

# 9<sup>th</sup> Users' Conference of IT4Innovations

30 – 31 October 2025

10:00 – 11:00 | Registration and networking

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

11:30 – 12:00 | Keynote I

*Chairperson: Martin Friák*

Machine-learning Optimization of Laser-driven Electron Accelerators  
[Petr Valenta](#) | [Extreme Light Infrastructure ERIC / ELI Beamlines Facility](#)

12:00 – 13:00 | Users' Talks I

Numerical Simulations at Karolina for Advancing Laser Plasma Research at Extreme Light Infrastructure - Nuclear Physics  
[Vojtěch Horný](#) | [Extreme Light Infrastructure](#) / [Nuclear Physics](#)

HPC-Accelerated Deep Learning Pipeline for Microhologram Dot Pattern Verification in Secure ID Document Authentication  
[Petra Svobodová](#) | [IT4Innovations](#)

Electronic Band Structure Calculations of Crystals on Noisy Quantum Simulators  
[Vojtěch Vašina](#) | [Institute of Physics of Materials of the CAS](#)

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

14:00 – 15:00 | Users' Talks II

*Chairperson: Branislav Janský*

Supercomputers and Synchrotrons: A New Era of Scientific Discovery  
[Štěpán Sklenák](#) | [J. Heyrovsky Institute of Physical Chemistry of the CAS](#)

Microstructural Analysis of Aluminide Coatings using Deep Learning-Driven Image Segmentation  
[Khyati Sethia](#) | [IT4Innovations](#)

Thermoelectric Effects of Structural Defects in Scandium Nitride Nanostructures  
[Luigi Cigarini](#) | [IT4Innovations](#)

15:00 – 15:20 | Accessing EuroHPC Systems | [Tomáš Karásek](#) | [IT4Innovations](#)

15:20 – 15:40 | Support from the High-Level Support Team (HLST) | [João Barbosa](#) | [IT4Innovations](#)

16:40 – 16:00 | Coffee Break

16:00 – 16:50 | Users' Council

16:50 – 17:20 | Keynote II

*Chairperson: Dominik Legut*

Model Complexity in All-Atom Plasma Membrane Simulations  
[Petra Čechová](#) | [CATRIN, Palacký University Olomouc](#)

17:20 – 18:20 | Users' Talks III

Translocation of Short Peptides through Carbon Nanotubes  
[Michal H. Kolář](#) | [University of Chemistry and Technology, Prague](#)

Atomic-Scale Insights into Graphene-Based Nanomaterials Interacting with Brain Cell Membranes  
[Andrea Nedělníková](#) | [CATRIN, Palacký University Olomouc](#)

Lipid Nanoparticles in Coarse-grained Resolution: From Internal Organization to Interaction with Cells  
[Markéta Paloncýová](#) | [CATRIN, Palacký University Olomouc](#)

18:20 - 21:00 | Conference Dinner & Poster Session

# 9<sup>th</sup> Users' Conference of IT4Innovations

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Friday, 31 October 2025

**09:00 – 09:30 | Keynote III**

Bridging Cosmological Simulations and High-Quality Visualizations using HPC resources  
[Petr Strakoš](#) | [IT4Innovations](#)

*Chairperson: Tomáš Kozubek*

**09:30 – 10:10 | Users' Talks IV**

CrSBr-MoS<sub>2</sub> Heterostructures and the Limits of VASP Parallelization  
[Athanasios Koliogiorgos](#) | [Charles University](#)

Nanowear in Molybdenum Disulfide Studied by Molecular Dynamics Simulations  
[Paolo Nicolini](#) | [Institute of Physics of the CAS](#)

**10:10 – 10:35 | Coffee Break**

**10:35 – 11:15 | Users' Talks V**

Antiferromagnetic Exchange Coupling across Transition Metal Films with Magnetic Elements  
[Dominik Legut](#) | [IT4Innovations](#)

Fine-tuning Stability of La-Ni-Sn-H Materials for Hydrogen Storage  
[Martin Friák](#) | [Institute of Physics of Materials of the CAS](#)

*Chairperson: Tomáš Kozubek*

**11:15 – 12:00 | From Supercomputing to Quantum Computing: Introduction of VLQ**

**12:00 – 13:00 | Lunch**