Rimei Chen
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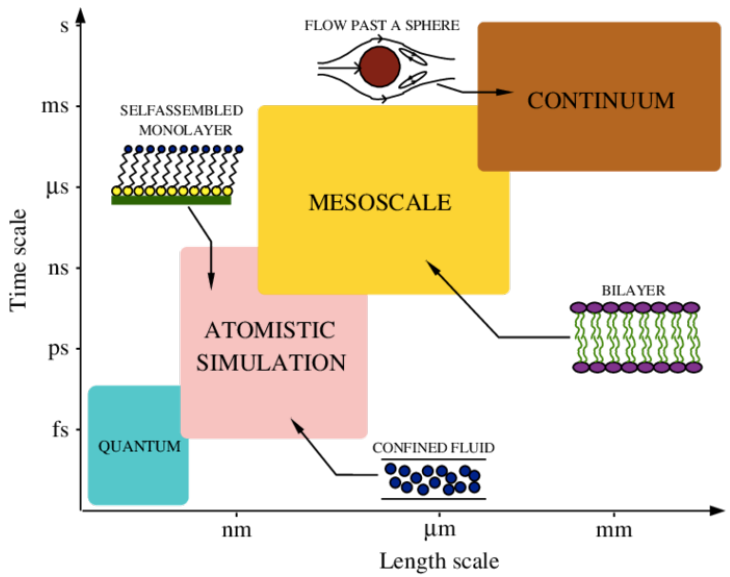
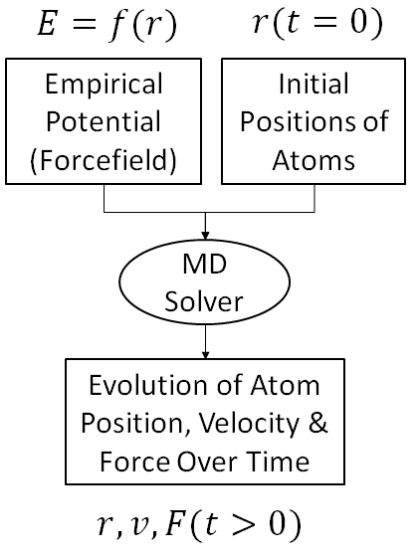
- Reactive molecular dynamics simulations of MoS_2 crystallization

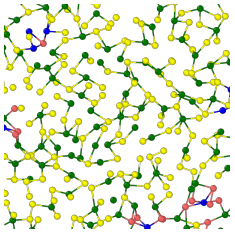




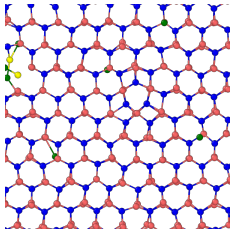
Molecular dynamics simulation: ns and nm

MD: solving Newton's equations of motion

Non-crystalline Mo
Non-crystalline S
Crystalline Mo
Crystalline S



Heat/shear



LAMMPS

Large-scale Atomic/Molecular Massively Parallel Simulator

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- Computational challenges
  1. Computational resource
  2. Computational preformation
     - Compiler
     - GPU

https://github.com/ucmerced/merced-cluster

Accelerator packages

GPU Package	for NVIDIA GPUs as well as OpenCL support
USER-INTEL Package	for Intel CPUs and Intel Xeon Phi
KOKKOS Package	for NVIDIA GPUs, Intel Xeon Phi, and OpenMP threading
USER-OMP Package	for OpenMP threading and generic CPU optimizations
OPT Package	generic CPU optimizations

Inverting this list, LAMMPS currently has acceleration support for three kinds of hardware, via the listed

Many-core CPUs	USER-INTEL, KOKKOS, USER-OMP, OPT packages
NVIDIA GPUs	GPU, KOKKOS packages
Intel Phi	USER-INTEL, KOKKOS packages