

WORKSHOP ANNOUNCEMENT

Grace Workshop – Atomistic Simulations with GRACE, LAMMPS and Modern Tools for Potential Validation

The **Institute of Physical Engineering** at the Faculty of Mechanical Engineering, Brno University of Technology, in cooperation with **ICAMS**, Ruhr University Bochum, Germany, is organizing a two-day workshop focused on modern approaches to interatomic potentials and atomistic simulations, with an emphasis on the **GRACE framework***.

The workshop will provide an introduction to the generation and validation of machine-learned interatomic potentials (GRACE), including practical sessions with Grace, AMS Tools, and LAMMPS.

Where:

Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2, Brno

When:

April 8–9, 2026

Fee:

attendance is free of charge

Registration:

send a registration e-mail to sestak@fme.vutbr.cz

Capacity:

max. 15 participants

Workshop organizer:

Dr. Petr Šesták (BUT)

GRACE introduction by:

Dr. Matouš Mrovec** (ICAMS)

Wednesday (April 8)

Introduction to GRACE and ACE potentials - differences between both approaches

Hands-on session (GRACE): preparation of training datasets, data handling and preprocessing, fitting of interatomic potentials

Time: **9:30 – 12:00**, lunch break, **13:30 – 16:30**

Thursday (April 9)

Validation and applications of interatomic potentials

Hands-on session (AMS & LAMMPS): validation workflows, LAMMPS simulations with GRACE/ACE potentials, extrapolation grade, and reliability assessment

Time: **9:30 – 12:00**, lunch break, **13:30 – 16:30**

Note

For the hands-on sessions, participants are required to bring their own laptop with an **SSH client** installed.

Assistance with setup can be provided during the workshop if needed.

The examples will be run on the local HPC cluster.

Useful links:

*<https://gracemaker.readthedocs.io/en/latest/>

**<https://www.icams.de/institute/icams/members/members-detail/?detail=1446>