

ANNOUNCEMENT

Workshop on molecular dynamics with LAMMPS

The Institute of Physical Engineering at Faculty of Mechanical Engineering, Brno University of Technology together with Nanomechanical Lab at Department of Structural Engineering, Norwegian University of Science and Technology organize a workshop on molecular dynamics simulations. The workshop will provide a basic introduction to molecular dynamics simulations and LAMMPS Molecular Dynamics Simulator (<https://www.lammps.org>).

where: Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2
when: 2 - 4. 8. 2022
level: beginners
fee: the attendance is free of charge
registration: send a registration e-mail to sestak@fme.vutbr.cz
capacity: 20 - 25 participants

Preliminary time schedule and topics

Tuesday (2.8.)	<i>Introduction to MD and Lammps.</i>	<i>Hands-on section using LAMMPS.</i>
time schedule	9:30 - 11:30	time for lunch
		13:00 - 16:00
Wednesday (3.8.)	<i>Introduction to MD force fields.</i>	<i>Hand-on section using LAMMPS.</i>
time schedule	9:30 - 11:30	time for lunch
		13:00 - 16:00
Thursday (4.8.)	<i>Introduction to MLFF – how to obtain reliable inter-atomic potentials via machine learning.</i>	<i>Hand-on section using VASP.</i>
time schedule	9:30 - 11:30	time for lunch
		13:00 - 16:00

Note:

For hands-on sessions it is necessary to bring your own laptop with an SSH client (Putty, MobaXterm, etc.) installed. We can help you with the installation during the workshop if necessary.

The hand-on sections will include example:

1. calculation of cohesive energy
2. polymer extension under tensile force
3. mechanical properties of nickel (with single grain-boundary, with polycrystalline structure)
4. characteristics of grain boundaries determined via machine learned force fields (VASP)

Further details about the workshop (exact location or other important information) will be sent to registered participants before the workshop.

The workshop is organized as a part of the EHP project no. EHP-CZ-ICP-3-012 that is focused on strengthening institutional cooperation between Czech and Norwegian universities and it helps to improve knowledge in atomistic simulations at both institutions.