Lecture #6
Whirlwind tour of more advanced topics

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7th LAMMPS Workshop Tutorial
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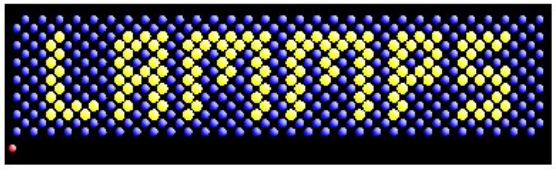

Center for Computing Research

Sandia National Laboratories

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National Nuclear Security Administration

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

Input script internal 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.html doc page

Lots of uses:

- One-time definition of values used in many places
  - or settable from command-line that invokes LAMMPS
- Many variable styles:
  - store strings or numbers or formulas, read from file
  - 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 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
- prd = parallel replica dynamics
- tad = temperature-accelerated dynamics
- neb = nudged-elastic band for barrier heights

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
  - shell cd subdir1
  - shell my_analyze out.file $n ${param}
  - see shell.html doc page
- Invoke Python functions from your script:
  - pass arguments to the function
  - return value(s) in variables
  - Python function can access LAMMPS data
  - Python code can be embedded in script or in another file
  - Richard Berger talk: Fri developers session
  - see Section 2 in Programmer Guide

LAMMPS packages

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- See Section 6.1 of User Guide for descriptions

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

Acceleration packages for CPUs and GPUs

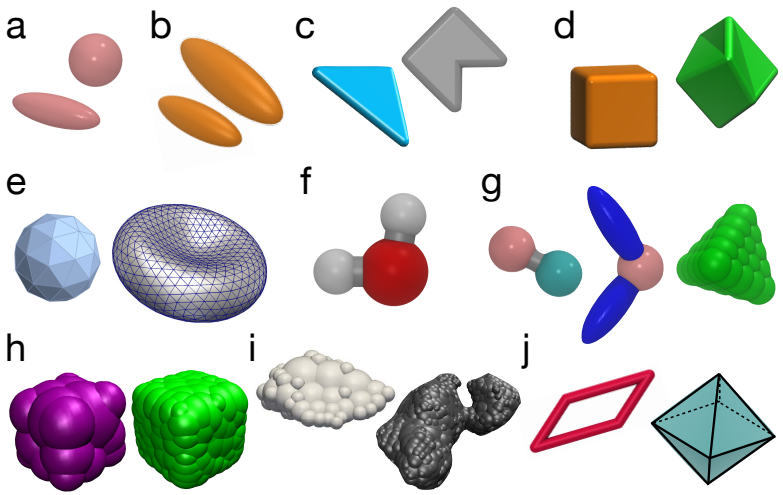
Each package has style variants optimized for specific hardware
See Section 7.4 of User Guide for details

- Four packages
  - GPU for GPUs
  - INTEL for Intel CPUs (and others)
  - KOKKOS for GPUs
  - OPENMP for OpenMP on multicore CPUs
  - Stan Moore talk: Wed late session on Kokkos
- GPU & KOKKOS now support NVIDIA, AMD, Intel GPUs
- Pair, bond/angle/etc, fix, compute, pppm styles
- Example: pair lj/cut $\Rightarrow$
  lj/cut/gpu, lj/cut/intel, lj/cut/kk, lj/cut/omp
- Invoke from command-line w/out changing input script

Coarse grained and meso/continuum scale models

Motivation: increase accessible length and time scales
See Section 6.1 of User Guide for package details
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 continnum-scale models
  - ATC = couple to finite elements
  - GRANULAR = granular systems
  - PERI = meshless continuum model for fracture
  - SPH, MACHDYN = smoothed particle hydro for liquids & solids



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- Data file must list bonds/angles/etc and FF params
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  - ch2lmp = CHARMM converter
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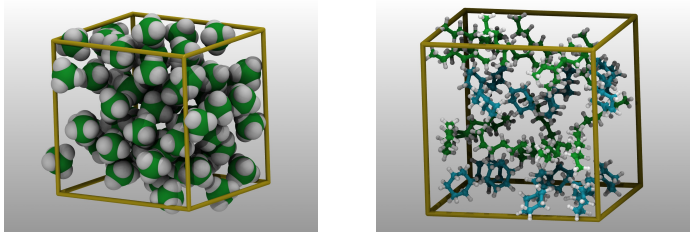
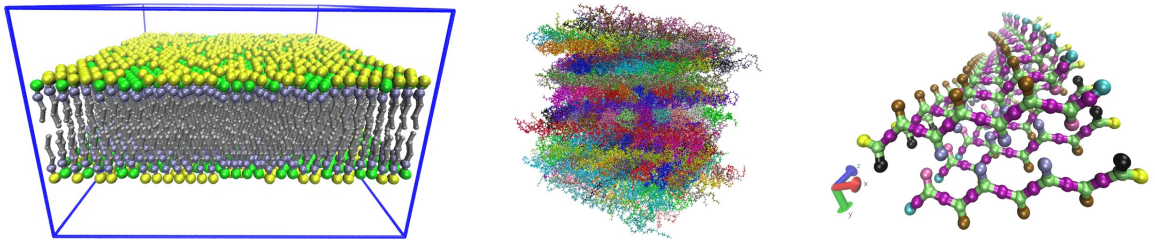
- 3rd-party builders which can create LAMMPS input
  - See website Pre/Post processing for free & commercial
  - VMD TopoTools, Moltemplate
  - Avogadro, Packmol, ATB (Auto Topology Builder)
  - Enhanced Monte Carlo, see breakout: Fri

Example systems created by builder tools

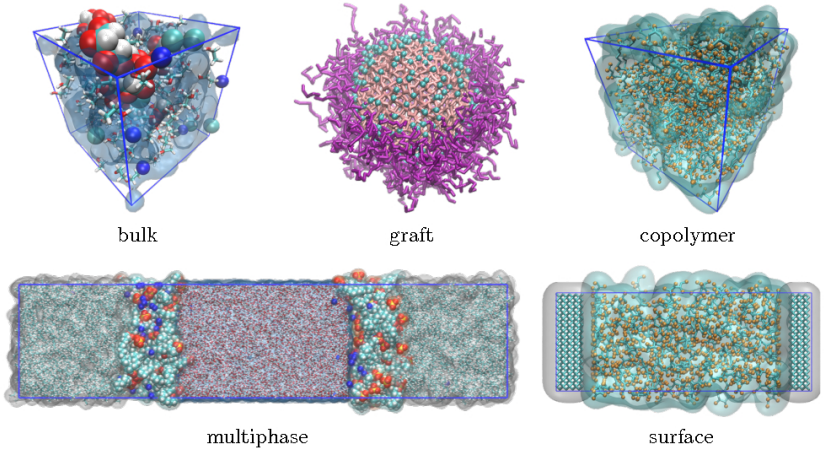
VMD TopoTools:



Moltemplate:



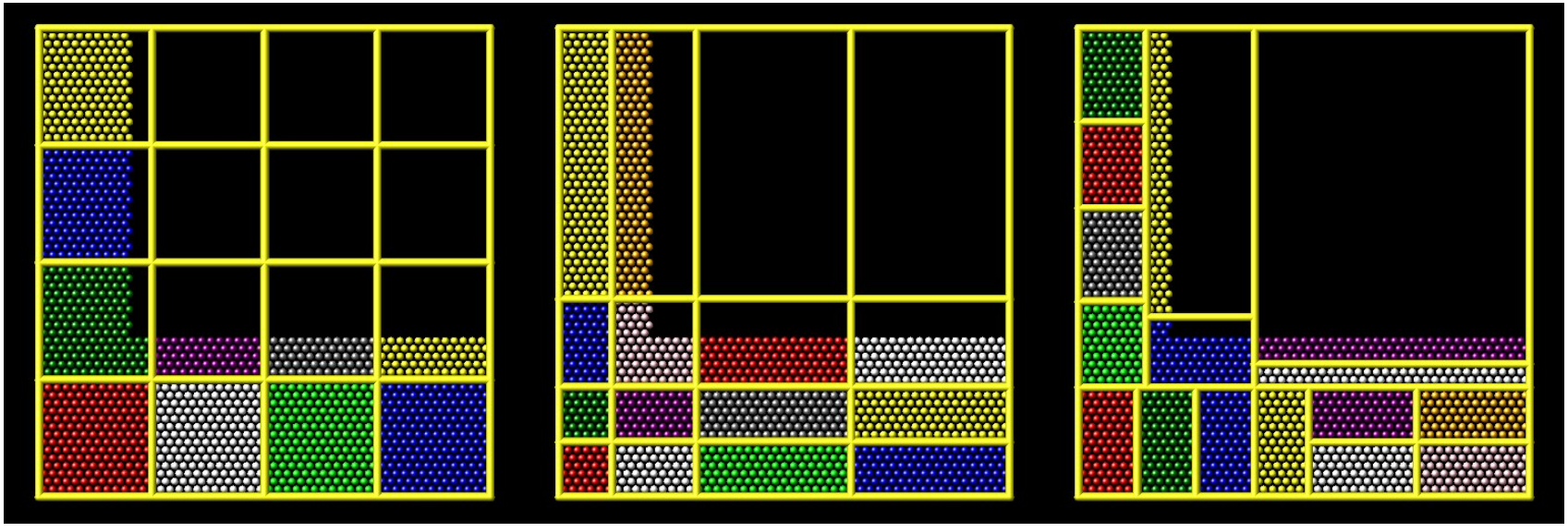
EMC:



Load balancing

- Use balance command for static balancing
- Use fix balance command for dynamic balancing

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



- 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, htfn, sd
- Via damped-dynamics minimization
  - min_style quickmin and fire
  - used for nudged-elastic band (NEB)

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

Final potpourri

- Units
  - see units.html doc page
  - currently 8 choices for unit systems
  - examples: lj, real, metal, cgs, si
  - all simulation input & output in one system
  - enables paticle-based models at any length scale
- Thermostats and barostats
  - see Section 8.2.3 and Section 8.2.4
  - one or more thermostats (by group)
  - single barostat for entire system
- Increase timestep size
  - fix shake command for rigid bonds (2 fs)
  - run_style respa command for hierarchical timesteps (4 fs)
  - hyper command for rare-event systems (10-1000x)