Supercomputer “Lomonosov”
LAMMPS
Practical seminar

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Plan

Part 1

1. Soft
2. Remote connection to “Lomonosov”
3. Few words about commands
4. Compilation, MPI implementations, running a job, queues …

Part 2

1. LAMMPS folder, manual, tools
2. Compiling of libraries
3. Compiling of LAMMPS
4. LAMMPS files
5. Making an input script
6. Example problems

Soft

To access the SC:

- Putty
- WinSCP

To check results obtained by LAMMPS:

- VMD (or other visualization program)
- “drawing” program (MATLAB, Origin etc.)

Linux commands

Basic commands:

- cd – change directory
- pwd – current position
- mc – midnight commander
- man - manual

Slurm commands:

- **mpienv**
- **sinfo**
- sbatch
- squeue
- srun

Compilation

- mpif90 (mpiifort)
- mpicxx (mpiicc)
- make

LAMMPS

- LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain.
- There is a version for Windows (both parallel and serial)

LAMMPS script

- **ensemble/system (simulation cell)**
- **potentials: potential energy and forces**(rules for atoms to move)
- **constrains: rules for ensemble to move, integration information**
- **statistics:** collect trajectories(post-processing data)
- technical commands

Simulation cell

- Read_data
- Read_restart
- Create_box (create_atoms etc.)

Interatomic potential

Pair_style
Bond_style
Angle_style
…

Constrains: rules for ensemble to move, integration information

- Fix command

Statistics and output

- compute command
- dump command
- write_restart command
- …