities of Extreme Scale Numerical Simulation

Present day supercomputers deliver a performnace beyond a Peta-Flop, that is 10^{15} floating point operations per second. In the coming decade, exa-scale computers will become feasible with a performance of even 10^{18} floating point operations per second. The availability of such computational power will open unprecedented opportunities, but it will come at a high price, not only for the machines themselves, but e.g. also for their energy consumption which is estimated to exceed 20 MW. For computational scientists these machines will pose enormous challenges, since new algorithms and software must be developed that can exploit massive parallel execution much beyond our current state of knowledge.

The lecture will illustrate the difficulties with examples from three projects. The first is a multigrid solver for finite elements, motivated by an application in geodynamics. Here the problem is to simulate the creeping flow of the earth mantle over a time period of about 100 million years with a resolution of up to a trillion elements such that a global meshing of the planet volume with a 1km mesh can be used. We will demonstrate that parallel multigrid solvers are suitable for this when advanced techniques such as a matrix-free design are implemented. The second example will deal with particulate systems modeled by the discrete element method with the goal of a direct numerical simulation of granular systems and particulate flows. Finally, we will discuss flow solvers using the Lattice-Boltzmann method with applications in additive manufacturing and food technology. All these algorithms are suitable for massively parallel systems.