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Guido Juckeland · Sunita Chandrasekaran (Eds.)

Tools and Techniques for High Performance Computing

Selected Workshops, HUST, SE-HER and WIHPC
Held in Conjunction with SC 2019
Denver, CO, USA, November 17–18, 2019
Revised Selected Papers

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Preface

The current proceedings combine 12 papers from three workshops co-located with the International Conference for High Performance Computing, Networking, Storage and Analysis (SC 2019). The workshops are HPC User Support Tools (HUST), Software Engineering for HPC-Enabled Research (SE-HER), and the Workshop on Interactive High Performance Computing (WIHPC). A description of each of the workshop is as follows:

The HUST workshop, held by Chris Bording (IBM Research, Hartree Centre), Elsa Gonsiorowski (Lawrence Livermore National Laboratory), and Karen Tomko (Ohio Supercomputing Center), has been the ideal forum for new and innovative tools such as XALT, SPACK, and Easybuild which have been widely announced to the broader HPC community. This has created communities and special interest groups surrounding these tools, many of which now hold their own BoFs, workshops, and tutorials at SC, ISC, and other HPC conferences. HUST will continue to provide a necessary forum for system administrators, user support team members, tool developers, policy makers, and end users. The workshop provided a forum to discuss support issues and we will provide a publication venue for current support developments. Best practices, user support tools, and any ideas to streamline user support at supercomputing centers are in the scope. HUST submitted four papers in total. For further details, please refer to the workshop website: https://hust-workshop.github.io/.

Developers who build research software for HPC or High Performance Data Analysis/Analytics (HPDA) face software engineering (SE) challenges at scales not often addressed by traditional SE approaches. For example, HPC and HPDA software developers must solve reliability, availability, and maintainability problems at extreme scales, consider reproducibility, understand domain specific constraints, deal with uncertainties inherent in scientific exploration, and efficiently use compute resources. SE researchers have developed tools and practices to support development tasks, including: requirements, design, validation and verification, testing, continuous integration, and maintenance. Because of the scale of HPC and HPDA, there is a need to adapt these SE tools/methods that are standard elsewhere. SE-HER 2019, held by Jeffrey C. Carver (University of Alabama), Anshu Dubey (Argonne National Laboratory), Neil Chue Hong (Software Sustainability Institute and Edinburgh Parallel Computing Center), and Daniel S. Katz (University of Illinois at Urbana-Champaign), brought together members of the SE and HPC/HPDA communities to present findings relative to these problems and to generate an agenda to advance software engineering tools and practices for HPC/HPDA software. For further details, please refer to the workshop website: http://SE4Science.org/workshops/seher19/.

Interactive exploration and analysis of large data sets, intelligent simulation ("cog-sim") workflows that combine interactive analysis and AI techniques with modeling and simulation, interactive preparation and debugging of large-scale scientific simulations, in-situ visualization, and application steering are all compelling

scenarios for exploratory science, design optimizations, and signal processing. However, a range of technical, organizational, and sociological challenges must be overcome to make these interactive workflows mainstream in HPC centers: What simulation scenarios or problem domains can benefit most from interactivity? How can we simplify the toolchain? What center policies are needed to support highly interactive workflows? WIHPC 2019, held by Michael Ringenburg (Cray Inc.), John Stone (University of Illinois at Urbana-Champaign), and Albert Reuther (MIT-Massachusetts Institute of Technology) on interactive high performance computing brought together domain scientists, tool developers, and HPC center administrators to identify the scientific impact and technical challenges of highly interactive access to HPC resources. For further details, please refer to the workshop website: https://sites.google.com/view/interactive-hpc/home.

Review Process

Papers from each workshop were peer reviewed with an average of three reviews per paper.

These proceedings include 12 papers in total, 4 from each of the 3 workshops. Each workshop put together a Steering and Program Committee of researchers and scientists spanning academia, national labs, and industries to drive the workshop and help with selecting high-quality papers.

February 2020

Guido Juckeland
Sunita Chandrasekaran

Organization

Annual Workshop on HPC User Support Tools (HUST)

Organizers

Chris Bording	IBM Research, Hartree Centre, UK
Elsa Gonsiorowski	Lawrence Livermore National Laboratory, USA
Karen Tomko	Ohio Supercomputing Center, USA

General Chair

Chris Bording	IBM Research, Hartree Centre, UK

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Elsa Gonsiorowski	Lawrence Livermore National Laboratory, USA
Karen Tomko	Ohio Supercomputing Center, USA

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Paul Kolano	NASA, USA
Kevin Manalo	PACE, Georgia Institute of Technology, USA
Robert McLay	TACC, USA
Abhinav Thota	Indiana University, USA

International Workshop on Software Engineering for HPC-Enabled Research (SE-HER)

Organizers

Jeffrey C. Carver	University of Alabama, USA
Anshu Dubey	Argonne National Laboratory, USA
Neil Chue Hong	Software Sustainability Institute and Edinburgh Parallel Computing Center, UK
Daniel S. Katz	University of Illinois at Urbana-Champaign, USA

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Damian Rouson	Sourcery Institute, USA
Manodeep Sinha	Swinburne University, Australia
Sophie Voisin	Oak Ridge National Laboratory, USA
Alexander Wagner	University of Tsukaba, Finland

Workshop on Interactive High-Performance Computing (WIHPC)

Organizers and Program Committee

Sadaf Alam	CSCS, Switzerland
Nicola Ferrier	Argonne National Laboratory, USA
Peter Messmer	NVIDIA, USA
Albert Reuther	MIT Lincoln Laboratory, USA
Michael Ringenburg	Cray Inc., USA
John Stone	University of Illinois at Urbana-Champaign, USA

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Contents

WIHPC – Workshop on Interactive High-Performance Computing