# Whirlwind tour of more advanced topics

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# Goals for this lecture

Tell you about ...

- Additional features and options in LAMMPS
- Where to go for more information about them

- Whirlwind fashion, one slide (or bullet!) per feature
- Not enough time to cover all the details
- But you can look into topics that interest you later

# Useful input script commands

Each of these is a command with its own doc page

General:

- info = print info about this LAMMPS executable
- include = insert commands from another script
- if = conditional, including elif and else options
- print = print message to the screen, can contain variables
- quit = force LAMMPS to exit

Used for looping:

- label = flag a position in the input script
- next = increment one or more variables
- jump = jump to a label

# Input script variable command

See variable command doc page

Lots of uses:

- One-time definition of values used in many places
  - also settable from command-line that invokes LAMMPS
- Many variable styles:
  - store strings or numbers or formulas
  - produce scalar or vector or per-atom values
- Formulas are C-like
  - use math functions, boolean logic, groups, regions, etc
  - use scalar or per-atom inputs
  - use output from computes, fixes, other variables
  - can be time-dependent or spatially-dependent
- Many LAMMPS commands allow variables as inputs
  - command invokes variable internally
  - example: define a time- or spatially-dependent E-field

# Input script action commands

Each of these is a command with its own doc page

Action = perform a simulation

- run = dynamics simulation (molecular dynamics)
- minimize = energy minimization (molecular statics)
- rerun = zero-step runs on snapshots from a dump file

Multi-replica simulations:

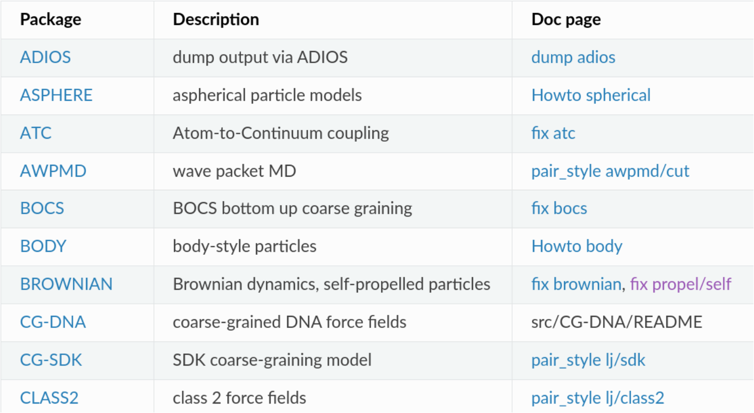
- temper = parallel tempering
- neb = nudged-elastic band for barrier heights
- prd = parallel replica dynamics
- tad = temperature-accelerated dynamics
- hyper = global or local hyperdynamics

# Three more input script features

- Run multiple simulations from one script
    - run N simulations on P procs split into M partitions
    - see Section 8.1.3 of User Guide
- Shell command to invoke an external program with args
    - example: shell cd subdir1
    - example: shell my_analyze.exe out.file $n ${param}
    - see shell command doc page
- Invoke Python functions from your script:
    - pass arguments to the function
    - return value(s) in variables
    - the Python function can access internal LAMMPS data
    - Python code can be embedded in script or in another file
    - see Section 2 in Programmer Guide

# LAMMPS packages

- Package = one or more style files with common theme
- Currently ∼90 package folders within src dir
- At compile time, optionally include individual packages or not
- See Section 6.1 of User Guide for one-liners, click for more



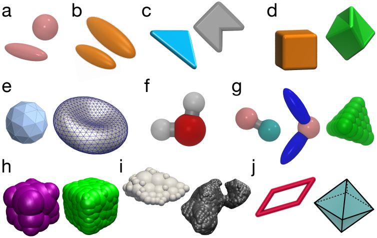
| Package | Description | Doc page |
|---|---|---|
| ADIOS | dump output via ADIOS | dump adios |
| ASPHERE | aspherical particle models | Howto spherical |
| ATC | Atom-to-Continuum coupling | fix atc |
| AWPMD | wave packet MD | pair_style awpmd/cut |
| BOCS | BOCS bottom up coarse graining | fix bocs |
| BODY | body-style particles | Howto body |
| BROWNIAN | Brownian dynamics, self-propelled particles | fix brownian, fix propel/self |
| CG-DNA | coarse-grained DNA force fields | src/CG-DNA/README |
| CG-SDK | SDK coarse-graining model | pair_style lj/sdk |
| CLASS2 | class 2 force fields | pair_style lj/class2 |

# Coarse grained and meso/continuum scale models

Motivation: increase accessible length and time scales

Some packages overlap these 3 categories

- Packages for coarse-grained (CG) models:
  - Bio systems: CG-DNA, CG-SDK
  - DPD variants: DPD-BASIC, DPD-MESO, DPD-REACT, DPD-SMOOTH
  - Surfaces: MANIFOLD
  - Multi-scaling CG: MSCG



- Packages for mesoscale models:
  - Aspherical particles: ASPHERE, BODY
  - Large particles: COLLOID
  - Rigid bodies: POEMS, RIGID
  - Solvent models: FLD, LATBOLTZ, SRD
  - Nanotubes: MESONT
- Packages for continum-scale models
  - ATC = couple to finite elements
  - GRANULAR = granular systems
  - PERI = meshless continuum model for fracture
  - SPH, MACHDYN = smoothed particle hydro for liquids & solids

# Examples of packages with unusual functionality

May not normally think of these in the context of MD

| | |
|---|---|
| ATC | Atom to continuum coupling via finite elements |
| DIFFRACTION | x-ray and electron diffraction intensities |
| LATBOLTZ | Lattice-Boltzman model |
| MC | Monte Carlo methods |
| MDI | Code coupling, e.g. for AIMD or QM/MM |
| ML-* | Variety of machine-learned potentials |
| PERI | Meshless continuum Peridynamics model |
| REACTION | Heuristic chemical reactions |
| RIGID | Rigid-body constraints |
| SPH | Smoothed particle hydrodynamics model |
| SPIN | Magnetic atomic spin dynamics |
| VORONOI | Voronoi tesselations around atoms/particles |

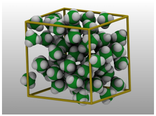
# Pre-processing tools to build complex molecular systems

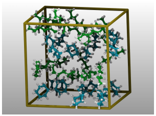
LAMMPS does not build molecular systems or
auto-magically assign force field parameters for you

- Data file must list bonds/angles/etc and FF params
- Converter programs:
    - ch2lmp = CHARMM converter
    - amber2lmp = AMBER converter
    - msi2lmp = Accelrys converter
    - see Section 10 of User Guide and lammps/tools dir
- 3rd-party builders which can create LAMMPS input
    - See website Pre/Post processing for free & commercial
    - VMD TopoTools, Moltemplate
    - Avogadro, Packmol, ATB (Auto Topology Builder)
    - Enhanced Monte Carlo – see breakout: Fri

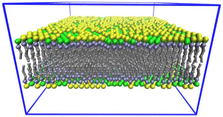
# Example systems created by builder tools

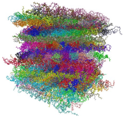
VMD TopoTools:

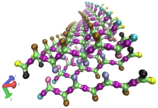




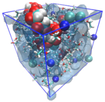
Moltemplate:



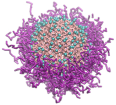




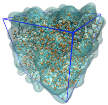
EMC:



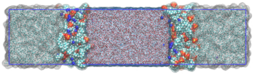
bulk



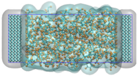
graft



copolymer



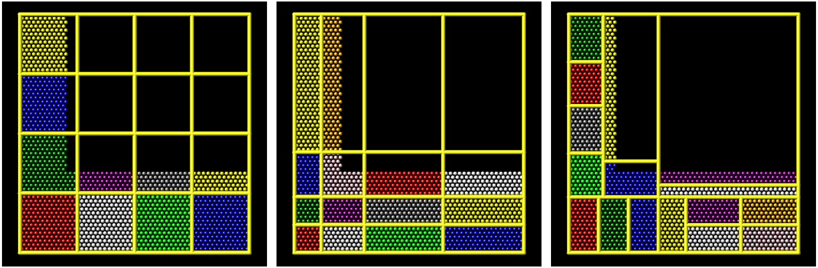
multiphase



surface

# Load balancing

- Can be especially useful for coarse-grained systems
- Use balance command for static balancing
- Use fix balance command for dynamic balancing



(A) Imbalanced (B) Adjust proc dividers (C) Recursive bisectioning

- Can balance by particle count, weighted particles, or CPU time

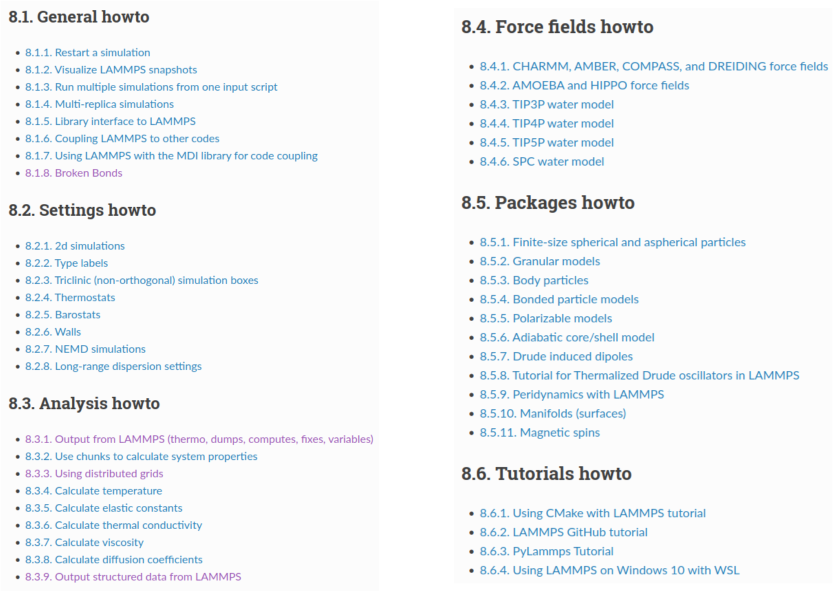
# Energy minimization

See minimize and min_style doc pages

- Via gradient-based minimization
  - min_style cg, hftn, sd
  - can include bond-length constraints, e.g. SHAKE
- Via damped-dynamics minimization
  - min_style quickmin and fire
  - also used for nudged-elastic band (NEB) calculations

- Possible to just un-overlap via usual dynamics
  - pair_style soft command
  - fix nve/limit and fix viscous commands

# 45 entries in Howto section 8 of User Guide



## 8.1. General howto

- 8.1.1. Restart a simulation
- 8.1.2. Visualize LAMMPS snapshots
- 8.1.3. Run multiple simulations from one input script
- 8.1.4. Multi-replica simulations
- 8.1.5. Library interface to LAMMPS
- 8.1.6. Coupling LAMMPS to other codes
- 8.1.7. Using LAMMPS with the MDI library for code coupling
- 8.1.8. Broken Bonds

## 8.2. Settings howto

- 8.2.1. 2d simulations
- 8.2.2. Type labels
- 8.2.3. Triclinic (non-orthogonal) simulation boxes
- 8.2.4. Thermostats
- 8.2.5. Barostats
- 8.2.6. Walls
- 8.2.7. NEMD simulations
- 8.2.8. Long-range dispersion settings

## 8.3. Analysis howto

- 8.3.1. Output from LAMMPS (thermo, dumps, computes, fixes, variables)
- 8.3.2. Use chunks to calculate system properties
- 8.3.3. Using distributed grids
- 8.3.4. Calculate temperature
- 8.3.5. Calculate elastic constants
- 8.3.6. Calculate thermal conductivity
- 8.3.7. Calculate viscosity
- 8.3.8. Calculate diffusion coefficients
- 8.3.9. Output structured data from LAMMPS

## 8.4. Force fields howto

- 8.4.1. CHARMM, AMBER, COMPASS, and DREIDING force fields
- 8.4.2. AMOEBA and HIPPO force fields
- 8.4.3. TIP3P water model
- 8.4.4. TIP4P water model
- 8.4.5. TIP5P water model
- 8.4.6. SPC water model

## 8.5. Packages howto

- 8.5.1. Finite-size spherical and aspherical particles
- 8.5.2. Granular models
- 8.5.3. Body particles
- 8.5.4. Bonded particle models
- 8.5.5. Polarizable models
- 8.5.6. Adiabatic core/shell model
- 8.5.7. Drude induced dipoles
- 8.5.8. Tutorial for Thermalized Drude oscillators in LAMMPS
- 8.5.9. Peridynamics with LAMMPS
- 8.5.10. Manifolds (surfaces)
- 8.5.11. Magnetic spins

## 8.6. Tutorials howto

- 8.6.1. Using CMake with LAMMPS tutorial
- 8.6.2. LAMMPS GitHub tutorial
- 8.6.3. PyLammps Tutorial
- 8.6.4. Using LAMMPS on Windows 10 with WSL