

5th Users' Conference of IT4Innovations

Tuesday, 9 November 2021

Poster session: I - Online (14:00 - 14:30)

time	[id] title	presenter
14:00	[91] Performance of k-Wave Toolbox on Multi-GPU Accelerated Clusters	VAVERKA, Filip JAROS, Jiri
14:00	[94] Preventing Deadlock in Non-uniform-timestep Distributed Pseudospectral Method	KADLUBIAK, Kristián
14:00	[93] Enhancement of ultrashort directional X-ray pulses	MASLAROVA, Dominika
14:00	[88] High-order magneto-hydrodynamic code with spontaneous magnetic fields generation	NIKL, Jan
14:00	[87] Inversion of the satellite-observed tidal magnetic fields in terms of three-dimensional upper-mantle electrical conductivity	Dr ŠACHL, Libor
14:00	[85] Exploring the complete conformational space of all 400 dipeptides by quantum chemical methods: Can we predict the protein structure "ab initio"?	KALVODA, Tadeas
14:00	[84] Towards Solvent Interactions in Modelling Infrared Spectra of Rhenium(I) Complex	MELČÁK, Martin
14:00	[83] k-Dispatch's Performance Modules for Advanced Workflow Submission	JAROS, Marta
14:00	[82] Handling C++ Exceptions in MPI Applications	JAROS, Jiri
14:00	[81] Hydrogen effect on the strength of the Fe ₃ Al alloy	Dr ŠESTÁK, Petr
14:00	[106] HyperQueue: Simplifying Usage of PBS/SLURM Clusters	BERÁNEK, Jakub
14:00	[67] PeptideCS: An extensive dataset mapping the potential energy surface of mono- and dipeptides	ANDRIS, Erik

Poster session: II - Online (14:30 - 15:00)

time	[id] title	presenter
14:30	[71] Reactive Molecular Dynamics Study on the Tribological Properties of Selected Vanadium Oxides	Dr DAŠIĆ, Miljan
14:30	[68] Segregation of oxygen impurities in transition metal nitride superlattices	ČERNÝ, Miroslav
14:30	[72] Crystallization of amorphous metals through molecular dynamics simulations	DWIVEDI, Prashant
14:30	[69] Determining the elastic properties of single grains in the ultrafine-grained W-Cr composite	KĄDZIELAWA, Andrzej Piotr
14:30	[73] Advances in the Evolutionary Design of Complex Cellular Automata	BIDLO, Michal
14:30	[70] Reactive Force Field for Molybdenum Disulfide Crystallization	PONOMAREV, Ilia
14:30	[76] Theoretical study of sublimation, local disorder and strain energies of crystalline caged hydrocarbons	TOUŠ, Petr
14:30	[77] ATLAS job submission systems for the IT4Innovation	Dr SVATOS, Michal

14:30	[101] Enhancement of Ion Acceleration by Laser-Pulse Shaping via Plasma Shutter	MATYS, Martin
14:30	[96] Calculation of NMR spin-spin couplings for intrinsically disordered proteins: a prospective tool to facilitate experimental NMR studies	GAFFOUR, Amina Mr KRISHNENDU, Bera
14:30	[95] HPC solver of Ising model: application in Material Design	DUJOVIĆ, Aleksandra
14:30	[100] Peptide Elongation in Carbon Nanotubes: An Atomistic Approach	CASTRO NEPOMUCENO, Felipe