Iceland Liechtenstein Norway grants

Workshop on molecular dynamics with LAMMPS

with the title „Atomistic modelling and molecular dynamics simulations in nanomechanics”

Dear participants,
as the workshops is approaching, we are sending you some information about its organization.

The workshop will be held at the Faculty of Mechanical Engineering, Brno University of Technology at address **Technická 2896/2, Brno, room: U8** (the first level of building A5).
Please see the details at the faculty map below.
https://www.fme.vutbr.cz/en/fakulta/planek/A5/1

The lecture room will be open since 9:00 and the lectures start at 9:30.
A small refreshment will be available during coffee breaks.
The internet access will be available via WiFi network.

Please find some information regarding the lectures below.

Tuesday and Wednesday - lectures and hands on sessions devoted to the LAMMPS code.
Examples used in these lectures represent sufficiently simple systems that can be calculated using a standard PC or laptop.
Therefore, there are two ways how to perform the calculations:
1. Run simulations on our local cluster Mark where the LAMMPS code has been already installed.
(If anybody doesn't have access to Mark cluster and plan to use it, then please let me know in advance. I will create an account for you.)
2. Install the LAMMPS code in your own laptop and run the calculations there.
(You can download it at the following link https://rpm.lammps.org/windows/64bit/. The examples have been tested with the following executable: 2022-06-24 08:19 LAMMPS-64bit-latest.exe).
It is also recommended to install **Ovito** and **Vesta** visualization software and Putty or MobaXterm as SSH client (if you plan to use the cluster Mark).

Thursday - Introduction to Machine-Learned Force Fields.
The examples will be calculated using the new version of the VASP code (6.3) at our cluster Mark.
This lecture requires a ssh client for the SSH connection:

- **MobaXterm**: https://mobaxterm.mobatek.net/ or Putty: https://www.putty.org/),
- **Vesta**: https://jp-minerals.org/vesta/en/
- **Ovito**: https://www.ovito.org/

Please do not hesitate to contact me in case of any additional questions regarding the workshop at my e-mail: sestak@fme.vutbr.cz.

Have a nice weekend and I am looking forward to see all of you on Tuesday morning.

With regards,
Petr Šesták
workshop organizer

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.