High Performance Computing 2019 Conference
September 2-6, 2019, Borovets, Bulgaria

SCIENTIFIC PROGRAM

Monday, September 2

Plenary Session

Lecture Hall A	
08:30 – 09:15	Registration
09:15 – 09:45	Opening: **Commissioner Mariya Gabriel** **Mrs. Karina Angelieva - Deputy Minister of Education and Science** **Acad. Julian Revalski - President of the Bulgarian Academy of Sciences**
9:45 – 10:15	**Bl. Sendov**, *Why supercomputers need super mathematics? (honorary lecture)*
10:15 – 11:05	**Thomas Lippert**, *Data intensive HPC applications and how to boost their computation on future modular supercomputers (plenary lecture)*
11:05 – 11:20	Coffee Break
Chair: Svetozar Margenov	
11:20 – 12:10	**Zahari Zlatev**, *Frontiers in Air Pollution Studies Combined with Advanced Climatic Scenarios (plenary lecture)*
12:10 – 12:40	**Daniel Verwaerde,** *Intensives Calculations in Nuclear Researches and Engineering (keynote lecture)*
12:40 – 13:10	**Thomas Schulthess** *Reflecting on the goal and baseline for exascale computing: a roadmap based on weather and climate simulations*
13:10 – 14:30	LUNCH Registration

Parallel Sessions

Lecture Hall A *Special Session "Application of Artificial Intelligence in Optimization and Modelling"*	**Lecture Hall B** *General Track + Special session "Advanced HPC Monte Carlo and Quasi-Monte Carlo Applications"*
Chair: Vassia Atanassova	Chair: Aneta Karaivanova
14:30 – 14:55 **A.Alexandrov**, R.Andreev**,** S. Ilchev**,** D.Batchvarov, A.Boneva, S.Ivanov, J.Doshev, *Modeling and simulation of Low Power Wireless Sensor Networks based on Generalized Nets*	14:30 – 15:10 **Asen Asenov**, *NanoElectronic Simulation Software (NESS): The first HPC TCAD open source platform (keynote lecture)*
14:55 – 15:20 **Kristina Kapanova,** Stoyan Markov, *Pipeline Algorithm for Simulating Large Neuronal Networks in Multi-core Environment*	
15:20 – 15:45 Vladimir Myasnichenko, Stefka Fidanova, **Rossen Mikhov,** Leoneed Kirilov, Nikolay Sdobnyakov**,** *Representation of Initial Temperature as a Function in Simulated Annealing Approach for Metal Nanoparticle Structures Modelling*	15:10 – 15:40 Josef Weinbub**, Mihail Nedjalkov**, *Computational Strategies for Two-Dimensional Wigner Monte Carlo (keynote lecture)*
15:45 – 16:10	15:40 – 16:10 **Svetozar Margenov,** *Applications Driven Approach in Evaluation of HPC Efficiency (keynote lecture)*
16:10 – 16:30	**Coffee Break**

Parallel Sessions

Lecture Hall A *Special session "Application of Artificial Intelligence in Optimization and Modelling"*	**Lecture Hall B** *Special session "Molecular Modelling and Simulation"*
Chair: Vassia Atanassova	Chair: Nevena Ilieva
16:30 – 16:55 Veselina Bureva, **Velichka Traneva,** Dafina Zoteva and Stoyan Tranev, *Generalized Net Model Simulation of Cluster Analysis using CLIQUE: Clustering in Quest*	16:30 – 16:55 **Damien Thompson**, *HPC-enabled predictive modelling of bio-inspired*

	nanostructured materials
16:55 – 17:20 Velichka Traneva and **Stoyan Tranev,** *An Intuitionistic Fuzzy Zero Suffix Method for Solving the Transportation Problem*	16:55 – 17:20 **Adam Liwo,** Emilia A. Lubecka, Cezary Czaplewski, Adam K. Sieradzan, *Simulations of protein structure, dynamics, and thermodynamics with the coarse-grained UNRES force field and massively parallel computers*
17:20 – 17:45 Kristina Kapanova and **Velislava Stoykova,** *Timeline Event Analysis of Social Network Communications Activity: the Case of Jan Kuciak*	17:20 – 17:45 **Ilian Todorov,** *Technical, scientific and data challenges for Molecular Simulation*
17:45 – 18:10	17:45 – 18:10 **Panel Discussion**

Tuesday, September 3

Keynote Session

Lecture Hall A	
Chair: Stoyan Markov	
09:00 – 09:40	**Owe Axelsson**, *A survey of optimal control problems for PDEs (keynote lecture)*
09:24 – 10:20	**Sinéad Ryan,** *HPC and Lattice QCD:progress and perspectives (keynote lecture)*
10:20 – 11:00	**Katrin Amunts,** *Computing the brain (keynote lecture)*
11:00 – 11:15	Coffee Break

Parallel Sessions

Lecture Hall A *Special session "Treatment of Large Scientific and Engineering Problems – Challenges and Their Solutions"*	**Lecture Hall B** *Special session "Application of Artificial Intelligence in Optimization and Modelling"*
Chair: Zahari Zlatev	Chair: Velichka Traneva
11:15 – 11:40 **Istvan Farago** and Fanni Dorner, *Extended Models of Epidemic Propagation*	11:15 – 11:40 Stefka Fidanova, **Velislava Stoykova,** *Teaching Supercomputers*
11:40 – 12:05 **A. Liolios,** G. Skodras, K. Georgiev and I. Georgiev, *A stochastic analysis of RC structures under progressive environmental collapse considering uncertainty and strengthening by ties*	11:40 – 12:05 I. Tsakovska, P. Alov, N. Ikonomov, **V. Atanassova,** P. Vassilev, O.Roeva, D. Jereva, I. Pajeva, K. Atanassov, T. Pencheva**,** *InterCriteria Analysis Implementation for Exploration of the Performance of Various Docking Scoring Functions*
12:05 – 12:30 G. Gadzhev, V. Ivanov, R. Valcheva, **K. Ganev** and H. Chervenkov, *HPC Simulations of the Present and Projected Future Climate of the Balkan Region*	12:05 – 12:30 **Yordanka Boneva,** Vladimir Ivanov**,** *Improvement of Traffic in Urban Environment through Signal Timing Optimization*
12:30 – 14:30 LUNCH	
13:30 – 14:30 Registration	

Parallel Sessions

Lecture Hall A *Special session "Treatment of Large Scientific and Engineering Problems – Challenges and Their Solutions"*	**Lecture Hall B** *Special session "Application of Artificial Intelligence in Optimization and Modeling"*
Chair: Istvan Farago	Chair: Velichka Traneva
14:30 – 14:55 Teshome Bayleyegn, István Faragó and **Ágnes Havasi**, *Generalized versions of Richardson extrapolation*	14:30 – 14:55 **A. Alexandrov,** R.Andreev, S.Ilchev, A.Boneva, S.Ivanov, and J.Doshev *WSN-based prediction model of microclimate in a city urbanized areas based on Extreme Learning and Kalman filter*

14:55 – 15:20 **Slavi Georgiev,** Lubin G. Vulkov, *Numerical Identification of Time-Dependent Volatility in European Options with Two-Stage Regime-Switching*	14:55 – 15:20 **Anna Wawrzyńczak-Szaban,** M. Berendt-Marchel, *Can the artificial neural network be applied to estimate the atmospheric contaminant transport?*
15:20 – 15:45 **Miglena Koleva**, Yuri Poveschenko, Lubin Vulkov *Numerical Simulation of Thermoelastic* *Nonlinear Waves in Fluid Saturated Porous Media with Nonlocal Darcy Law*	15:20 – 15:45 Krassimir Atanassov, **Veselina Bureva**, *Four operations over extended intuitionistic fuzzy index matrices and some of their applications*
15:45 – 16:10 **Dean Palejev,** Mladen Savov, *Estimating the Statistical Power of the Benjamini-Hochberg Procedure*	15:45 – 16:10 Rumen Ketipov, Georgi Kostadinov, Plamen Petrov, Iliyan Zankinski, **Todor Balabanov**, *Genetic Algorithm Based Formula Generation for Curve Fitting in Time Series Forecasting Implemented as Mobile Distributed Computing*
16:10 – 16:30	**Coffee Break**

Parallel Sessions

Lecture Hall A *Special session "Treatment of Large Scientific and Engineering Problems – Challenges and Their Solutions"*	**Lecture Hall B** Special session *"Molecular Modeling and Simulation"*
Chair: Tzvetan Ostromsky	Chair: Andrey Milchev
16:30 – 16:55 V. Ivanov, **R. Valcheva,** G. Gadzhev, *HPC Simulations of the Extreme Thermal Conditions in the Balkan Region with RegCM4*	16:30 – 16:55 **Sonya Tsibranska,** Anela Ivanova, Slavka Tcholakova, Nikolai Denkov**,** *Structure of dense adsorption layers of escin at the air-water interface studied by molecular dynamics simulations*
16:55 – 17:20 **Matthias Ehrhardt**, *High-Order Methods for Parabolic Equations in Multiple Space Dimensions for Option Pricing Problems*	16:55 – 17:20 **Fatmegyul Mustan**, Anela Ivanova, Slavka Tcholakova, *Effect of Ca2+ on the kinetics of adsorption of LAS and SLES molecules studied by molecular dynamics*
17:20 – 17:45 **Anton G. Artemov,** *Approximate Matrix Multiplication Using the Chunks and Tasks Programming Model*	17:20 – 17:45 **Stefan Ivanov,** *Bridging solute molecules mediate RNase A - ligand binding*
17:45- 18:10 D. Barantiev, E. Batchvarova, **H. Kirova** and O. Gueorguiev,	18:10 – 18:35 **Nevena Zaharieva,** Irini Doytchinova and Ivan Dimitrov,

Numerical Modeling of Extreme Wind Profiles Measured with SODAR in a Coastal Area	*Immunogenicity Prediction of Bacterial Proteins by Machine Learning Algorithms*
18:10- 18:35 Abdallah Bradji, **Moussa Ziggaf** *A Convergence Result of a Linear SUSHI Scheme Using Characteristics Method for a Semi-Linear Parabolic Equation*	18:10 – 18:35
18:35- 19:00 Bangti Jin, **Raytcho Lazarov**, Joseph Pasciak, and Zhi Zhou *Recent Advances in Numerical Treatment of Fractional PDEs. A Concise Overwiew*	

Wednesday, September 4

Parallel Sessions

Lecture Hall A *General track*	**Lecture Hall B** *Special session "Advanced HPC Monte Carlo and Quasi-Monte Carlo Applications"*
Chair: Andrey Andreev	Chair: Vassil Alexandrov
09:00 – 09:25 Hristo Chervenkov, **Kiril Slavov,** *ETCCDI Climate Indices for Assessment of the Recent Climate over Southeast Europe*	09:00 – 09:25 E. Atanassov, T. Gurov, M. Durchova, S. Ivanovska, **A. Karaivanova**, *On the performance of a class of quasi-Monte Carlo algorithms on diverse HPC Systems*
09:25 – 09:50 **Hristo Chervenkov,** Valery Spiridonov, *Sensitivity of Selected ETCCDI Climate Indices from the Calculation Method for Projected Future Climate*	09:25 – 09:50 **E. Atanassov,** S. Ivanovska, A. Karaivanova *Optimization of the direction numbers of the Sobol sequences*
09:50 – 10:15 **Michael Quell**, Georgios Diamantopoulos, Andreas Hossinger, Siegfried Selberherr, and Josef Weinbub, *Parallelized Bottom-Up Correction in Hierarchical Re-Distancing forTopography Simulation*	09:50 – 10:15 Vassil Alexsandrov, **Maya Neytcheva,** *Utilizing Monte Carlo-based approximate inverses as preconditioners for discrete linear elasticity problems*
10:15 – 10:40 **Venelin Todorov**, Ivan Dimov, Tzvetan Ostromsky, Zahari Zlatev, *Advanced quasi-Monte Carlo algorithms for Multidimensional Integrals in Air Pollution Modelling*	10:15 – 10:40 Anton Lebedev, **Vassil Alexandrov** *Advanced Monte Carlo Methods for Linear Algebra on Advanced Accelerator Architectures*

10:40 – 11:05 **Andrey Andreev,** Milena Racheva, *Finite Element Approximation for the Sturm-Liouville Problem with Quadratic Eigenvalue Parameter*	10:40 – 11:05 **Behrouz Fathi-Vajargah,** Vassil Alexandrov, Kolsoum Yousefpanah, Anton Lebedev, *Enhancing Monte Carlo and quasi-Monte Carlo methods for Solving Underdetermined, Overdetermined and Singular Linear Systems*
11:05 – 12:30 LUNCH	
12:30 – 19:00 EXCURSION	

Thursday, September 5

Plenary Session

Lecture Hall A	
Chair: Ivan Dimov	
09:00 – 09:50	**Jack Dongarra,** *High Performance Computing and Big Data: Challenges for the Future (plenary lecture)*
9:50 – 10:40	**Wil Schilders,** *The role of mathware within (Euro)HPC (plenary lecture)*
10:40 – 11:00	**Coffee Break**

Parallel Sessions

Lecture Hall A *Special session "Molecular Modeling and Simulation"*	**Lecture Hall B** *Special session "Modeling, Simulation; Optimization in a Data-rich Environment"*
Chair: Ilian Todorov	*Chair: Wil Schilders*
11:00 – 11:25 **Nevena Ilieva** *HPC perspective of topological protein folding*	11:00 – 11:25 **Zoltan Horvath,** *European projects for HPC: MSO4SC and HiDALGO*
12:15 – 12:40 **Mateusz Chwastyk,** Ewa A. Panek, Jan Malinowski, Mariusz Jaskólski, Marek Cieplak, *Statistical properties of cavities in proteins and their complexes*	11:25 – 11:50 **Christophe Prud'homme** *High-Performance Computing to optimize energy in existing buildings*

11:50 – 12:15 **Elena Lilkova,** Nevena Ilieva, Peicho Petkov, Leandar Litov**,** *Self-association evidence for partially intrinsically disordered antimicrobial peptides via long-scale MD simulations: a case study*	11:50 – 12:15 **A. Lotfi,** D. Marcsa, Z. Horvath, C.Prud'homme, V. Chabannes, *Coupled magnetothermal simulation of electric motors with applications*
12:15 – 12:40 **Andrey Milchev,** *New Insights into the Physics of Liquid-Crystalline Systems from Large-Scale Molecular Dynamics Simulations*	12:15 – 12:40 **Janez Povh**, *BiqBin: moving boundaries for NP-hard problems by HPC*
12:40 – 14:30 LUNCH	
Lecture Hall A *Special session "Molecular Modeling and Simulation*	**Lecture Hall B** *Special session "Modeling, Simulation; Optimization in a Data-rich Environment"*
Chair: Ilian Todorov	Chair: Zoltan Horvath
14:30 – 14:55 **Michael Seaton,** *Technical and scientific challenges of mesoscopic modelling with HPC*	14:30 – 14:55 Zoltan Horvath, Tamas Budai, Akos Kovacs, **Bence Liszkai,** *The Digital Twin of Urban Air Pollution*
14:55 – 15:20 **Peicho Petkov,** Stoyan Markov, Valentin Pavlov, *Large-scale molecular dynamics simulations on Modular Supercomputing Architecture with Gromacs*	14:55 – 15:20 **Mariane Clausel,** *Textual data analysis*
15:20 – 15:35 *Session Summary*	15:20 – 15:45 **Veronique Maume-Deschamps,** *Sensitivity analysis of the insurance process' Digital twin*
Special session "Treatment of Large Scientific and Engineering Problems – Challenges and Their Solutions" Chair: Agnes Havasi	
15:35 – 16:00 **Miklos Mincsovics,** *Different Types of Stability and Convergence of Linear Multistep Methods*	15:45 – 16:10 **Bertrand Maury**, *Real time data-based computation of pedestrian uxes: methodological and technological issues*

16:00 – 16:25 Georgi Gadzhev, **Kostadin Ganev,** *HPC Simulations of the Atmospheric Composition Climate of Bulgaria*	16:10-16:35 **Todor Stoilov,** Krasimira Stoilova, Miroslav Vladimirov, *Modeling and Assessment of Financial Investments by Portfolio Optimization on Stock Exchange*
16:35 – 16:50	**Coffee Break**

Discussion Session

Lecture Hall A	
Moderators: Thomas Skordas	
16:50- 19:00	**Thomas Lippert (PRACE), Svetozar Margenov(CoE), Vit Vondrak (IT4Innovations national supercomputing center), Kosta Ganev (NSP), Nevena Ilieva (NSP), Aneta Karaivanova (NCHDC), Volodimyr Saviak (HPE), Kalin Penev**, ***(Global Scalable Optimisation)*** *Presentation of HPC projects, programs and challenges*
19:30 – 23:00 OFFICIAL DINNER	

Friday, September 6

Lecture Hall A

Lecture Hall B	
Chair: Jack Dongarra	
09:00- 09:40	**Jean Gonnord,** *Europe back in the HPC big leagues (Building the industrial HPC ecosystem to support the EU digital challenge and secure EU independent and competitive HPC supply) (keynote lecture)*
09:40 – 10:10	**Robert Adamski,** *HPC and AI convergence - Intel roadmap and tools (keynote lecture)*
10:10- 10:35	**Ivan Blagoev,** *Method for evaluating the vulnerability of random number generators for cryptographic protection in information systems*
10:35 – 11:00	**Tzvetan Ostromsky,** Venelin Todorov, Ivan Dimov, Zahari Zlatev, *Sensitivity Studies of an Air Pollution Model by Using Efficient Stochastic Algorithms for Multidimensional Numerical Integration*
11:00 – 11:25	**Yuri Dimitrov,** Venelin Todorov, Ivan Dimov, *Second Order Shifted Approximations for the First Derivative*

12:00 DEPARTURE