

Commenced Publication in 2007

Founding and Former Series Editors:

Alfredo Cuzzocrea, Xiaoyong Du, Orhun Kara, Ting Liu, Dominik Ślęzak,
and Xiaokang Yang

Editorial Board

Simone Diniz Junqueira Barbosa

*Pontifical Catholic University of Rio de Janeiro (PUC-Rio),
Rio de Janeiro, Brazil*

Phoebe Chen

La Trobe University, Melbourne, Australia

Joaquim Filipe

Polytechnic Institute of Setúbal, Setúbal, Portugal

Igor Kotenko

*St. Petersburg Institute for Informatics and Automation of the Russian
Academy of Sciences, St. Petersburg, Russia*

Krishna M. Sivalingam

Indian Institute of Technology Madras, Chennai, India

Takashi Washio

Osaka University, Osaka, Japan

Junsong Yuan

Nanyang Technological University, Singapore, Singapore

Lizhu Zhou

Tsinghua University, Beijing, China

More information about this series at <http://www.springer.com/series/7899>

Vladimir Voevodin · Sergey Sobolev (Eds.)

Supercomputing

Third Russian Supercomputing Days, RuSCDays 2017
Moscow, Russia, September 25–26, 2017
Revised Selected Papers



Springer

Editors

Vladimir Voevodin 
Research Computing Center (RCC)
Moscow State University
Moscow
Russia

Sergey Sobolev 
Moscow State University
Moscow
Russia

ISSN 1865-0929

ISSN 1865-0937 (electronic)

Communications in Computer and Information Science

ISBN 978-3-319-71254-3

ISBN 978-3-319-71255-0 (eBook)

<https://doi.org/10.1007/978-3-319-71255-0>

Library of Congress Control Number: 2017959610

© Springer International Publishing AG 2017

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, express 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.

Printed on acid-free paper

This Springer imprint is published by Springer Nature

The registered company is Springer International Publishing AG

The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Preface

The Third Russian Supercomputing Days Conference (RuSCDays 2017) was held September 25–26, 2017, in Moscow, Russia. It was organized by the Supercomputing Consortium of Russian Universities and the Federal Agency for Scientific Organizations. The conference was supported by the Russian Foundation for Basic Research and our respected platinum educational partner (Intel), platinum sponsors (T-Platforms, NVIDIA, RSC), gold sponsor (Mellanox), and silver sponsors (Almaz-SP, Atos, Dell EMC, IBM, Xilinx). The conference was organized in a partnership with the ISC High-Performance conference series and the NESUS project.

The conference was born in 2015 as a union of several supercomputing events in Russia and quickly became one of the most notable Russian supercomputing meetings. The conference caters to the interests of a wide range of representatives from science, industry, business, education, government, and students – anyone connected to the development or the use of supercomputing technologies. The conference topics cover all aspects of supercomputing technologies: software and hardware design, solving large tasks, application of supercomputing technologies in industry, exaflops computing issues, supercomputing co-design technologies, supercomputing education, and others.

All papers submitted to the conference were reviewed by three referees in the first review round. The papers were evaluated according to the quality of relevance to the conference topics, scientific contribution, presentation, approbation, and related works description. After notification of the conditional acceptance of a paper, the second review round was arranged. It was aimed at the final polishing of papers and also at evaluating the authors work after the referees' comments. After the conference, the final selection was made, and the 42 best works were carefully selected to be included in this volume.

The proceedings editors would like to thank all conference committee members, especially the Organizing and Program Committee members as well as other referees and reviewers for their contributions. We also thank Springer for producing these high-quality proceedings of RuSCDays 2017.

October 2017

Vladimir Voevodin
Sergey Sobolev

Organization

The Third Russian Supercomputing Days Conference (RuSCDays 2017) was organized by the Supercomputing Consortium of Russian Universities and the Federal Agency for Scientific Organizations, Russia. The conference organization coordinator was Moscow State University Research Computing Center.

Steering Committee

V.A. Sadovnichiy (Chair)	Moscow State University, Russia
V.B. Betelin (Co-chair)	Russian Academy of Sciences, Moscow, Russia
A.V. Tikhonravov (Co-chair)	Moscow State University, Russia
J. Dongarra (Co-chair)	University of Tennessee, Knoxville, USA
A.I. Borovkov	Peter the Great Saint-Petersburg Polytechnic University, Russia
VI.V. Voevodin	Moscow State University, Russia
V.P. Gergel	Lobachevsky State University of Nizhni Novgorod, Russia
G.S. Elizarov	NII Kvant, Moscow, Russia
V.V. Elagin	Hewlett Packard Enterprise, Moscow, Russia
A.K. Kim	MCST, Moscow, Russia
E.V. Kudryashova	Northern (Arctic) Federal University, Arkhangelsk, Russia
N.S. Mester	Intel, Moscow, Russia
E.I. Moiseev	Moscow State University, Russia
A.A. Moskovskiy	RSC Group, Moscow, Russia
V.Yu. Opanasenko	T-Platforms, Moscow, Russia
G.I. Savin	Joint Supercomputer Center, Russia
V.A. Soyfer	Russian Academy of Sciences, Moscow, Russia
L.B. Sokolinskiy	Samara University, Russia
I.A. Sokolov	South Ural State University, Chelyabinsk, Russia
R.G. Strongin	Russian Academy of Sciences, Moscow, Russia
A.N. Tomilin	Lobachevsky State University of Nizhni Novgorod, Russia
A.R. Khokhlov	Institute for System Programming of the Russian Academy of Sciences, Moscow, Russia
B.N. Chetverushkin	Moscow State University, Russia
E.V. Chuprunov	Keldysh Institutes of Applied Mathematics, Russia
A.L. Shestakov	Russian Academy of Sciences, Moscow, Russia
	Lobachevsky State University of Nizhni Novgorod, Russia
	South Ural State University, Chelyabinsk, Russia

Program Committee

VI.V. Voevodin (Chair)	Moscow State University, Russia
R.M. Shagaliev (Co-chair)	Russian Federal Nuclear Center, Sarov, Russia
M.V. Yakobovskiy (Co-chair)	Keldysh Institutes of Applied Mathematics, Russian Academy of Sciences, Moscow, Russia
T. Sterling (Co-chair)	Indiana University, Bloomington, USA
A.I. Avetisyan	Institute for System Programming of the Russian Academy of Sciences, Moscow, Russia
D. Bader	Georgia Institute of Technology, Atlanta, USA
P. Balaji	Argonne National Laboratory, USA
M.R. Biktimirov	Russian Academy of Sciences, Moscow, Russia
A.V. Bukhanovskiy	ITMO University, Saint Petersburg, Russia
J. Carretero	University Carlos III of Madrid, Spain
V.E. Velikhov	National Research Center Kurchatov Institute, Moscow, Russia
V.Yu. Volkonskiy	MCST, Moscow, Russia
V.M. Volokhov	Institute of Problems of Chemical Physics of Russian Academy of Sciences, Chernogolovka, Russia
R.K. Gazizov	Ufa State Aviation Technical University, Russia
B.M. Glinsky	Institute of Computational Mathematics and Mathematical Geophysics, Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia
V.M. Goloviznin	Moscow State University, Russia
V.A. Ilyin	National Research Center Kurchatov Institute, Moscow, Russia
I.A. Kalyaev	NII MVS, South Federal University, Taganrog, Russia
H. Kobayashi	Tohoku University, Japan
V.V. Korenkov	Joint Institute for Nuclear Research, Dubna, Russia
V.A. Kryukov	Keldysh Institutes of Applied Mathematics, Russian Academy of Sciences, Moscow, Russia
J. Kunkel	University of Hamburg, Germany
J. Labarta	Barcelona Supercomputing Center, Spain
A. Lastovetsky	University College Dublin, Ireland
M.P. Lobachev	Krylov State Research Centre, Saint Petersburg, Russia
Y. Lu	National University of Defense Technology, Changsha, Hunan, China
T. Ludwig	German Climate Computing Center, Hamburg, Germany
V.N. Lykosov	Institute of Numerical Mathematics, Russian Academy of Sciences, Moscow, Russia
M. Michalewicz	University of Warsaw, Poland
L. Mirtaheri	Kharazmi University, Tehran, Iran

A.V. Nemukhin	Moscow State University, Russia
G.V. Osipov	Lobachevsky State University of Nizhni Novgorod, Russia
A.V. Semyanov	Lobachevsky State University of Nizhni Novgorod, Russia
Ya.D. Sergeev	Lobachevsky State University of Nizhni Novgorod, Russia
H. Sithole	Centre for High Performance Computing, Cape Town, South Africa
A.V. Smirnov	Moscow State University, Russia
R.G. Strongin	Lobachevsky State University of Nizhni Novgorod, Russia
H. Takizawa	Tohoku University, Japan
M. Tauer	University of Delaware, Newark, USA
H. Torsten	ETH Zurich, Switzerland
V.E. Turlapov	Lobachevsky State University of Nizhni Novgorod, Russia
E.E. Tyryshnikov	Institute of Numerical Mathematics, Russian Academy of Sciences, Moscow, Russia
V.A. Fursov	Samara University, Russia
L.E. Khaymina	Northern (Arctic) Federal University, Arkhangelsk, Russia
B.M. Shabanov	Joint Supercomputer Center, Russian Academy of Sciences, Moscow, Russia
N.N. Shabrov	Peter the Great Saint-Petersburg Polytechnic University, Russia
L.N. Shchur	Higher School of Economics, Moscow, Russia
R. Wyrzykowski	Czestochowa University of Technology, Poland
M. Yokokawa	Kobe University, Japan

Industrial Committee

A.A. Aksenov (Co-chair)	Tesis, Moscow, Russia
V.E. Velikhov (Co-chair)	National Research Center Kurchatov Institute, Moscow, Russia
V.Yu. Opanasenko (Co-chair)	T-Platforms, Moscow, Russia
Yu.Ya. Boldyrev	Peter the Great Saint-Petersburg Polytechnic University, Russia
M.A. Bolshukhin	Afrikantov Experimental Design Bureau for Mechanical Engineering, Nizhny Novgorod, Russia
R.K. Gazizov	Ufa State Aviation Technical University, Russia
M.P. Lobachev	Krylov State Research Centre, Saint Petersburg, Russia
V.Ya. Modorskiy	Perm National Research Polytechnic University, Russia

A.P. Skibin	Gidropress, Podolsk, Russia
S. Stoyanov	T-Services, Moscow, Russia
N.N. Shabrov	Peter the Great Saint-Petersburg Polytechnic University, Russia
A.B. Shmelev	RSC Group, Moscow, Russia
S.V. Strizhak	Hewlett-Packard, Moscow, Russia

Educational Committee

V.P. Gergel (Co-chair)	Lobachevsky State University of Nizhni Novgorod, Russia
VI.V. Voevodin (Co-chair)	Moscow State University, Russia
L.B. Sokolinskiy (Co-chair)	South Ural State University, Chelyabinsk, Russia
Yu.Ya. Boldyrev	Peter the Great Saint-Petersburg Polytechnic University, Russia
A.V. Bukhanovskiy	ITMO University, Saint Petersburg, Russia
R.K. Gazizov	Ufa State Aviation Technical University, Russia
S.A. Ivanov	Hewlett-Packard, Moscow, Russia
I.B. Meerov	Lobachevsky State University of Nizhni Novgorod, Russia
V.Ya. Modorskiy	Perm National Research Polytechnic University, Russia
I.O. Odintsov	RSC Group, Saint Petersburg, Russia
N.N. Popova	Moscow State University, Russia
O.A. Yufryakova	Northern (Arctic) Federal University, Arkhangelsk, Russia

Organizing Committee

VI.V. Voevodin (Chair)	Moscow State University, Russia
V.P. Gergel (Co-chair)	Lobachevsky State University of Nizhni Novgorod, Russia
V.Yu. Opanasenko (Co-chair)	T-Platforms, Moscow, Russia
B.M. Shabanov (Co-chair)	Joint Supercomputer Center, Russian Academy of Sciences, Moscow, Russia
S.I. Sobolev (Scientific Secretary)	Moscow State University, Russia
A.A. Aksenov	Tesis, Moscow, Russia
A.P. Antonova	Moscow State University, Russia
K.A. Barkalov	Lobachevsky State University of Nizhni Novgorod, Russia
M.R. Biktimirov	Russian Academy of Sciences, Moscow, Russia
O.A. Gorbachev	RSC Group, Moscow, Russia
V.A. Grishagin	Lobachevsky State University of Nizhni Novgorod, Russia
V.V. Korenkov	Joint Institute for Nuclear Research, Dubna, Russia

I.B. Meerov

Lobachevsky State University of Nizhni Novgorod,
Russia

I.M. Nikolskiy

Moscow State University, Russia

N.N. Popova

Moscow State University, Russia

N.M. Rudenko

Moscow State University, Russia

L.B. Sokolinskiy

South Ural State University, Chelyabinsk, Russia

V.M. Stepanenko

Moscow State University, Russia

A.V. Tikhonravov

Moscow State University, Russia

A.Yu. Chernyavskiy

Moscow State University, Russia

M.V. Yakobovskiy

Keldysh Institutes of Applied Mathematics, Russian
Academy of Sciences, Moscow, Russia



Contents

Parallel Algorithms

Parallel Numerical Methods Course for Future Scientists and Engineers	3
<i>Iosif Meyerov, Sergey Bastrakov, Konstantin Barkalov, Alexander Sysoyev, and Victor Gergel</i>	
GPU Acceleration of Dense Matrix and Block Operations for Lanczos Method for Systems over Large Prime Finite Field	14
<i>Nikolai Zamarashkin and Dmitry Zheltkov</i>	
Means for Fast Performance of the Distributed Associative Operations in Supercomputers	27
<i>Gennady Stetsyura</i>	
Scalability Evaluation of NSLP Algorithm for Solving Non-Stationary Linear Programming Problems on Cluster Computing Systems	40
<i>Irina Sokolinskaya and Leonid B. Sokolinsky</i>	
Dynamic Optimization of Linear Solver Parameters in Mathematical Modelling of Unsteady Processes	54
<i>Dmitry Bagaev, Igor Konshin, and Kirill Nikitin</i>	
Optimization of Numerical Algorithms for Solving Inverse Problems of Ultrasonic Tomography on a Supercomputer	67
<i>Sergey Romanov</i>	
The Comparison of Large-Scale Graph Processing Algorithms Implementation Methods for Intel KNL and NVIDIA GPU	80
<i>Ilya Afanasyev and Vladimir Voevodin</i>	
Two Approaches to Speeding Up Dynamics Simulation for a Low Dimension Mechanical System	95
<i>Stepan Orlov, Alexey Kuzin, and Nikolay Shabrov</i>	
Solving Time-Consuming Global Optimization Problems with Globalizer Software System	108
<i>Alexander Sysoyev, Konstantin Barkalov, Vladislav Sovrasov, Ilya Lebedev, and Victor Gergel</i>	
An Approach for Parallel Solving the Multicriterial Optimization Problems with Non-convex Constraints	121
<i>Victor Gergel and Evgeny Kozinov</i>	

Increasing Performance of the Quantum Trajectory Method by Grouping Trajectories	136
<i>Alexey Liniov, Valentin Volokitin, Iosif Meyerov, Mikhail Ivanchenko, and Sergey Denisov</i>	
Tensor Train Global Optimization: Application to Docking in the Configuration Space with a Large Number of Dimensions	151
<i>A.V. Sulimov, D.A. Zheltkov, I.V. Oferkin, D.C. Kutow, E.V. Katkova, E.E. Tyryshnikov, and V.B. Sulimov</i>	
On the Parallel Least Square Approaches in the Krylov Subspaces	168
<i>V.P. Il'in</i>	
Supercomputer Simulation	
Simulation of Seismic Waves Propagation in Multiscale Media: Impact of Cavernous/Fractured Reservoirs	183
<i>Vladimir Tcheverda, Victor Kostin, Galina Reshetova, and Vadim Lisitsa</i>	
Computational Modeling of Turbulent Structuring of Molecular Clouds Based on High Resolution Calculating Schemes	194
<i>Boris Rybakin, Valery Goryachev, and Stepan Ageev</i>	
The Combinatorial Modelling Approach to Study Sustainable Energy Development of Vietnam	207
<i>Aleksey Edelev, Valeriy Zorkaltsev, Sergey Gorsky, Doan Van Binh, and Nguyen Hoai Nam</i>	
Ani3D-Extension of Parallel Platform INMOST and Hydrodynamic Applications	219
<i>Vasily Kramarenko, Igor Konshin, and Yuri Vassilevski</i>	
Numerical Simulation of Light Propagation Through Composite and Anisotropic Media Using Supercomputers	229
<i>Roman Galev, Alexey Kudryavtsev, and Sergey Trashkeev</i>	
The Technology of Nesting a Regional Ocean Model into a Global One Using a Computational Platform for Massively Parallel Computers CMF	241
<i>Alexandr Koromyslov, Rashit Ibrayev, and Maxim Kaurkin</i>	
Parallel Heterogeneous Multi-classifier System for Decision Making in Algorithmic Trading	251
<i>Yuri Zelenkov</i>	
Smoothed-Particle Hydrodynamics Models: Implementation Features on GPUs	266
<i>Sergey Khrapov and Alexander Khoperskov</i>	

The Integrated Approach to Solving Large-Size Physical Problems on Supercomputers	278
<i>Boris Glinsky, Igor Kulikov, Igor Chernykh, Alexey Snytnikov, Anna Sapetina, and Dmitry Weins</i>	
Further Development of the Parallel Program Complex of SL-AV Atmosphere Model	290
<i>Mikhail Tolstykh, Rostislav Fadeev, Gordey Goyman, and Vladimir Shashkin</i>	
The Supercomputer Simulation of Nanocomposite Components and Transport Processes in the Li-ion Power Sources of New Types	299
<i>V.M. Volokhov, D.A. Varlamov, T.S. Zyubina, A.S. Zyubin, A.V. Volokhov, and E.S. Amosova</i>	
Possibility of Physical Detonation in the Flow of vibrationally Preexcited Hydrogen in a Shock Tube	313
<i>Sergey V. Kulikov, Nadezda A. Chervonnaya, and Olga N. Ternovaya</i>	
Supercomputer Modelling of Electromagnetic Wave Scattering with Boundary Integral Equation Method	325
<i>Andrey Aparinov, Alexey Setukha, and Stanislav Stavtsev</i>	
Parallel FDTD Solver with Optimal Topology and Dynamic Balancing	337
<i>Gleb Balykov</i>	
High Performance Architectures, Tools and Technologies	
Retrospective Satellite Data in the Cloud: An Array DBMS Approach	351
<i>Ramon Antonio Rodriges Zalipynis, Anton Bryukhov, and Evgeniy Pozdeev</i>	
The Architecture of Specialized GPU Clusters Used for Solving the Inverse Problems of 3D Low-Frequency Ultrasonic Tomography	363
<i>Alexander Goncharsky and Sergey Seryozhnikov</i>	
The Energy Consumption Analysis for the Multispectral Infrared Satellite Images Processing Algorithm	376
<i>Ekaterina Tyutlyanova, Sergey Konyukhov, Igor Odintsov, and Alexander Moskovsky</i>	
Automatic SIMD Vectorization of Loops: Issues, Energy Efficiency and Performance on Intel Processors	388
<i>Olga Moldovanova and Mikhail Kurnosov</i>	
Improving the Performance of an AstroPhi Code for Massively Parallel Supercomputers Using Roofline Analysis	400
<i>Boris Glinsky, Igor Kulikov, and Igor Chernykh</i>	

Using Simulation to Improve Workflow Scheduling in Heterogeneous Computing Systems	407
<i>Alexey Nazarenko and Oleg Sukhoroslov</i>	
C++ Playground for Numerical Integration Method Developers.	418
<i>Stepan Orlov</i>	
Efficiency Analysis of Intel and AMD x86_64 Architectures for Ab Initio Calculations: A Case Study of VASP	430
<i>Vladimir Stegailov and Vyacheslav Vecher</i>	
Design of Advanced Reconfigurable Computer Systems with Liquid Cooling	442
<i>Ilya Levin, Alexey Dordopulo, Alexander Fedorov, and Yury Doronchenko</i>	
RAML-Based Mock Service Generator for Microservice Applications Testing	456
<i>Nikita Ashikhmin, Gleb Radchenko, and Andrei Tchernykh</i>	
Architecture of Middleware to Provide the Multiscale Modelling Using Coupling Templates	468
<i>Alexey Liniov, Valentina Kustikova, Alexander Sysoyev, Maxim Zhiltsov, Igor Polyakov, Denis Nasonov, and Nikolay Butakov</i>	
Anticipation Scheduling in Grid with Stakeholders Preferences	482
<i>Victor Toporkov, Dmitry Yemelyanov, and Anna Toporkova</i>	
The State-of-the-Art Trends in Education Strategy for Sustainable Development of the High Performance Computing Ecosystem	494
<i>Sergey Mosin</i>	
A Service-Oriented Infrastructure for Teaching Big Data Technologies	505
<i>Oleg Sukhoroslov</i>	
JobDigest – Detailed System Monitoring-Based Supercomputer Application Behavior Analysis	516
<i>Dmitry Nikitenko, Alexander Antonov, Pavel Shvets, Sergey Sobolev, Konstantin Stefanov, Vadim Voevodin, Vladimir Voevodin, and Sergey Zhumatiy</i>	
Author Index	531