University of Cologne

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Workshop on Efficiency in Computational Science

University of Cologne
25th September 2019

Outline

This workshop brings together researchers in the field of computational science to share and discuss their work where it relates to efficiency. Here, efficiency is understood in a very broad sense, including numerical method development, serial and parallel algorithms, implementation, and hardware aspects. The intention is to provide an informal environment that encourages the exchange of novel ideas and untested approaches. Therefore, the speakers are asked to put an emphasis on work in progress and unsolved issues, and to not restrict themselves to sharing "camera-ready" results only. Ultimately, the goal is to get a fresh perspective on common challenges, to establish new connections across institutional and discipline boundaries, and to identify potential for future scientific collaborations.

Agenda

13:00	**Welcome**
13:10	**Efficiency challenges in adaptive parallel multiphysics simulations** *Dr. Michael Schlottke-Lakemper, University of Cologne*
13:40	**Current HPC developments in the TRACE flow solver** *Dr. Georg Geiser, DLR Cologne*
14:10	**Towards Large Scale Continual Learning on Modular High Performance Computers** *Dr. Jenia Jitsev, Forschungszentrum Jülich*
14:40	**Coffee break**
15:20	**Vectorization of high-order DG and adaptive linearization** *Dr. Harald Klimach, University of Siegen*
15:50	**Promises and Challenges of Dispersion Relation Preserving Finite Difference Methods** *Dr. Viktor Linders, Lund University*
16:20	**Structural modelling for helicopter simulation – or: making small problems even smaller** *Melven Roehrig-Zoellner/Dr. Max Kontak, DLR Cologne*
16:50	**Coffee, discussions & open end**

Organization

The workshop will take place at the Mathematical Institute, University of Cologne, Weyertal 86–90, 50931 Cologne, in “Seminarraum I” (room 005 on the ground floor). Each talk has a slot of 30 minutes, which includes five minutes that should be reserved for discussions. Guests are welcome and invited to join for both the talks and discussions.

Abstracts

Efficiency challenges in adaptive parallel multiphysics simulations
Dr. Michael Schlottke-Lakemper, University of Cologne
Coupled multiphysics simulations pose particular challenges when trying to scale to a large number of processes. Problems such as data exchange, adaption, dynamic load balancing, or the synchronization between solvers are either nonexistent in single-physics applications or become considerably more complex in multi-system setups. In this talk, a scalable approach for multiphysics simulations will be presented, where multiple solvers share a single hierarchical Cartesian mesh. In addition, open questions regarding the efficient execution of multi-solver configurations, and some possible solutions, will be discussed.

Current HPC developments in the TRACE flow solver
Dr. Georg Geiser, DLR Cologne
A brief overview of the TRACE flow solver and current developments w.r.t. high performance computing is given. This includes advanced partitioning techniques for structured multi-block grids and a cooperative multi-task scheduler supporting asynchronous communication patterns with context switching. In addition, first results of a code modernization for SIMD-friendliness are presented.

Towards Large Scale Continual Learning on Modular High Performance Computers
Dr. Jenia Jitsev, Forschungszentrum Jülich
In the talk I will outline the opportunities and challenges towards removing current severe limitations in training robust generic transferable models from large data streams and progress towards neural architectures that are capable of continual learning. Continual learning posits set of abilities to receive streams of incoming, unlabeled data without any clear task boundaries and digest them into a progressively growing generic model without functional collapse. Using this generic model, learning network should be able to deal with variety of multiple tasks and diversity of specific domains without any additional external supervision or necessity to freeze or otherwise manually tune learning, showing increasingly better learning performance across tasks and domains as learning progresses (learning to learn). Apart from the core algorithmic challenge to designing such learning systems, learning of such a versatile model will require active generation of large amounts of highly variable data and will thus put high computational demand on data generation and training of networks. HPC facililites will therefore become indispensable for growing such general AI.

Vectorization of high-order DG and adaptive linearization
Dr. Harald Klimach, University of Siegen
I will briefly discuss a concept of local linearization that can easily be achieved in a modal discontinuous Galerkin discretization. It enables adaptive efficient computations for problems like direct aeroacoustic simulations where only small fractions of the overall computational domain need to be computed with nonlinear equations. For the efficient computation of these schemes we employ the NEC Aurora TSUBASA vector system. I will show how the vector system can be exploited for high-order discretization and present some first performance evaluations on a single Aurora node.

Promises and Challenges of Dispersion Relation Preserving Finite Difference Methods
Dr. Viktor Linders, Lund University
It is well known that maximizing the formal order of accuracy with respect to the bandwidth of a finite difference stencil may lead to a sub-optimal numerical scheme for problems involving high frequency waves over large time spans. Errors materialize as incorrect phase and group velocities, which may drastically distort the numerical solution. An attractive alternative is the family of dispersion relation preserving (DRP) schemes with improved resolution of high frequency solution components. This talk aims to outline the benefits of such schemes for severely under-resolved problems as well as discussing some of the difficulties inherent to these methods.

Structural modelling for helicopter simulation – or: making small problems even smaller
Melven Roehrig-Zoellner/Dr. Max Kontak, DLR Cologne
We present algorithmic and implementation aspects of our work on a software for helicopter simulation from a joint project with the DLR Institute for Flight Systems. In this talk we focus on the structural dynamics of (rigid) multibody systems and flexible beams. Both already represent small problems compared to, e.g., large scale CFD simulations (we have usually less than 100-1000 DOFs). However, several cases of application of the software require us to make these problems even smaller (we'll give a motivation for that in the talk!). We exploit C++ template-programming to obtain a modular software design and to still be able to obtain reasonable performance with small data: examples include efficient automatic differentiation as well as a fast 1D discontinuous Galerkin method. We discuss the underlying software design ideas and show results for the performance and accuracy of our approach.