

6th Users' Conference of IT4Innovations

November 3 and 4, 2022 / IT4Innovations

10:00 - 11:00 | Registration and networking

11:00 - 11:30 | Welcome and IT4Innovations news

11:30 - 12:00 | KEYNOTE I

An All-Atom Simulation Model of the Outer-Cell Interaction Network
[Denys BIRIUKOV | Institute of Organic Chemistry and Biochemistry of the CAS](#)

12:00 - 13:00 | Users' Talks I

Lipid Nanoparticles for RNA Delivery – Morphology Revealed by Coarse-Grained Simulations
[Marketa PALONCYOVA | Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute \(CATRIN\), Palacky University Olomouc](#)

Interactions of Macrocyclic Inhibitors with STING Protein – Novel Route to Treat Cancer and Chronic Hepatitis B

[Lubomir RULISEK | Institute of Organic Chemistry and Biochemistry of the CAS](#)

Anisotropy, Local disorder and polymorphism of crystalline biogenic acids
[Ctirad CERVINKA | Department of Physical Chemistry, UCT Prague](#)

13:00 - 14:00 | Lunch & Poster Session

14:00 - 14:45 | Users' Talks II

Large-scale atomistic simulations of the bacterial ribosome
[Michal H. KOLAR | University of Chemistry and Technology](#)

Phylogenomics of Heterolobosea
[Tomas PANEK | Charles University](#)

14:45 - 15:30 | USERS' COUNCIL

15:30 - 16:00 | Coffee break

16:00 - 16:30 | KEYNOTE II

Challenges of LHC Computing on HPC
[Jiri CHUDOBA | FZU - Institute of Physics of the CAS](#)

16:30 - 17:50 | Users' Talks III

Moving-mesh radiation-hydrodynamic modelling of astrophysical transients: methods and first results
[Diego CALDERON | Institute of Theoretical Physics, Charles University](#)

Benchmarking Barбора, Karolina and LUMI Using the k-Wave Toolbox
[Jiri JAROS | Brno University of Technology](#)

Excitation of wide band gap materials from first principles: studying the role of laser polarization using real-space real-time time-dependent density functional theory
[Thibault J.-Y. DERRIEN | HiLASE Centre - Institute of Physics](#)

Computational advances in the modelling of radiative interactions in the PALM LES model
[Pavel KRC | Institute of Computer Science of the CAS](#)

17:50 - 18:00 | Break

18:00 - 21:00 | Conference Dinner & Poster Session

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09:00 - 09:30 | KEYNOTE III

Using large-scale pre-trained models for building speech applications

[Oldrich PLCHOT](#) | [Brno University of Technology](#)

09:30 - 10:50 | Users' Talks IV

Electrons and Phonons in uranium hydrides - potential energy storage materials

[Dominik LEGUT](#) | [IT4Innovations](#)

Non-Covalent Interactions Atlas benchmark database

[Jan REZAC](#) | [Institute of Organic Chemistry and Biochemistry of the CAS](#)

Using the power of supercomputers to design new catalysts for selective oxidation reactions

[Stepan SKLENAK](#) | [J. Heyrovsky Institute of Physical Chemistry of the CAS](#)

Electrostatic and Electromagnetic fields as a knob to control nanofriction in nanostructured materials

[Antonio CAMMARATA](#) | [Czech Technical University in Prague](#)

10:50 - 11:00 | Coffee break

11:00 - 12:00 | Users' Talks V

Impact of disorder on materials properties of Ni-Mn-Sn alloys

[Martin FRIAK](#) | [Institute of Physics of Materials of the CAS](#)

Reactive Neural Network Potentials for Zeolites with Density Functional Theory Accuracy

[Lukas GRAJCIAR](#) | [Charles University in Prague](#)

Large scale atomistic models based on machine learned force fields for grain boundary segregation in bcc iron

[Petr SESTAK](#) | [CEITEC, Brno University of Technology](#)

12:00 - 13:00 | Lunch