

# Topic 10: Parallel Numerical Algorithms

## (Introduction)

Julien Langou, Matthias Bolten, Laura Grigori, and Marian Vajteršić

Topic Committee

The solution of large-scale problems in Computational Science and Engineering relies on the availability of accurate, robust and efficient numerical algorithms and software that are able to exploit the power offered by modern computer architectures. Such algorithms and software provide building blocks for prototyping and developing novel applications, and for improving existing ones, by relieving the developers from details concerning numerical methods as well as their implementation in new computing environments.

The topic includes many different aspects, ranging from fundamental algorithmic concepts, to their efficient implementation on modern parallel architectures, such as multicore and multi-GPU systems, to their application in design and prototyping scientific simulation software, as well as to performance analysis.

From the papers submitted to this year's Euro-Par, the topic of Parallel Numerical Algorithms involving these themes attracted submissions from various continents. Each paper received at least four reviews and finally five were selected for presentation following extensive discussions between members of Euro-Par's Program Committee.

Kuzmin, Luisier and Schenk describe a parallelization based on techniques used for sparse direct solvers to compute selected entries of the inverse of a sparse matrix. The technique is successfully applied in the context of quantum transport calculation.

Agullo, Buttari, Guermouche and Lopez presents an implementation of the multifrontal QR factorization based on the StarPU runtime. The parallelism related to the factorization of each frontal matrix as well as the parallelism available among different frontal matrices and exposed by the separator tree is exploited. The authors show that a runtime system as StarPU can be successfully used to implement sparse/irregular matrix computations. The paper confirms the interest of runtime systems, even for sparse computations.

Schindewolf, Rocker, Karl and Heuveline compare different ways of implementing the Conjugate Graduate method (CG) on multi-core CPUs. The authors apply transactional memory technique and show that a "pipeline" CG method enables to speedup execution time by reducing communication and synchronization costs.

Lotz, Naumann, Sagebaum, and Schanen explain how to compute the discrete adjoint, with the Algorithmic Differentiation (AD) tool "dco", within the PETSc framework. Technical work described includes management by AD of the BLAS and LAPACK used in PETSc, and differentiation of the MPI communications involved (with a focus on persistent communication). This strategy to obtain

discrete adjoints targets difficult situations, involving libraries and tools at various functionality levels (PETSc, BLAS/LAPACK), as well as MPI parallelism. These situations will occur typically in large, real-life applications. This strategy makes full use of the versatility of overloading-based AD.

Schreiber, Weinzierl, and Bungartz focus on solvers for partial differential equations and consider dynamically adaptive grids arising from spacetrees. The authors use the fact that such grids have an underlying tree formalism and use it to decompose such grids into clusters on-the-fly. The authors also describe an approach for dynamically adaptive cluster reordering and skipping. The algorithms are implemented using OpenMP tasks and TBB based on a depth-first traversal of trees.

These five papers provide a selected overview of recent developments in the design and implementation of numerical methods on modern parallel architectures.

It is appropriate, at this time, to thank the authors who submitted papers to our topic and to congratulate those whose papers were accepted. We are especially grateful to the referees who provided us with carefully written and informative reviews. Finally, we thank the conference organizers for providing the opportunity to the participants to present and discuss the state-of-the-art in Parallel Processing in the beautiful city of Aachen.