2ND USERS' CONFERENCE OF IT4INNOVATIONS

November 7, 2018
IT4Innovations National Supercomputing Center

08:00–09:00   **Registration and networking**

09:00–09:30   **Welcome and IT4Innovations news**

09:30–10:00   **KEYNOTE 1**

Dominik Legut | IT4Innovations
„Ultrafast demagnetization dynamics at $M2,3$ edges of hcp Co – first-principles calculations"

10:00–10:30   **Coffee break**

10:30–12:00   **Users talks I**

Jan Řezáč | Czech Academy of Sciences
„Efficient quantum-mechanical calculations for computer-aided drug design"

Martin Beseda | IT4Innovations
„lib4neuro - a library for artificial neural networks calculations in (not only) molecular physics"

Miroslav Černý | CEITEC, Brno University of Technology
„Interface-induced toughening of nitride superlattices"

Stanislav Böhm | IT4Innovations
„Snailwatch: Did you make it slow?"

Miroslav Rubeš | Czech Academy of Sciences
„Temperature dependence of carbon monoxide adsorption in H-FER zeolite"

David Wagenknecht | Charles University
„Alloy analogy model: Fully relativistic electrical transport with phonons, magnons, and chemical disorder"

12:00–13:00   **Lunch & poster session**

13:00–13:30   **KEYNOTE 2**

Richard Wünsch | Czech Academy of Sciences
„Origin of globular clusters: star formation in the most extreme conditions"

13:30–15:00 Users talks II

Stella Skiadopoulou | IT4Innovations
„Magnetoelectric excitations in the polar antiferromagnets Ni-based tellurates"

Michal H. Kolář | University of Chemistry and Technology, Prague
„Structure and Dynamics of a Ribosome-Regulatory Peptide"

Rhys Taylor | Czech Academy of Sciences
„Optically dark hydrogen clouds in the Virgo galaxy cluster"

Marek Ingr | Tomas Bata University in Zlín
„Binding of hyaluronan and its neutral analog by TSG-6 Link domain"

Ondřej Meca | IT4Innovations
„Workflow for Parallel Processing of Sequential Mesh Databases"

Benjamin Irving | Czech Technical University in Prague
„Predicting Tribological Properties of Low-Dimensional Materials"

15:00–15:30 Coffee break

15:30–16:15 Users Council

16:15–17:45 Users talks III

Alberto Fraile | Czech Technical University in Prague
„Jacob's Ladder: Prime numbers in 2d"

Martin Mokrejš | IT4Innovations
„Assembling diploid genome of Cobitis taenia using Illumina short reads"

Jiří Klimeš | Charles University
„Towards an accurate theoretical description of extended systems"

Lukáš Grajciar | Charles University
„Hydrolysis of zeolites: new insights from biased ab initio molecular dynamics"

Jaroslav Resler | Czech Academy of Sciences
„Radiative transfer model for the microscale urban climate model PALM-4U"

Daniel Holý | Czech Academy of Sciences
„Ion binding at lipid bilayers"

17:45–20:00 Conference dinner & poster session