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# Parallel Processing and Applied Mathematics

12th International Conference, PPAM 2017 Lublin, Poland, September 10–13, 2017 Revised Selected Papers, Part II



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#### **Preface**

This volume comprises the proceedings of the 12th International Conference on Parallel Processing and Applied Mathematics – PPAM 2017, which was held in Lublin, Poland, September 10–13, 2017. It was organized by the Department of Computer and Information Science of the Czestochowa University of Technology together with Maria Curie-Skłodowska University in Lublin, under the patronage of the Committee of Informatics of the Polish Academy of Sciences, in technical cooperation with the IEEE Computer Society and ICT COST Action IC1305 "Network for Sustainable Ultrascale Computing (NESUS)". The main organizer was Roman Wyrzykowski.

PPAM is a biennial conference. Ten previous events have been held in different places in Poland since 1994. The proceedings of the last six conferences have been published by Springer in the *Lecture Notes in Computer Science* series (Nałęczów, 2001, vol. 2328; Częstochowa, 2003, vol. 3019; Poznań, 2005, vol. 3911; Gdańsk, 2007, vol. 4967; Wrocław, 2009, vols. 6067 and 6068; Toruń, 2011, vols. 7203 and 7204; Warsaw, 2013, vols. 8384 and 8385; Kraków, 2015, vols. 9573 and 9574).

The PPAM conferences have become an international forum for the exchange of ideas between researchers involved in parallel and distributed computing, including theory and applications, as well as applied and computational mathematics. The focus of PPAM 2017 was on models, algorithms, and software tools that facilitate efficient and convenient utilization of modern parallel and distributed computing architectures, as well as on large-scale applications, including big data and machine learning problems.

This meeting gathered more than 170 participants from 25 countries. A strict review process resulted in the acceptance of 100 contributed papers for publication in the conference proceedings, while approximately 42% of the submissions were rejected. For regular tracks of the conference, 49 papers were selected from 98 submissions, giving an acceptance rate of 50%.

The regular tracks covered such important fields of parallel/distributed/cloud computing and applied mathematics as:

- Numerical algorithms and parallel scientific computing, including parallel matrix factorizations and particle methods in simulations
- Task-based paradigm of parallel computing
- GPU computing
- Parallel non-numerical algorithms
- Performance evaluation of parallel algorithms and applications
- Environments and frameworks for parallel/distributed/cloud computing
- Applications of parallel computing
- Soft computing with applications

The invited talks were presented by:

- Rosa Badia from the Barcelona Supercomputing Center (Spain)
- Franck Cappello from the Argonne National Laboratory (USA)
- Cris Cecka from NVIDIA and Stanford University (USA)
- Jack Dongarra from the University of Tennessee and ORNL (USA)
- Thomas Fahringer from the University of Innsbruck (Austria)
- Dominik Göddeke from the University of Stuttgart (Germany)
- William Gropp from the University of Illinois Urbana-Champaign (USA)
- Georg Hager from the University of Erlangen-Nurnberg (Germany)
- Alexey Lastovetsky from the University College Dublin (Ireland)
- Satoshi Matsuoka from the Tokyo Institute of Technology (Japan)
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- Manish Parashar from Rutgers University (USA)
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- Andrei Tchernykh from the CICESE Research Center (Mexico)
- Jeffrey Vetter from the Oak Ridge National Laboratory and Georgia Institute of Technology (USA)

Important and integral parts of the PPAM 2017 conference were the workshops:

- Workshop on Models, Algorithms, and Methodologies for Hierarchical Parallelism in New HPC Systems organized by Giulliano Laccetti and Marco Lapegna from the University of Naples Federico II (Italy), and Raffaele Montella from the University of Naples Parthenope (Italy)
- Workshop on Power and Energy Aspects of Computation PEAC 2017 organized by Ariel Oleksiak from the Poznan Supercomputing and Networking Center (Poland) and Laurent Lefevre from Inria (France)
- Workshop on Scheduling for Parallel Computing SPC 2017 organized by Maciej Drozdowski from the Poznań University of Technology (Poland)
- The 7th Workshop on Language-Based Parallel Programming Models WLPP 2017 organized by Ami Marowka from Bar-Ilan University (Israel)
- Workshop on PGAS Programming organized by Piotr Bała from Warsaw University (Poland)
- Special Session on Parallel Matrix Factorizations organized by Marian Vajtersic from the University of Salzburg (Austria) and Slovak Academy of Sciences
- Minisymposium on HPC Applications in Physical Sciences organized by Grzegorz Kamieniarz and Wojciech Florek from the A. Mickiewicz University in Poznań (Poland)
- Minisymposium on High-Performance Computing Interval Methods organized by Bartłomiej J. Kubica from Warsaw University of Technology (Poland)
- Workshop on Complex Collective Systems organized by Paweł Topa and Jarosław Wąs from the AGH University of Science and Technology in Kraków (Poland)

The PPAM 2017 meeting began with three tutorials:

- Scientific Computing with GPUs, by Dominik Göddeke from the University of Stuttgart (Germany) and Robert Strzodka from Heidelberg University (Germany)
- Advanced OpenMP Tutorial, by Dirk Schmidl from RWTH Aachen University (Germany)
- Parallel Computing in Java, by Piotr Bała from Warsaw University (Poland), and Marek Nowicki from the Nicolaus Copernicus University in Toruń (Poland)

A new topic at PPAM 2017 was "Particle Methods in Simulations." Particle-based and Lagrangian formulations are all-time classics in supercomputing and have been wrestling with classic mesh-based approaches such as finite elements for quite a while now, in terms of computational expressiveness and efficiency. Computationally, particle formalisms benefit from very costly inter-particle interactions. These interactions with high arithmetic intensity make them reasonably "low-hanging" fruits in supercomputing with its notoriously limited bandwidth and high concurrency.

Surprisingly, PPAM 2017 was shaped by articles that give up on expensive particle-particle interactions: discrete element methods (DEM) study rigid bodies which interact only rarely once they are in contact, while particle-in-cell (PIC) methods use the physical expressiveness of Lagrangian descriptions but make the particles interact solely locally with a surrounding grid. It is obvious that the lack of direct long-range particle-particle interaction increases the concurrency of the algorithms. Yet, it comes at a price. With low arithmetic intensity, all data structures have to be extremely fine-tuned to perform on modern hardware, and load-balancing has to be lightweight. Codes cannot afford to resort data inefficiently all the time, move around too much data, or work with data structures that are ill-suited for vector processing, while notably the algorithmic parts with limited vectorization potential have to be revisited and maybe rewritten for emerging processors tailored toward stream processing.

The new session "Particle Methods in Simulations" provided a platform for some presentations with interesting and significant contributions addressing these challenges:

- Contact problems are rephrased as continuous minimization problems coupled with a posteriori validity checks, which allows codes to vectorize at least the first step aggressively (by K. Krestenitis, T. Weinzierl, and T. Koziara)
- Classic PIC is recasted into a single-touch algorithm with only few synchronization points, which releases pressure from the memory subsystem (by Y. Barsamian, A. Chargueraud, and A. Ketterlin)
- Cell-based shared memory parallelization of PIC is revised from a scheduling point of view and tailored parallelization schemes are developed, which anticipate the enormous per-cell load imbalances resulting from clustered particles (by A. Larin et al.)
- Particle sorting algorithms are revisited that make the particles be stored in memory
  in the way they are later accessed by the algorithm even though the particles tend to
  move through the domain quickly (by A. Dorobisz et al).

Another new topic at PPAM 2017 was "Task-Based Paradigm of Parallel Computing." Task-based parallel programming models have appeared in the recent years as an alternative to traditional parallel programming models, both for fine-grain and

coarse-grain parallelism. In this paradigm, the task is the unit of execution and traditionally a data-dependency graph of the application tasks represents the application. From this graph, the potential parallelism of the application is exploited, enabling an asynchronous execution of the tasks that do not require explicit fork-join structures.

Research topics in the area are multiple, from the specification of the syntax or programming interfaces, the definition of new scheduling and resource management algorithms that take into account different metrics, the design of the interfaces with the actual infrastructure, or new algorithms specified in this parallel paradigm. As an example of the success of this paradigm, the OpenMP standard has adopted this paradigm in its latest releases.

This topic was presented at PPAM 2017 in the form of a session that consisted of several presentations from various topics:

- "A Proposal for a Unified Interface for Task-Based Programming Models That Enables the Execution of Applications in Multiple Parallel Environments" (by A. Zafari)
- "A Comparison of Time and Energy Oriented Scheduling for Task-Based Programs, Which Is Based on Real Measured Data for the Tasks Leading to Diverse Effects Concerning Time, Energy, and Power Consumption" (by T. Rauber and G. Rünger)
- "A Study of a Set of Experiments with the Sparse Cholesky Decomposition on Multicore Platforms, Using a Parametrized Task Graph Implementation" (by I. Duff and F. Lopez)
- "A Task-Based Algorithm for Reordering the Eigenvalues of a Matrix in Real Schur Form, Which Is Realized on Top of the StarPU Runtime System" (by M. Myllykoski)

A new topic at PPAM 2017 was the "Special Session on Parallel Matrix Factorizations." Nowadays, in order to meet demands of high-performance computing, it is necessary to pay serious attention to the development of fast, reliable, and communication-efficient algorithms for solving kernel linear algebra problems. Tasks that lead to matrix decomposition computations are undoubtedly some of the most frequent problems encountered in this field. Therefore, the aim of the special session was to present new results from parallel linear algebra with an emphasis on methods and algorithms for factorizations and decompositions of large sparse and dense matrices. Both theoretical aspects and software issues related to this problem area were considered for submission.

The topics of the special session focused on: (a) efficient algorithms for the EVD/SVD/NMF decompositions of large matrices, their design and analysis; (b) implementation of parallel matrix factorization algorithms on parallel CPU and GPU systems; (c) usage of parallel matrix factorizations for solving problems arising in scientific and technical applications. Seven papers were accepted for presentation, which covered the session topics. Geographically, the authors were dispersed among two continents and five countries. The individual themes of the contributions included:

"New Preconditioning for the One-Sided Block-Jacobi Singular Value Decomposition Algorithm" (by M. Bečka, G. Okša, and E. Vidličková)

- "Using the Cholesky QR Method in the Full-Blocked One-Sided Jacobi Algorithm"
   (by S. Kudo and Y. Yamamoto)
- "Parallel Divide-and-Conquer Algorithm for Solving Tridiagonal Eigenvalue Problems on Manycore Systems" (by Y. Hirota and I. Toshiyuki)
- "Structure-Preserving Technique in the Block SS-Hankel Method for Solving Hermitian Generalized Eigenvalue Problems" (by A. Imakura, Y. Futamura, and T. Sakurai)
- "Parallel Inverse of Non-Hermitian Block Tridiagonal Matrices" (by L. Spellacy and D. Golden)
- "Tunability of a New Hessenberg Reduction Algorithm Using Parallel Cache Assignment" (by M. Eljammaly, L. Karlsson, and B. Kågström)
- "Convergence and Parallelization of Nonnegative Matrix Factorization (NMF) with Newton Iteration" (by R. Kutil, M. Flatz, and M. Vajtersic).

The organizers are indebted to the PPAM 2017 sponsors, whose support was vital for the success of the conference. The main sponsor was the Intel Corporation. Another important sponsor was Lenovo. We thank all the members of the international Program Committee and additional reviewers for their diligent work in refereeing the submitted papers. Finally, we thank all the local organizers from the Częstochowa University of Technology, and Maria Curie-Skłodowska University in Lublin, who helped us run the event very smoothly. We are especially indebted to Grażyna Kołakowska, Urszula Kroczewska, Łukasz Kuczyński, Adam Tomaś, and Marcin Woźniak from the Częstochowa University of Technology; and to Przemysław Stpiczyński and Beata Bylina from Maria Curie-Skłodowska University. Also, Paweł Gepner from Intel offered great help in organizing social events for PPAM 2017, including the excursion to the Zamoyski Palace in Kozłówka and the concert of the youth accordion orchestra "Arti Sentemo" at the Royal Castle in Lublin.

We hope that this volume will be useful to you. We would like everyone who reads it to feel invited to the next conference, PPAM 2019, which will be held during September 8–11, 2019, in Białystok, the largest city in northeastern Poland, located close to the world-famous Białowieża Forest.

January 2018

Roman Wyrzykowski Jack Dongarra Ewa Deelman Konrad Karczewski

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# **Contents - Part II**

Workshop on Models, Algorithms and Methodologies

for Hybrid Parallelism in New HPC Systems	
An Experience Report on (Auto-)tuning of Mesh-Based PDE Solvers on Shared Memory Systems	3
Using GPGPU Accelerated Interpolation Algorithms for Marine Bathymetry Processing with On-Premises and Cloud Based Computational Resources	14
Relaxing the Correctness Conditions on Concurrent Data Structures for Multicore CPUs. A Numerical Case Study	25
Energy Analysis of a 4D Variational Data Assimilation Algorithm and Evaluation on ARM-Based HPC Systems	37
Performance Assessment of the Incremental Strong Constraints 4DVAR Algorithm in ROMS	18
Evaluation of HCM: A New Model to Predict the Execution Time of Regular Parallel Applications on a Heterogeneous Cluster	58
Workshop on Power and Energy Aspects of Computations (PEAC 2017)	
Applicability of the Empirical Mode Decomposition for Power  Traces of Large-Scale Applications	71

Efficiency Analysis of Intel, AMD and Nvidia 64-Bit Hardware for Memory-Bound Problems: A Case Study of Ab Initio Calculations with VASP	81
GPU Power Modeling of HPC Applications for the Simulation of Heterogeneous Clouds	91
Bi-cluster Parallel Computing in Bioinformatics – Performance and Eco-Efficiency	102
Performance and Energy Analysis of Scientific Workloads  Executing on LPSoCs	113
Energy Efficient Dynamic Load Balancing over MultiGPU  Heterogeneous Systems	123
Workshop on Scheduling for Parallel Computing (SPC 2017)	
Scheduling Data Gathering with Maximum Lateness Objective  Joanna Berlińska	135
Fair Scheduling in Grid VOs with Anticipation Heuristic	145
A Security-Driven Approach to Online Job Scheduling in IaaS Cloud Computing Systems	156
Dynamic Load Balancing Algorithm for Heterogeneous Clusters  Tiago Marques do Nascimento, Rodrigo Weber dos Santos, and Marcelo Lobosco	166
Multi-Objective Extremal Optimization in Processor Load Balancing for Distributed Programs	176

Contents - Part II

XVII

# XVIII Contents - Part II

Fault-Tolerance Mechanisms for the Java Parallel Codes Implemented with the PCJ Library	298
Exploring Graph Analytics with the PCJ Toolbox	308
Big Data Analytics in Java with PCJ Library: Performance Comparison with Hadoop	318
Performance Comparison of Graph BFS Implemented in MapReduce and PGAS Programming Models	328
Minisymposium on HPC Applications in Physical Sciences	
Efficient Parallel Generation of Many-Nucleon Basis for Large-Scale Ab Initio Nuclear Structure Calculations	341
Parallel Exact Diagonalization Approach to Large Molecular Nanomagnets Modelling	351
Application of Numerical Quantum Transfer-Matrix Approach in the Randomly Diluted Quantum Spin Chains	359
Minisymposium on High Performance Computing Interval Methods	
A New Method for Solving Nonlinear Interval and Fuzzy Equations Ludmila Dymova and Pavel Sevastjanov	371
Role of Hull-Consistency in the HIBA_USNE Multithreaded Solver for Nonlinear Systems	381
Parallel Computing of Linear Systems with Linearly Dependent Intervals in MATLAB	391

Contents – Part II	XI
What Decision to Make in a Conflict Situation Under Interval Uncertainty:  Efficient Algorithms for the Hurwicz Approach	40
Practical Need for Algebraic (Equality-Type) Solutions of Interval Equations and for Extended-Zero Solutions	41
Workshop on Complex Collective Systems	
Application of Local Search with Perturbation Inspired by Cellular Automata for Heuristic Optimization of Sensor Network Coverage Problem	42
A Fuzzy Logic Inspired Cellular Automata Based Model for Simulating Crowd Evacuation Processes	43
Nondeterministic Cellular Automaton for Modelling Urban Traffic with Self-organizing Control	44
Towards Multi-Agent Simulations Accelerated by GPU	45
Tournament-Based Convection Selection in Evolutionary Algorithms	460
Multi-agent Systems Programmed Visually with Google Blockly Szymon Górowski, Robert Maguda, and Paweł Topa	470
Author Index	483

# **Contents – Part I**

Numerical Algorithms and Parallel Scientific Computing	
Advances in Incremental PCA Algorithms	3
Algorithms for Forward and Backward Solution of the Fokker-Planck Equation in the Heliospheric Transport of Cosmic Rays  Anna Wawrzynczak, Renata Modzelewska, and Agnieszka Gil	14
Efficient Evaluation of Matrix Polynomials	24
A Comparison of Soft-Fault Error Models in the Parallel Preconditioned Flexible GMRES	36
Multilayer Approach for Joint Direct and Transposed Sparse Matrix  Vector Multiplication for Multithreaded CPUs	47
Comparison of Parallel Time-Periodic Navier-Stokes Solvers	57
Blocked Algorithms for Robust Solution of Triangular Linear Systems Carl Christian Kjelgaard Mikkelsen and Lars Karlsson	68
A Comparison of Accuracy and Efficiency of Parallel Solvers for Fractional Power Diffusion Problems	79
Efficient Cross Section Reconstruction on Modern Multi and Many Core Architectures	90
Parallel Assembly of ACA BEM Matrices on Xeon Phi Clusters	101
Stochastic Bounds for Markov Chains on Intel Xeon Phi Coprocessor	111

## **Particle Methods in Simulations**

123
133
145
156
169
185
197
207
219
232

NVIDIA GPUs Scalability to Solve Multiple (Batch) Tridiagonal Systems Implementation of cuThomasBatch	243
Two-Echelon System Stochastic Optimization with R and CUDA  Witold Andrzejewski, Maciej Drozdowski, Gang Mu, and Yong Chao Sun	254
Parallel Hierarchical Agglomerative Clustering for fMRI Data	265
Parallel Non-numerical Algorithms	
Two Parallelization Schemes for the Induction of Nondeterministic Finite  Automata on PCs	279
Approximating Personalized Katz Centrality in Dynamic Graphs Eisha Nathan and David A. Bader	290
Graph-Based Speculative Query Execution for RDBMS	303
A GPU Implementation of Bulk Execution of the Dynamic Programming for the Optimal Polygon Triangulation	314
Performance Evaluation of Parallel Algorithms and Applications	
Early Performance Evaluation of the Hybrid Cluster with Torus Interconnect Aimed at Molecular-Dynamics Simulations	327
Load Balancing for CPU-GPU Coupling in Computational Fluid Dynamics	337
Implementation and Performance Analysis of 2.5D-PDGEMM on the K Computer	348

Contents - Part I XXIII

An Approach for Detecting Abnormal Parallel Applications Based on Time Series Analysis Methods	3
Prediction of the Inter-Node Communication Costs of a New Gyrokinetic Code with Toroidal Domain	3
Andreas Jocksch, Noé Ohana, Emmanuel Lanti, Aaron Scheinberg, Stephan Brunner, Claudio Gheller, and Laurent Villard	
D-Spline Performance Tuning Method Flexibly Responsive to Execution	
Time Perturbation	3
Environments and Frameworks for Parallel/Distributed/Cloud Computing	
Dfuntest: A Testing Framework for Distributed Applications	3
Security Monitoring and Analytics in the Context of HPC	
Processing Model	4
Multidimensional Performance and Scalability Analysis for Diverse	
Applications Based on System Monitoring Data	4
Bridging the Gap Between HPC and Cloud Using HyperFlow	
and PaaSage  Dennis Hoppe, Yosandra Sandoval, Anthony Sulistio, Maciej Malawski, Bartosz Balis, Maciej Pawlik, Kamil Figiela, Dariusz Krol, Michal Orzechowski, Jacek Kitowski, and Marian Bubak	4
A Memory Efficient Parallel All-Pairs Computation Framework:	
Computation – Communication Overlap	4
Automatic Parallelization of ANSI C to CUDA C Programs  Jan Kwiatkowski and Dzanan Bajgoric	4
Consistency Models for Global Scalable Data Access Services Michał Wrzeszcz, Darin Nikolow, Tomasz Lichoń, Rafał Słota, Łukasz Dutka, Renata G. Słota, and Jacek Kitowski	4

Applications of Parallel Computing	
Global State Monitoring in Optimization of Parallel  Event–Driven Simulation	483
High Performance Optimization of Independent Component Analysis Algorithm for EEG Data	495
Continuous and Discrete Models of Melanoma Progression Simulated in Multi-GPU Environment	505
Early Experience on Using Knights Landing Processors for Lattice Boltzmann Applications	519
Soft Computing with Applications	
Towards a Model of Semi-supervised Learning for the Syntactic Pattern Recognition-Based Electrical Load Prediction System	533
Parallel Processing of Color Digital Images for Linguistic Description of Their Content	544
Co-evolution of Fitness Predictors and Deep Neural Networks	555
Performance Evaluation of DBN Learning on Intel Multi- and Manycore Architectures	565
Special Session on Parallel Matrix Factorizations	
On the Tunability of a New Hessenberg Reduction Algorithm Using Parallel Cache Assignment	579
New Preconditioning for the One-Sided Block-Jacobi SVD Algorithm	590

Contents - Part I XXV

# XXVI Contents - Part I

Structure-Preserving Technique in the Block SS–Hankel Method for Solving Hermitian Generalized Eigenvalue Problems	
On Using the Cholesky QR Method in the Full-Blocked One-Sided  Jacobi Algorithm	612
Parallel Divide-and-Conquer Algorithm for Solving Tridiagonal Eigenvalue Problems on Manycore Systems	623
Partial Inverses of Complex Block Tridiagonal Matrices	634
Parallel Nonnegative Matrix Factorization Based on Newton Iteration with Improved Convergence Behavior	646
Author Index	657