

Preface

Current high-performance computing (HPC) systems consist of complex configurations with a massive number of components that are very likely heterogeneous and typically have a limited amount of memory per component. These hardware and software configurations can change dynamically owing to fault recovery or power saving procedures. To make efficient use of such systems, complex software components require programming layers structured in deep hierarchies. Additionally, applications increasingly use HPC systems for data analytics and complex workflows. Therefore, the successful development of software for scientific computations requires collaboration between domain scientists on one hand and computer science/HPC experts on the other.

JARA-HPC is the high-performance computing section of JARA, the Jülich Aachen Research Alliance. This alliance represents a cooperative venture between RWTH Aachen University and Forschungszentrum Jülich. This cooperative relationship goes beyond the mere juxtaposition of university and non-university research and teaching and represents a pioneering model in Germany. Scientists from JARA-HPC combine in-depth knowledge of massively parallel computing architectures with expertise in specific research fields. Within JARA-HPC, distinct research teams embodied by simulation laboratories (SimLabs) provide support to communities in diverse computational science disciplines. At the same time, HPC experts in cross-sectional groups provide support to the SimLabs in the form of services needed by a broader spectrum of scientific communities, such as performance optimization for software codes and visualization of simulation data.

Since its establishment, JARA-HPC has proven that close interdisciplinary mixing of domain-specific knowledge and HPC expertise is a concept that is key for success in scientific software. This success has been substantiated by the in-depth collaborations which have reaped synergies from a diverse knowledge base during the development of complex scientific codes. JARA-HPC established the JARA-HPC Symposium (JHPCS) to pass on its collected experience and complement it with the experience developed by other HPC development teams. In the long term, the aim of the JHPCS is to motivate broader discussion on various aspects of HPC application development among experts at an international scale. Participants in the symposium are given the opportunity for a profound exchange with colleagues from different research fields utilizing HPC systems in their scientific work.

This volume contains the papers presented at the First JHPCS held during October 3–4, 2016 in Aachen, Germany. The JHPCS Program Committee received a total of 26 submissions. Each submission was reviewed by at least two Program Committee members as well as additional external reviewers in a single-blind peer review. Owing to the above-average quality of the submissions, the Program Committee decided to accept 21 papers on diverse topics, such as coupling methods and strategies in computational fluid dynamics (CFD), performance portability and applications in HPC,

as well as provenance tracking for large-scale simulations. The symposium program included a keynote talk by Viktor Eijkhout from the Texas Advanced Computing Center (TACC) on “Parallel Programming for the 21st Century.” Furthermore, it featured a half-day workshop that focused on CFD-related aeroacoustic research with a mix of invited talks and paper submissions. Overall, the program reflected the anticipated broad spectrum of topics and brought together several communities active in HPC software development.

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