

Message from the PDSEC-18 Workshop Chairs

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Welcome to the 19th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC-18), held on May 25, 2018 in Vancouver, Canada, in conjunction with the 32nd IEEE International Parallel and Distributed Processing Symposium (IPDPS 2018).

The field of high performance computing has earned prominence through advances in electronic and integrated technologies. The scientific and engineering application domains have a key role in shaping future research and development activities in academia and industry, especially when the solution of large and complex problems must cope with tight timing schedules. Current times are very exciting and the years to come will witness a proliferation in the use of parallel and distributed systems. As in previous years, we saw a continuation in the increase in the use of board-level massively parallel processors for scientific applications, with one half of the papers of the workshop utilizing GP-GPUs, FGPA's and manycore processors for this purpose. In terms of parallel techniques, the workshop hosted papers on Hierarchical Equations of Motion, ordinary differential equations, tensors, and least-squares methods. It also hosted systems papers on task-TAG runtime systems and HPC virtualization. Application areas included geophysics, high precision middleware, and ice sheet modelling.

An emerging application in medical science requiring massive amounts of parallel processing is cardiac electrophysiology. This year we were delighted to have Dr Johannes Langguth, Research Scientist at Simula, Norway, deliver the PDSEC-18 keynote speech *Heterogeneous HPC Computations in Cardiac Electrophysiology*.

We were also honoured to host invited talks from two long-serving PDSEC Program Committee Members: *Space-Time Parallelization is Feasible for Highly Non-linear Simulations* by Prof. Eric Aubanel, University of New Brunswick; and *Robust Scheduling for Scientific Applications in Parallel and Distributed Environments* by Prof. Ioana Banicescu, Mississippi State University.

For this year's workshop we have received many high-

quality submissions from Asia Pacific, Australia, Europe, North America and South America. In a peer-reviewing phase with at least 3 reviews per paper, the submissions were judged by originality, relevance, technical quality, and clarity of presentation. Based on the reviews, we decided to accept 10 high-quality papers for presentation in the technical program of PDSEC-18.

This year we are pleased to announce that the Best Paper Award went to Matthias Noack, Alexander Reinefeld, Tobias Kramer and Thomas Steinke for their paper *DM-HEOM: A Portable and Scalable Solver-Framework for the Hierarchical Equations of Motion*.

The annual PDSEC workshop brings together researchers from computer science, applied mathematics and other application areas of high-performance computing to present, discuss and exchange ideas, results, work in progress and experiences in the area of parallel and distributed computing for problems in science and engineering applications.

The program for this workshop is the result of hard and excellent work of many others. We would like to express our sincere appreciation to all authors for their valuable contributions and to all program committee members and external reviewers for their cooperation and diligent work in completing the workshop program under a very tight schedule. Last but not least, we thank Erik Saule (University of North Carolina) and Jaroslaw Zola (The State University of New York), the IPDPS 2018 Workshops Chair and Vice-Chair, and Kyle Chard (University of Chicago) and Moustafa AbdelBaky (Rutgers University), the IPDPS 2018 Workshops Proceedings Chair and Vice-Chair, for helping and encouraging the inclusion of the PDSEC-18 workshop in IPDPS Workshops 2018.

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PDSEC-18 KEYNOTE SPEECH DETAILS

Heterogeneous GPU-CPU computing for Electro-cardiac Simulations.

Dr Johannes Langguth, Simula, Norway (keynote speech).

Abstract:

Detailed organ-scale simulations of calcium handling and electrical signal transmission in the human heart require stochastic simulation of a large number of ion channels in each cell, which consumes immense processing power for the simulation of a single heartbeat, thereby creating the need for large scale parallel implementations. We present codes for solving such cardiac models on structured and unstructured meshes, and discuss the challenges involved in modernizing these codes to run on heterogeneous supercomputers. We focus on the interaction between OpenMP, MPI, and CUDA in such computations, as well as optimizations to communication and vector processing, and illustrate practical experiences with these applications on different supercomputers.

About the Speaker:

Johannes Langguth is a research scientist at Simula research laboratory, Oslo, Norway. He received his PhD in computer science from the University of Bergen in 2011, followed by a postdoctoral appointment at ENS Lyon, France. His research interests include computer architecture, parallel algorithms, computational social science, and high-performance scientific computing on multi-core CPUs and GPUs.

PDSEC-18 INVITED SPEECH DETAILS (I)

Space-Time Parallelization is Feasible for Highly Nonlinear Simulations, Prof. Eric Aubanel, University of New Brunswick (invited talk).

Abstract:

Realistic simulation of time-dependent processes requires long time evolution using very small time steps in order to resolve phenomena at different time scales. Traditional spatial parallelism offers some performance gain, which however may be insufficient. The parareal algorithm parallelizes partial differential equations by time decomposition, and has been employed for a range of physical problems. It faces particular challenges in the case of highly nonlinear dynamics, where the parareal corrections can cause significant instability. This talk describes strategies that have been used to deal with this instability, including grid coarsening techniques, filtering of grid-dependent features, and multi-stage convergence techniques, in the context of turbulent flow in computational fluid dynamics.

About the Speaker:

Dr. Eric Aubanel is a Professor in the Faculty of Computer Science at The University of New Brunswick, Canada. He received his Bachelors of Science from Trent University and his PhD from Queen's University. Eric's current research includes the development of tools and algorithms to support scientific computing on heterogeneous distributed resources, including manycore accelerators. He is also beginning a study of the cognitive aspects of parallel programming. In 2016 he published a graduate textbook on parallel computing, *Elements of Parallel Computing*, with CRC Press. He is a member the IBM CASA (Centre for Advanced Studies - Atlantic), where he has participated in projects on performance optimization of managed runtimes.

PDSEC-18 INVITED SPEECH DETAILS (II)

Robust Scheduling for Scientific Applications in Parallel and Distributed Environments, Prof. Ioana Banicescu, Mississippi State University (invited talk).

Abstract:

Computational problems in science and engineering are continuously increasing in size and complexity, and their solutions can often be made tractable only by using parallel and distributed computing environments with state-of-the-art techniques and tools. Such computational environments are prone to irregular behavior due to unpredictable variations in problem, algorithm and system characteristics. In situations where application execution times are stochastic in nature and the availability of resources is uncertain, a robustness study of resource allocations and application scheduling is required to guarantee a desired level of performance. This talk will reveal highlights of the past and ongoing work on such a robustness study, including models, heuristics, and a framework for robust allocations and scheduling of scientific applications in heterogeneous environments. Moreover, robustness prediction and evaluation will be described for scheduling arbitrarily divisible workloads for computational intensive and communication intensive scientific applications, thus underscoring the power of analytical prediction of the robustness of resource allocations and application scheduling in various computational environments. The significance of the robustness study using stochastic models in providing a cost-effective and low overhead analysis of robust allocation and scheduling will also be discussed.

About the Speaker:

Ioana Banicescu is a professor in the Department of Computer Science and Engineering at Mississippi State University (MSU). Between 2010 and 2017, she was also a Director of the Center for Cloud and Autonomic Computing at MSU, and a Co-Director of the National Science Foundation Center for Cloud and Autonomic Computing. She received the Diploma in Engineering (Electronics and Telecommunications) from Polytechnic University - Bucharest, and the MS and the PhD degrees in Computer Science from New York University - Polytechnic Institute. Professor Banicescu's research focus is on performance optimization for problems in computational science, autonomic computing and graph analytics. Her research interests include parallel algorithms, scientific computing,

scheduling, and performance modeling, analysis and prediction. Professor Banicescu is the recipient of a number of awards for research and scholarship from the National Science Foundation. She serves on numerous scientific panels for advanced research grants in the US and Europe, on journal editorial boards, and on the steering and program committees of a number of international conferences, symposia and workshops. She served on the Executive Board and Advisory Board of the IEEE Technical Committee on Parallel Processing (TCPP).