Project LAMMPS-Freeride

Large-scale simulations of semi-crystalline polymers

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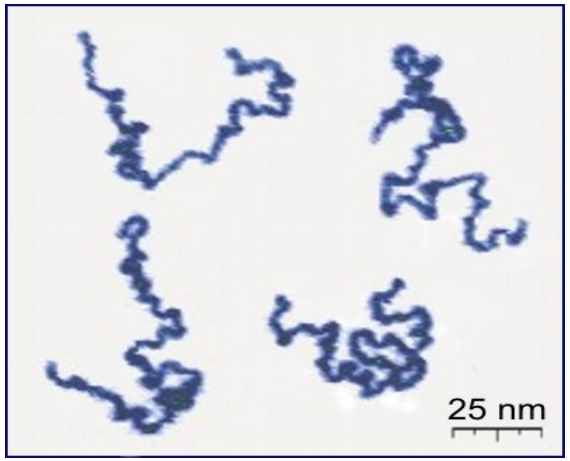
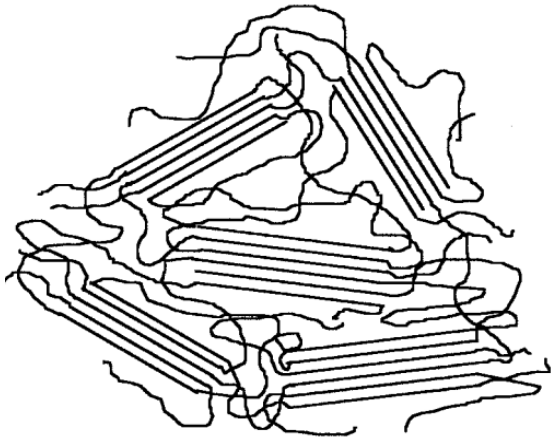
Slot time: 05/04-08/04

Semi-crystalline polymers



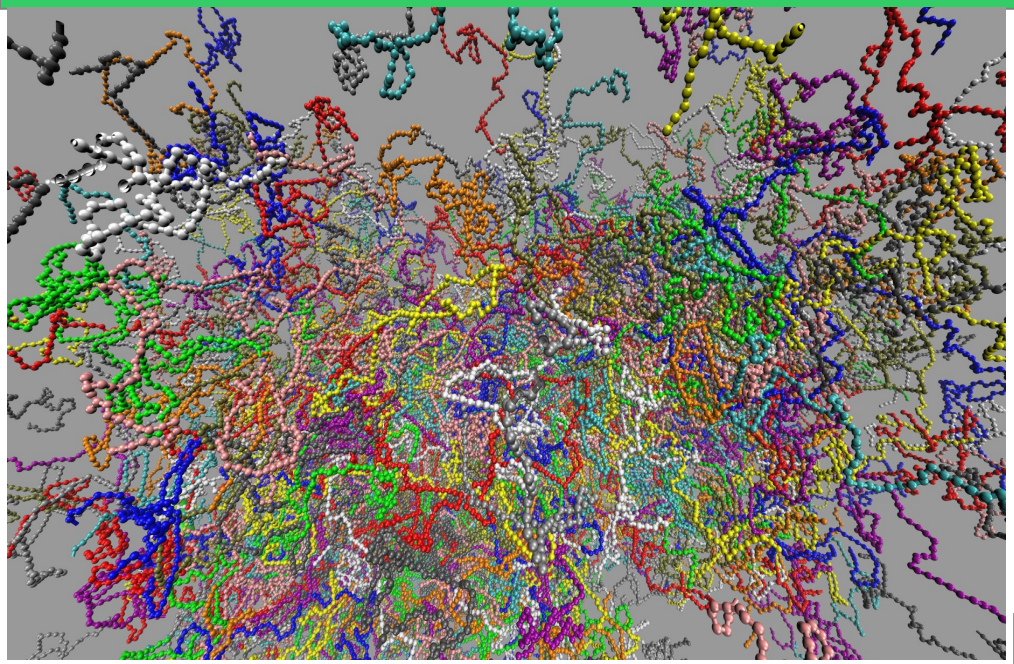
Cooling



Intriguing mechanical properties

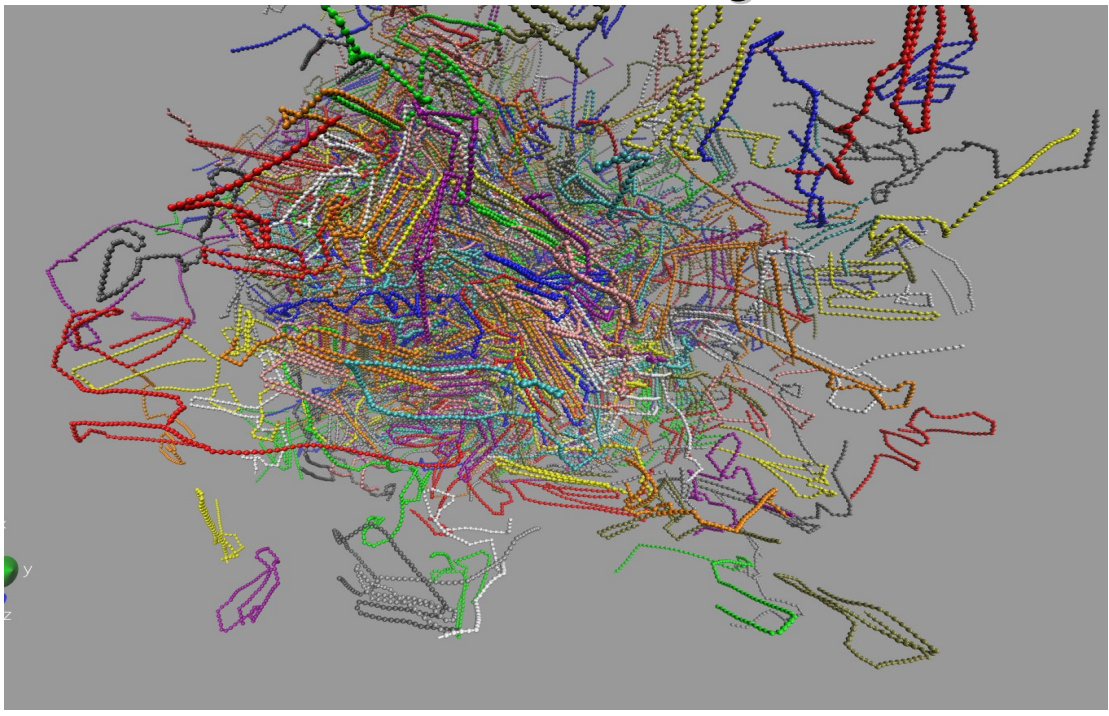
Number of monomers $10^5 - 10^6$ → Parallel Computing LAMMPS

Simulation results



Before Cooling

After Cooling



Large-scale simulations: LAMMPS

LAMMPS: **L**arge-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator (http://lammps.sandia.gov/)

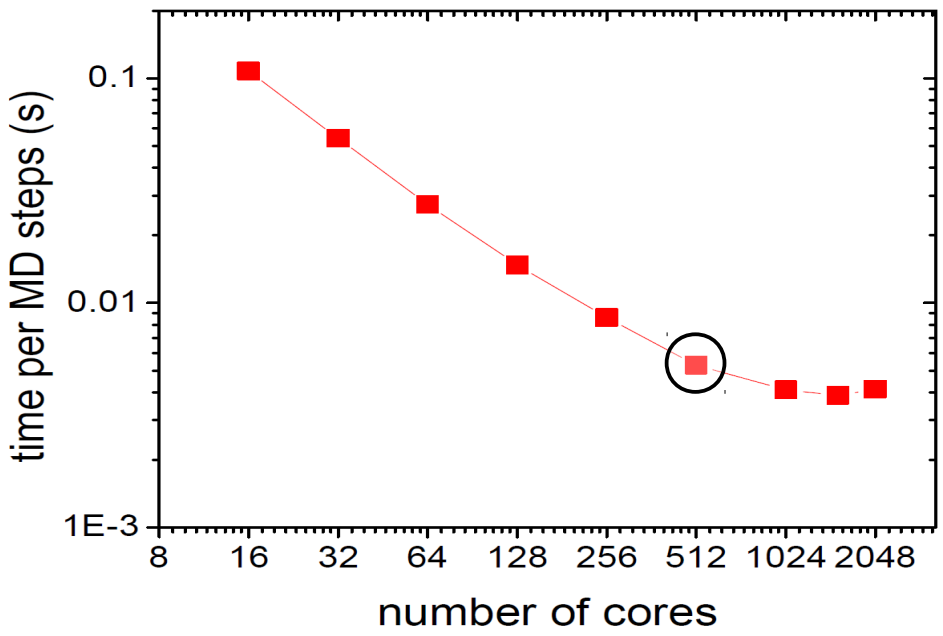
Applications: soft materials (biomolecules, polymers) and solid-state materials (metals, semiconductors)

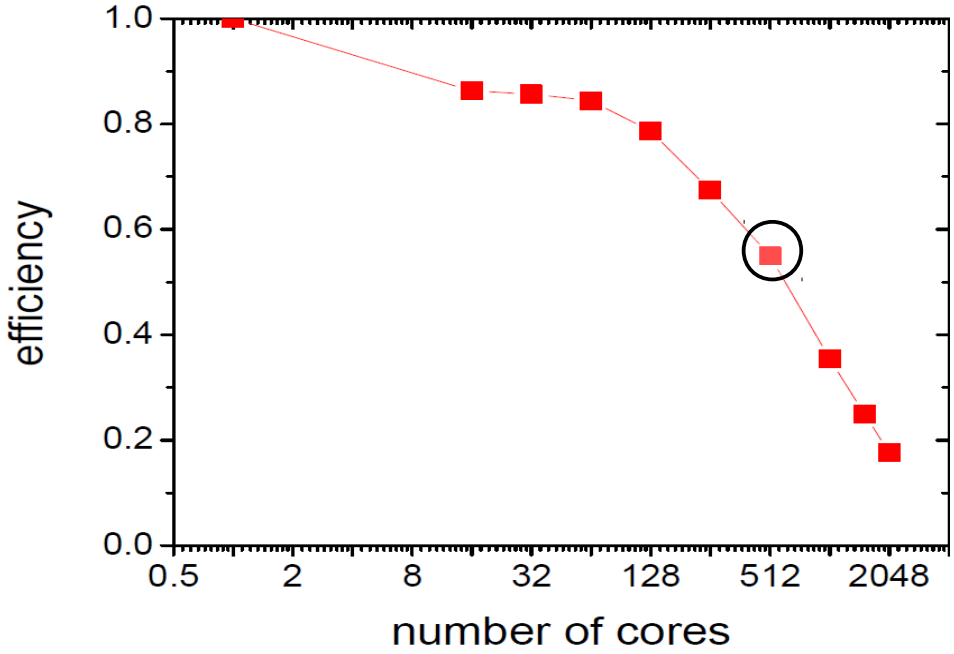
Advantages:

- Open source
- Parallel computing using MPI and spatial-decomposition of the simulation domain.

Big system 1 million particles
requires
Large number of processors

Performance of froggy cluster





MD simulations:

- **1.1 millions particles**
- run for 50000 timestep
- **677.56 Mb** used in total

$$\text{efficiency} = \frac{t_1}{\text{ncpu} * t_{\text{ncpu}}}$$

Optimum number of particles per CPU 2250 roughly
512 cores

Two simulations: Cooling experiments 1.15 M and 4.3 M

Simulation results