RWTH Aachen

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Fifth SIAM Workshop on Combinatorial Scientific Computing, May 19–21, 2011, Darmstadt, Germany

Markus Beckers, Johannes Lotz, Viktor Mosenkis and Uwe Naumann (Editors)

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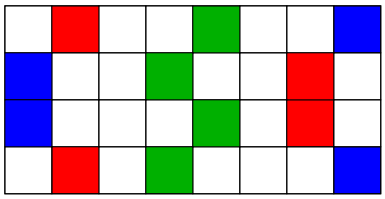

Abstracts

Markus Beckers, Johannes Lotz, Viktor Mosenkis, and Uwe Naumann (Editors)
LuFG Informatik 12: Software and Tools for Computational Engineering
RWTH Aachen University, Germany

The human desire for meaningful numerical simulation of physical, chemical, and biological phenomena in science and engineering has been increasing with the growing performance of the continuously improving computer systems. As a result of this development, we are (and will always be) faced with a large (and growing) number of highly complex numerical simulation codes that run at the limit of the available high-performance computing resources. These codes often result from the discretization of systems of differential equations. The runtime correlates with the resolution that often needs to be very high in order to capture the real behavior of the underlying system. There is no doubt that the available hardware will always be used to the extreme. Improvements in the runtime of the simulations need to be sought through research in numerical algorithms and their efficient implementation on parallel architectures.

Many of the resulting problems are combinatorial in nature. Most of those are known to be computationally hard in the sense that efficient (polynomial in the required time and memory space) algorithms for their exact solution are unlikely to exist. For example, we have to deal with partitioning, elimination ordering, coloring, and matching problems for graphs and hypergraphs in various contexts. A good approximation of the solution to these abstract problems may lead to a significant decrease in the runtime of numerical programs that implement solvers for partial differential equations, nonlinear optimization algorithms, or solvers for generalized Eigenvalue problems. Problem sizes are typically now in the millions of unknowns; and with emerging large-scale computing systems, this size is expected to increase by a factor of thousand over the next five years. Moreover, simulations are increasingly used in design optimization and parameter identification which is even more complex and requires the highest possible computational performance and fundamental enabling algorithmic technology.

What binds together the community of combinatorial scientific computing is the focus on practical use of graph algorithms and combinatorial algorithms to address a variety of different problems that all arise in scientific computing. This shared common denominator allows us to interact productively and to advance the state of the art in several different problem areas.

The Fifth SIAM Workshop on Combinatorial Scientific Computing represents another important milestone. Three CSC experts have been invited to present plenary talks on various important aspects of CSC:

- Thomas F. Coleman (University of Waterloo, Canada): *Efficient Automatic Differentiation for Nonlinear Systems and Continuous Optimization (by using graphs)*; joint with SIAM Workshop on Optimization;
- Burkhard Monien (Paderborn University, Germany): *Recent Trends in Graph Partitioning for Scientific Computing*;
- Trond Steihaug (Bergen University, Norway): *Sparse Matrix Structures and Higher Derivatives.*

This collection of extended abstracts covers all accepted contributed oral and poster presentations. It is meant to give both participants of CSC11 and other interested readers an overview of recent results and ongoing research and development projects in the area of Combinatorial Scientific Computing.