2018 IEEE/ACM 9th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA 2018)

Dallas, Texas, USA 12 November 2018



IEEE Catalog Number: ISBN:

CFP18A63-POD 978-1-7281-0177-4

Copyright \odot 2018 by the Institute of Electrical and Electronics Engineers, Inc. All Rights Reserved

Copyright and Reprint Permissions: Abstracting is permitted with credit to the source. Libraries are permitted to photocopy beyond the limit of U.S. copyright law for private use of patrons those articles in this volume that carry a code at the bottom of the first page, provided the per-copy fee indicated in the code is paid through Copyright Clearance Center, 222 Rosewood Drive, Danvers, MA 01923.

For other copying, reprint or republication permission, write to IEEE Copyrights Manager, IEEE Service Center, 445 Hoes Lane, Piscataway, NJ 08854. All rights reserved.

*** This is a print representation of what appears in the IEEE Digital Library. Some format issues inherent in the e-media version may also appear in this print version.

 IEEE Catalog Number:
 CFP18A63-POD

 ISBN (Print-On-Demand):
 978-1-7281-0177-4

 ISBN (Online):
 978-1-7281-0176-7

Additional Copies of This Publication Are Available From:

Curran Associates, Inc 57 Morehouse Lane Red Hook, NY 12571 USA Phone: (845) 758-0400 Fax: (845) 758-2633

E-mail: curran@proceedings.com Web: www.proceedings.com



2018 IEEE/ACM 9th **Workshop on Latest Advances in Scalable Algorithms for Large-Scale** Systems (ScalA) **ScalA 2018**

Table of Contents

Session 2

Event-Triggered Communication in Parallel Computing .1
Communication Reduced Multi-time-step Algorithm for Real-Time Wind Simulation on GPU-based Supercomputers 9
Naoyuki Onodera (Japan Atomic Energy Agency), Yasuhiro Idomura (Japan Atomic Energy Agency), Yussuf Ali (Japan Atomic Energy Agency), and Takashi Shimokawabe (The University of Tokyo)
Communication Avoiding Multigrid Preconditioned Conjugate Gradient Method for Extreme Scale Multiphase CFD Simulations .1.7
Non-collective Scalable Global Network Based on Local Communications .25

Session 3

Iterative Randomized Algorithms for Low Rank Approximation of Tera-scale Matrices with

Small Spectral Gaps .33.

Chander Iyer (Rensselaer Polytechnic Institute), Alex Gittens
(Rensselaer Polytechnic Institute), Christopher Carothers (Rensselaer
Polytechnic Institute), and Petros Drineas (Purdue University)

Shift-Collapse Acceleration of Generalized Polarizable Reactive Molecular Dynamics for Machine Learning-Assisted Computational Synthesis of Layered Materials .41..... Kuang Liu (University of Southern California), Subodh Tiwari (University of Southern California), Chunyang Sheng (University of Southern California), Aravind Krishnamoorthy (University of Southern California), Sungwook Hong (University of Southern California), Pankai Rajak (University of Southern California), Rajiv K. Kalia (University of Southern California), Aiichiro Nakano (University of Southern California), Ken-ichi Nomura (University of Southern California), Priya Vashishta (University of Southern California), Manaschai Kunaseth (National Science and Technology Development Agency, Thailand), Saber Naserifar (Materials and Process Simulation Center, California Institute of Technology), William A. Goddard III (Materials and Process Simulation Center, California Institute of Technology), Ye Luo (Argonne Leadership Computing Facility, Argonne National Laboratory). Nichols A. Romero (Argonne Leadership Computing Facility. Argonne National Laboratory), and Fuyuki Shimojo (Department of Physics, Kumamoto University, Japan) Machine Learning-Aided Numerical Linear Algebra: Convolutional Neural Networks for the Efficient Preconditioner Generation .49. Markus Goetz (Karlsruhe Institute of Technology) and Hartwig Anzt (Karlsruhe Institute of Technology) **Session 4** Low Thread-Count Gustavson: A Multithreaded Algorithm for Sparse Matrix-Matrix Multiplication Using Perfect Hashing .57.

James J. Elliott (Sandia National Laboratories) and Christopher M. Siefert (Sandia National Laboratories) A General-Purpose Hierarchical Mesh Partitioning Method with Node Balancing Strategies for Large-Scale Numerical Simulations .65. Fande Kong (Idaho National Laboratory), Roy H. Stogner (The University of Texas, Austin), Derek R. Gaston (Idaho National Laboratory), John W. Peterson (Idaho National Laboratory), Cody J. Permann (Idaho National Laboratory), Andrew E. Slaughter (Idaho National Laboratory), and Richard C. Martineau (Idaho National Laboratory) Dynamic Load Balancing of Plasma and Flow Simulations 73. Gerrett Diamond (Rensselaer Polytechnic Institute (RPI)), Cameron W. Smith (Rensselaer Polytechnic Institute (RPI)), Eisung Yoon (Ulsan National Institute of Science and Technology), and Mark S. Shephard (Rensselaer Polytechnic Institute (RPI)) On Advanced Monte Carlo Methods for Linear Algebra on Advanced Accelerator Architectures .81..... Anton Lebedev (Institute for Theoretical Physics, University of Tuebingen) and Vassil Alexandrov (ICREA, Barcelona Supercomputing Centre)