

Session Program

November 9, 2021

5th Users' Conference of IT4Innovations

Poster session

IT4Innovations, Online

Tue, November 9

2:00 PM

Poster session: I

Session | Location: IT4Innovations, Online

2:00 – 2:30 PM

Preventing Deadlock in Non-uniform-timestep Distributed Pseudospectral Method

Speaker

Kristián Kadlubiak

2:00 – 2:30 PM

Enhancement of ultrashort directional X-ray pulses

Speaker

Dominika Maslarova

2:00 – 2:30 PM

Inversion of the satellite-observed tidal magnetic fields in terms of three-dimensional upper-mantle electrical conductivity

Speaker

Dr Libor Šachl

2:00 – 2:30 PM

High-order magneto-hydrodynamic code with spontaneous magnetic fields generation

Speaker

Jan Nikl

2:00 – 2:30 PM

Exploring the complete conformational space of all 400 dipeptides by quantum chemical methods: Can we predict the protein structure "ab initio"?

Speaker

Tadeas Kalvoda

2:00 – 2:30 PM

Towards Solvent Interactions in Modelling Infrared Spectra of Rhenium(I) Complex

Speaker

Martin Melčák

2:00 – 2:30 PM

k-Dispatch's Performance Modules for Advanced Workflow Submission

Speaker

Marta Jaros

2:00 – 2:30 PM

Handling C++ Exceptions in MPI Applications

Speaker

Jiri Jaros

2:00 – 2:30 PM

Hydrogen effect on the strength of the Fe₃Al alloy

Speaker

Dr Petr Šesták

2:00 – 2:30 PM **HyperQueue: Simplifying Usage of PBS/SLURM Clusters**

Speaker

Jakub Beránek

2:00 – 2:30 PM

PeptideCS: An extensive dataset mapping the potential energy surface of mono- and dipeptides

Speaker

Erik Andris

2:00 – 2:30 PM **Performance of k-Wave Toolbox on Multi-GPU Accelerated Clusters**

Speakers

Filip Vaverka, Jiri Jaros

2:30 PM

2:30 PM

Poster session: II

Session | Location: IT4Innovations, Online

2:30 – 3:00 PM

Reactive Molecular Dynamics Study on the Tribological Properties of Selected Vanadium Oxides

Speaker

Dr Miljan Dašić

2:30 – 3:00 PM **ATLAS job submission systems for the IT4Innovation**

Speaker

Dr Michal Svatos

2:30 – 3:00 PM

Enhancement of Ion Acceleration by Laser-Pulse Shaping via Plasma Shutter

Speaker

Martin Matys

2:30 – 3:00 PM

Calculation of NMR spin-spin couplings for intrinsically disordered proteins: a prospective tool to facilitate experimental NMR studies

Speakers

Amina Gaffour, Mr Bera Krishnendu

2:30 – 3:00 PM **HPC solver of Ising model: application in Material Design**

Speaker

Aleksandra Dujović

2:30 – 3:00 PM **Peptide Elongation in Carbon Nanotubes: An Atomistic Approach**

Speaker

Felipe Castro Nepomuceno

2:30 – 3:00 PM **Reactive Force Field for Molybdenum Disulfide Crystallization**

Speaker

Iliia Ponomarev

2:30 – 3:00 PM **Advances in the Evolutionary Design of Complex Cellular Automata**

Speaker
Michal Bidlo

2:30 - 3:00 PM

Determining the elastic properties of single grains in the ultrafine-grained W-Cr composite

Speaker
Andrzej Piotr Kądziaława

2:30 - 3:00 PM

Crystallization of amorphous metals through molecular dynamics simulations

Speaker
Prashant Dwivedi

2:30 - 3:00 PM

Segregation of oxygen impurities in transition metal nitride superlattices

Speaker
Miroslav Černý

2:30 - 3:00 PM

Theoretical study of sublimation, local disorder and strain energies of crystalline caged hydrocarbons

Speaker
Petr Touš

3:00 PM