

HIGH PERFORMANCE COMPUTING IN SCIENCE AND ENGINEERING

MAY 20 - 23, 2019, **HOTEL SOLÁŇ**

organized by

IT4Innovations National Supercomputing Center
VŠB Technical University of Ostrava, Czech Republic

Scientific programme

Monday, May 20

- 10:00 – 12:00 *Registration of participants*
- 12:00 – 14:00 *Lunch*
Chairman: Tomáš Kozubek
- 14:00 – 14:30 *Opening – Tomáš Kozubek, Vít Vondrák*
- 14:30 – 15:15 **Garth N. Wells: High performance computing for complex engineering systems**
- 15:15 – 16:00 **Dominik Göddeke: Enabling PDE software frameworks for exascale**
- 16:00 – 16:30 *Coffee break*
Chairman: Jakub Šístek
- 16:30 – 17:00 **Ondřej Meca, Lubomír Říha, Tomáš Brzobohatý: Workflow for parallel processing of sequential mesh databases**
- 17:00 – 17:30 **Erin Carson, Zdeněk Strakoš: On the cost of iterative computations**
- 17:30 – 18:30 **Jennifer Scott, Miroslav Tůma: Stretching for linear least squares - strengths and limitations**
Jakub Klinkovský, Tomáš Oberhuber, Radek Fučík: Computational study of MGSR- and CWY-based GMRES variants applied to two-phase flow in porous media
Pavel Eichler, Radek Fučík: A modified immersed boundary-lattice Boltzmann method for incompressible fluid flow in 2D and 3D on GPU
- 19:00 *Welcome grill party*

Tuesday, May 21

- 07:30 – 09:00 *Breakfast*
Chairman: Miroslav Tůma
- 09:00 – 09:45 Daniela di Serafino: **Accelerating split Bregman methods for sparse data recovery with joint l1-type regularizers**
- 09:45 – 10:30 Ben Cox, Jiří Jaroš, Bradley Treeby: **k-space models of acoustic wave propagation**
- 10:30 – 11:00 *Coffee break*
Chairman: Jiří Jaroš
- 11:00 – 11:30 Jaroslav Křivánek: **From nuclear reactors to pretty pictures and 3D prints: computational challenges**
- 11:30 – 12:30 Jakub Budiský: **Heterogeneous media in biological ultrasound simulations**
Filip Vaverka, Bradley E. Treeby, Jiří Jaroš: **Performance of pseudo-spectral codes on DGX-2 Server: k-Wave Ultrasound Simulations**
Radim Blaheta, Michal Béréš, Simona Domesová, Tomáš Luber: **HPC in applied geosciences: multiphysics and uncertainties**
- 12:30 – 14:00 *Lunch*
- 14:00 – 19:00 *Networking time (trip to Wallachian Open Air Museum, hiking, or wellness)*
- 19:00 – 20:00 *Dinner*
- 20:00 *Poster session with a short presentation per poster*

Wednesday, May 22

- 07:30 – 09:00 *Breakfast*
Chairman: Tomáš Oberhuber
- 09:00 – 09:45 Andrea Bartolini: **Datacenter Automation – AI, big-data, and application awareness for green and smart supercomputers**
- 09:45 – 10:30 Stefano Zampini: **BDDC and FETI-DP methods in PETSc**
- 10:30 – 11:00 *Coffee break*
Chairman: Petr Tichý
- 11:00 – 11:30 Jakub Šístek, Pavel Kůs: **A parallel multilevel domain decomposition solver and its application to adaptive FEM**
- 11:30 – 12:30 Ondřej Vysocký, Lubomír Říha, Andrea Bartolini: **Application instrumentation for performance analysis and tuning**
Zdeněk Dostál, Oldřich Vlach, Tomáš Brzobohatý: **Improving the convergence of TFETI for contact problems by adaptive augmentation**
Raphael Watschinger, Günther Of: **Fast directional matrix-vector multiplications – algorithm and parameter study**
- 12:30 – 14:00 Lunch
Chairman: Dalibor Lukáš
- 14:00 – 14:45 Günther Of, Stefan Dohr, Jan Zapletal, Michal Merta, Michal Kravčenko: **A parallel space-time boundary element method for the heat equation**
- 14:45 – 15:15 Pavel Kůs, Andreas Marek, Hermann Lederer: **Eigensolvers in the ELPA library**
- 15:15 – 16:00 Laura Grigori, Jan Papež, Radek Stompor: **Solving CMB parametric component separation problem using subspace recycling**
Dalibor Lukáš, Ivo Peterek, Ladislav Foltyn: **A coupling of parareal and domain decomposition methods for the 2d heat equation**
- 16:00 – 16:30 *Coffee break*
Chairman: Zdeněk Dostál
- 16:30 – 17:00 Giuseppe Accaputo, Peter M. Derlet, Peter Arbenz: **Solving large-scale interior eigenvalue problems to investigate the vibrational properties of the boson peak regime in amorphous materials**
- 17:00 – 18:00 Dalibor Lukáš: **A uniform parallel framework to large-scale simulations of 3d wave-type equations**
Dejan Brkić, Pavel Praks: **Efficient friction loss modelling using approximations of special functions**
Karel Tůma, Mohsen Rezaee, Stanisław Stupkiewicz: **Three-dimensional multiphase martensitic transformations in shape memory alloys**
- 19:00 *Conference dinner*

Thursday, May 23

- 07:30 – 09:00 *Breakfast*
Chairman: Peter Arbenz
- 09:00 – 09:45 Jakub Kurzak: **SLATE: Software for Linear Algebra Targeting Exascale**
- 09:45 – 10:30 Frédéric Hecht, Ionut Danaila, Pierre Jolivet, Frédéric Nataf, Pierre-Henri Tournier, Victorita Dolean: **Numerical simulation in physics and engineering with FreeFem++**
- 10:30 – 11:00 *Coffee break*
Chairman: Radim Blaheta
- 11:00 – 12:30 Jakub Solovský, Radek Fučík, Jakub Šístek: **Simulation of two-phase flow in porous media using MHFEM with BDDC in 2D and 3D**
- Tomáš Oberhuber, Jakub Klinkovský, Aleš Wodecky, Vít Hanousek, Radek Fučík: **TNL: Numerical library for modern parallel architectures**
- Josef Šlapal: **A closure operator for the digital plane**
- Michal Svatoš, Jiří Chudoba, Petr Vokáč: **ATLAS job submission system for Salomon HPC based on ARC-CE**
- 12:30 – 14:00 *Lunch, discussion, closing*

Poster session with a short presentation per poster (Tuesday at 20:00)

<i>Authors</i>	<i>Titles</i>
S. Arul	Optimization and highly parallel implementation of domain decomposition based solvers for water-turbines simulations
<u>M. Béréš</u> , S. Domesová, R. Blaheta	Modeling hydro-mechanical processes in fractured porous media
<u>J. Blahoš</u>	Large scale nonlinear modelling and simulation of whole engine models
<u>G. Bordovský</u> , J. Jaroš	On the complexity of photoacoustic tomography: a trade-off between image quality and computational cost
<u>J. Březina</u> , J. Stebel, P. Exner, M. Špetlík	Multilevel Monte Carlo and homogenisation for transport processes in fractured porous media
<u>T. Brzobohatý</u> , O. Meca, L. Říha	Parallel preprocessing of sequential mesh databases
<u>R. Cimrman</u> , J. Vackář, M. Novák	A software for generating and optimizing pseudopotentials
<u>M. Čermák</u> , S. Sysala, J. Valdman	On vectorized MATLAB implementation of elastoplastic problems
<u>S. Domesová</u> , M. Béréš, R. Blaheta	Deflation for sequences of linear systems for efficient implementation of Bayesian inversion
D. Dlouhá, <u>V. Dubovský</u>	On evaporation estimates
M. Jaroš	Scientific workflow management framework
G. Jenovencio	Parallel scalability of quasi-cyclic turbine models using FETI-like methods
<u>K. Kadlubiak</u> , J. Jaroš, B. E. Treeby	Impact of higher order integration scheme on elastic wave simulation
<u>M. Kravčenko</u> , M. Merta, J. Zapletal	A parallel multi-domain scattering in BEM4I
F. Kukliš	Fast reconstruction of photoacoustic images
J. Vondřejc, D. Liu, <u>M. Ladecký</u> , H. G. Matthies	FFT-based homogenisation accelerated by low-rank approximation
T. Luber	Exploring poroelasticity with FEniCS
<u>C. Matonoha</u> , Š. Papáček	Numerical optimization of the non-axisymmetric bleaching pattern for FRAP experiments
<u>M. Merta</u> , J. Zapletal, G. Of, S. Dohr	A parallel space-time boundary element method for the heat equation

- G. Nečasová, P. Veigend, V. Šátek **Taylor series based solution of ODE systems**
- T. Panoc, O. Meca, L. Říha,
T. Brzobohatý **Optimization of the parallel solver execution time with evolutionary and swarm algorithms**
- Š. Papáček, R. Filip, K. Petera **Modeling and simulation of macroalgae growth within integrated multitrophic aquaculture systems**
- P. Pařík, J. G. Kim **Efficient implementation of the enhanced Craig-Bampton method**
- M. Jaroš, P. Strakoš, L. Říha,
F. Siddi, A. Goralczyk, S. Stuvél,
P. Vazquez **Rendering of path-traced open-movie Spring in Blender Cycles on Intel Xeon Phi (KNC)**
- Švihlová H., Hron J. **Mathematical modelling in biomechanics**
- R. Vavřík, T. Brzobohatý, O. Meca,
L. Říha **ESPRESO FEM – Highly parallel finite element package for engineering simulations**