

## Founding Editors

Gerhard Goos

*Karlsruhe Institute of Technology, Karlsruhe, Germany*

Juris Hartmanis

*Cornell University, Ithaca, NY, USA*

## Editorial Board Members

Elisa Bertino

*Purdue University, West Lafayette, IN, USA*

Wen Gao

*Peking University, Beijing, China*

Bernhard Steffen 

*TU Dortmund University, Dortmund, Germany*

Gerhard Woeginger 

*RWTH Aachen, Aachen, Germany*

Moti Yung

*Columbia University, New York, NY, USA*

More information about this series at <http://www.springer.com/series/7407>


Heike Jagode · Hartwig Anzt ·  
Guido Juckeland · Hatem Ltaief (Eds.)


# High Performance Computing

ISC High Performance 2020 International Workshops  
Frankfurt, Germany, June 21–25, 2020  
Revised Selected Papers

### Editors

Heike Jagode   
University of Tennessee at Knoxville  
Knoxville, TN, USA

Guido Juckeland   
Computational Science  
Helmholtz-Zentrum Dresden Rossendorf  
Dresden, Sachsen, Germany

Hartwig Anzt   
Department of Mathematics  
KIT für Technologie Karlsruhe  
Karlsruhe, Baden-Württemberg, Germany

Hatem Ltaief  
Extreme Computing Research Center  
King Abdullah University of Science  
and Technology  
Thuwal, Saudi Arabia

ISSN 0302-9743 ISSN 1611-3349 (electronic)  
Lecture Notes in Computer Science  
ISBN 978-3-030-59850-1 ISBN 978-3-030-59851-8 (eBook)  
<https://doi.org/10.1007/978-3-030-59851-8>

LNCS Sublibrary: SL1 – Theoretical Computer Science and General Issues

© Springer Nature Switzerland AG 2020

Chapters 6, 19 and 24 are licensed under the terms of the Creative Commons Attribution 4.0 International License (<http://creativecommons.org/licenses/by/4.0/>). For further details see license information in the chapters.

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG  
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

# Preface

Without a doubt, 2020 has been a different kind of year for all of us, and so it was for the 35th ISC High Performance conference, which became known as ISC 2020 Digital. As the name suggests, the organizing team around David Keyes (KAUST, Saudi Arabia) successfully adapted the conference to an all-digital format by providing a significant portion of the program via web conferencing. While we should not forget the importance of in-person interaction and socializing, the video streaming of the accepted papers, focus sessions, and invited talks enabled unprecedented access and dissemination of new research findings for the high-performance computing community.

The ISC High Performance workshop series has been a complementary component of the main conference since 2015, and – sustained by its continued success – a renewed workshop program was presented at the ISC 2020 Digital event under the leadership of workshops chair Heike Jagode (The University of Tennessee at Knoxville, USA) and deputy chair Hartwig Anzt (Karlsruhe Institute of Technology, Germany). Guido Juckeland (Helmholtz-Zentrum Dresden-Rossendorf, Germany) and Hatem Ltaief (KAUST, Saudi Arabia) joined the team as proceedings chair and deputy chair, respectively, and managed the organization of the workshops' proceedings.

All workshops were selected with a peer-review process by an international committee of 21 experts in the field from all over Europe, the USA, and Asia. For the digital version of the conference, we offered all of the accepted workshops the flexibility to postpone their workshop to ISC 2021 and run a virtual workshop in the ISC 2020 edition. In the end, 10 of the 23 accepted workshops decided to organize a virtual version of their event, which we greatly appreciate given the extra effort put forth by everyone involved.

Like in the 2019 edition, the ISC workshops were composed of two types of workshops: workshops with proceedings (early deadline) and workshops without proceedings (later deadline). While we had 16 workshops with proceedings accepted, only 7 out of those decided to offer a digital version this year. Given all of these challenges, the quality of this year's ISC workshops proceedings is impressive. In total, we have 25 high-quality papers that all underwent thorough reviews. Each chapter of the book contains the accepted and revised papers for one of the workshops. For some workshops, an additional preface describes the review process and provides a summary of the outcome.

With the hope that, perhaps next year, we will be able to once again host ISC High Performance in person, we want to thank our Workshops Committee members, organizers of workshops, and all contributors. We are proud to present the latest findings on

topics related to research, development, and the application of large-scale, high-performance systems.

August 2020

Heike Jagode  
Hartwig Anzt  
Guido Juckeland  
Hatem Ltaief

# Organization

## Workshops Committee

Emmanuel Agullo	Inria, France
Hartwig Anzt	Karlsruhe Institute of Technology, Germany, and The University of Tennessee, Knoxville, USA
Richard Barrett	Sandia National Laboratories, USA
Roy Campbell	Department of Defense, USA
Florina Ciorba	University of Basel, Switzerland
Anthony Danalis	The University of Tennessee, Knoxville, USA
Manuel F. Dolz	Universitat Jaume I, Spain
Nick Forrington	Arm, USA
Karl Fuerlinger	Ludwig Maximilian University of Munich (LMU), Germany
Judit Gimenez Lucas	Barcelona Supercomputing Center, Spain
Thomas Gruber	University of Erlangen-Nuremberg, Erlangen Regional Computing Center, Germany
Joachim Hein	Lund University, Sweden
David Henty	The University of Edinburgh, UK
Marc-Andre Hermanns	RWTH Aachen University, Germany
Kevin Huck	University of Oregon, USA
Sascha Hunold	TU Wien, Austria
Heike Jagode	The University of Tennessee, Knoxville, USA
Eileen Kühn	Karlsruhe Institute of Technology, Germany
Diana Moise	Cray, HPE, Switzerland
Tapasya Patki	Lawrence Livermore National Laboratory, USA
Jelena Pjesivac-Grbovic	Verily Life Sciences LLC, Google LLC, USA
Philip Roth	Oak Ridge National Laboratory, USA
Ana Lucia Varbanescu	University of Amsterdam, The Netherlands

## Proceedings Chairs

Guido Juckeland	Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany
Hatem Ltaief	KAUST, Saudi Arabia

# Contents

## First Workshop on Compiler-Assisted Correctness Checking and Performance Optimization for HPC (C3PO'20)

Compiler-Assisted Type-Safe Checkpointing. . . . .	5
<i>Jan-Patrick Lehr, Alexander Hück, Moritz Fischer, and Christian Bischof</i>	
Static Analysis to Enhance Programmability and Performance in OmpSs-2. . .	19
<i>Adrian Munera, Sara Royuela, Roger Ferrer, Raul Peñacoba, and Eduardo Quiñones</i>	
Automatic Detection of MPI Assertions . . . . .	34
<i>Tim Jammer, Christian Iwainsky, and Christian Bischof</i>	
Automatic Code Motion to Extend MPI Nonblocking Overlap Window. . . .	43
<i>Van Man Nguyen, Emmanuelle Saillard, Julien Jaeger, Denis Barthou, and Patrick Carribault</i>	

## First International Workshop on the Application of Machine Learning Techniques to Computational Fluid Dynamics Simulations and Analysis (CFDML)

Complete Deep Computer-Vision Methodology for Investigating Hydrodynamic Instabilities . . . . .	61
<i>Re'em Harel, Matan Rusanovsky, Yehonatan Fridman, Assaf Shimony, and Gal Oren</i>	
Prediction of Acoustic Fields Using a Lattice-Boltzmann Method and Deep Learning . . . . .	81
<i>Mario Rüttgers, Seong-Ryong Koh, Jenia Jitsev, Wolfgang Schröder, and Andreas Lintermann</i>	
Unsupervised Learning of Particle Image Velocimetry . . . . .	102
<i>Mingrui Zhang and Matthew D. Piggott</i>	
Reduced Order Modeling of Dynamical Systems Using Artificial Neural Networks Applied to Water Circulation . . . . .	116
<i>Alberto Costa Nogueira Jr., João Lucas de Sousa Almeida, Guillaume Auger, and Campbell D. Watson</i>	

Parameter Identification of RANS Turbulence Model Using  
Physics-Embedded Neural Network. . . . . 137  
*Shirui Luo, Madhu Vellakal, Seid Koric, Volodymyr Kindratenko,  
and Jiahuan Cui*

**HPC I/O in the Data Center Workshop (HPC-IODC)**

Investigating the Overhead of the REST Protocol When Using Cloud  
Services for HPC Storage. . . . . 161  
*Frank Gadban, Julian Kunkel, and Thomas Ludwig*

Characterizing I/O Optimization Effect Through Holistic Log Data Analysis  
of Parallel File Systems and Interconnects . . . . . 177  
*Yuichi Tsujita, Yoshitaka Furutani, Hajime Hida, Keiji Yamamoto,  
and Atsuya Uno*

The Importance of Temporal Behavior When Classifying Job IO Patterns  
Using Machine Learning Techniques. . . . . 191  
*Eugen Betke and Julian Kunkel*

**1st Workshop “Machine Learning on HPC Systems” (MLHPCS)**

GOPHER, an HPC Framework for Large Scale Graph Exploration  
and Inference . . . . . 211  
*Marc Josep-Fabregó, Xavier Teruel, Victor Gimenez-Abalos,  
Davide Cirillo, Dario Garcia-Gasulla, Sergio Alvarez-Napagao,  
Marta García-Gasulla, Eduard Ayguadé, and Alfonso Valencia*

Ensembles of Networks Produced from Neural Architecture Search. . . . . 223  
*Emily J. Herron, Steven R. Young, and Thomas E. Potok*

SmartPred: Unsupervised Hard Disk Failure Detection. . . . . 235  
*Philipp Rombach and Janis Keuper*

**1st International Workshop on Monitoring and Data Analytics  
(MODA20)**

Application IO Analysis with Lustre Monitoring Using LASSi  
for ARCHER . . . . . 255  
*Karthee Sivalingam and Harvey Richardson*

AI-Driven Holistic Approach to Energy Efficient HPC . . . . . 267  
*Robert Tracey, Lan Hoang, Felix Subelet, and Vadim Elisseev*

Characterizing HPC Performance Variation with Monitoring  
and Unsupervised Learning . . . . . 280  
*Gence Ozer, Alessio Netti, Daniele Tafani, and Martin Schulz*

## 15th Workshop on Virtualization in High-Performance Cloud Computing (VHPC'20)

Service Function Chaining Based on Segment Routing Using P4 and SR-IOV (P4-SFC) . . . . .	297
<i>Andreas Stockmayer, Stephan Hinselmann, Marco Häberle, and Michael Menth</i>	
Seamlessly Managing HPC Workloads Through Kubernetes . . . . .	310
<i>Sergio López-Huguet, J. Damià Segrelles, Marek Kasztelnik, Marian Bubak, and Ignacio Blanquer</i>	
Interference-Aware Orchestration in Kubernetes . . . . .	321
<i>Achilleas Tzenetopoulos, Dimosthenis Masouros, Sotirios Xydis, and Dimitrios Soudris</i>	
RustyHermit: A Scalable, Rust-Based Virtual Execution Environment . . . . .	331
<i>Stefan Lankes, Jonathan Klimt, Jens Breitbart, and Simon Pickartz</i>	
Rootless Containers with Podman for HPC . . . . .	343
<i>Holger Gantikow, Steffen Walter, and Christoph Reich</i>	
Bioinformatics Application with Kubeflow for Batch Processing in Clouds . . . . .	355
<i>David Yu Yuan and Tony Wildish</i>	
Converging HPC, Big Data and Cloud Technologies for Precision Agriculture Data Analytics on Supercomputers . . . . .	368
<i>Yiannis Georgiou, Naweiluo Zhou, Li Zhong, Dennis Hoppe, Marcin Pospieszny, Nikela Papadopoulou, Kostis Nikas, Orestis Lagkas Nikolos, Pavlos Kranas, Sophia Karagiorgou, Eric Pascolo, Michael Mercier, and Pedro Velho</i>	
Author Index . . . . .	381