

Preface

Advanced Computing

The opening statement of this book, one of the key conclusions of the 2005 PITAC report, labels *Advanced Computing* and *computational science applications* as fields of research with high scientific and economic relevance. Today, computational science and engineering (CSE) has become a highly interdisciplinary, challenging, and thriving scientific domain of increasing importance and visibility in research, development, and education. Its essence involves modelling and computations – in particular (numerical) simulations – on computer systems ranging from standard PC to supercomputers. Thus, CSE applications have always been a driving force of computing technologies, especially progressing the field of supercomputing.

However, regarding *advanced computing technologies*, an increasing gap is observed between what should be possible in theory – due to recent advancements in algorithms, hardware, and networks – and what can really be achieved in practice. While increase of hardware performance (Moore’s law) and considerations on complexity and accuracy of algorithms were driving this field over the last decades, new limiting factors are now encountered: hardware awareness and ubiquitous parallelism due to many-core systems (to name only two such issues) transform computing into a multifaceted process spawning modelling, algorithmics, parallel programming, and even hardware design; simulation data are produced to an extent and resolution which makes their mere handling, their analysis and, thus, the extraction and representation of relevant information a serious challenge – especially if to be done interactively; the development of software for high-performance computing (HPC), ranging from specialised single-application codes to general problem-solving environments, has thus become an increasingly complex process, comparable to what we have known for decades from other fields, and it needs sophisticated language and tool support as well as a substantial professionalisation.

Hence, to be able to exploit future (super)computers at their full potential and to expand the research frontiers mentioned above, a concerted effort is necessary in *Advanced Computing* – which is thus defined as HPC together with all its enabling

technologies crucial to tackle the old and new bottlenecks. Such an endeavour must combine computing technologies and applications and bring together the HPC community as well as application specialists with experts from the enabling technologies.

The Munich Centre of Advanced Computing

Starting from these considerations, in 2008, the *Munich Centre of Advanced Computing* (MAC) has been established as an independent research consortium and common roof for computing-related activities of research groups at Technische Universität München (TUM) – together with several partner institutions, such as the Leibniz Supercomputing Centre, the Max-Planck Institute for Astrophysics, or the Department of Geophysics of Ludwig-Maximilians-Universität München. On the funding side, MAC started on two pillars: eight projects cofinanced by the State of Bavaria and by TUM and two projects established in the framework of a strategic partnership between TUM and KAUST, the King Abdullah University of Science and Technology, in Jeddah, Saudi Arabia. Fostering a structured programme for PhD studies, MAC is participating in TUM's International Graduate School of Science and Engineering (IGSSE). All MAC PhD students thus engaged in IGSSE's research training programme – one of the cornerstones being a 3-month research visit at an international partner institute.

Articles in These Proceedings

The present proceedings volume combines 11 articles that review research work and results from the MAC project teams. The first two articles, by Schillinger et al. and Benk et al. focus on the Finite Cell Method and on Immersed Boundary Methods, respectively, and thus on the question how to efficiently and accurately discretise problems with complicated domain boundaries on structured (adaptive) Cartesian grids, in order to simplify mesh generation and improve computational performance. Cai et al. discuss how micro- and macroscale modelling can be combined for accurate simulation of porous media flow, with CO₂-sequestration as the intended application. Simon and Ulbrich present their work on optimal control problems for this application area.

As an example for the development of novel mathematical algorithms, Böhm and Ulbrich present a Newton-CG method for full-waveform seismic inversion. Roderus et al. demonstrate how advancing both mathematical and computational algorithms can lead to substantial improvement of the performance of established computational science codes on HPC platforms – their focus being on density functional theory as application. Kraja et al. in their article, put the HPC platforms first in the development chain and discuss how to design HPC architectures for

given applications; here, on-board processing for SAR image reconstruction on spacecrafts is considered. As simulation tasks and codes, respectively, become more and more complex, systematic software engineering has become imperative – Li et al. address this question via a requirements engineering approach for a software package in computational seismology.

The following two articles both address interactive simulations: while by Knežević et al. present an interactive computing framework for engineering applications, in particular, Benzina et al. introduce a framework that uses surrogate models based on sparse grids to allow interactive handling of high-dimensional simulation data. Both projects used the FRAVE – a flexible, reconfigurable visualisation environment installed at MAC – for their studies. Tönnis et al. as our last article in these proceedings, focus on the developers and users of such interactive simulation and visualisation environments: they present experiences and findings regarding ergonomic aspects of setting up and working with the FRAVE.

Taken altogether, the articles thus provide an overview of research in MAC from 2008 to 2012 and cover (nearly) the entire simulation pipeline.

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