Building a reusable LAMMPS script library

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overview

Motivation

Evolving simulation strategies

Implementation details

Examples

Closing
motivation

Something done once will likely need doing again... after I’ve forgotten how to do it.
motivation

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Research workflow:

- Question ➔ Plan ➔ Develop ➔ Test ➔ Execute ➔ Answer
  - simulation
  - debug
  - revise
  - propose

Goal: loop more efficiently
  - code re-use
  - friendly documentation
simulation strategy v0.1

Model: one script per job

▶ create new script when needed
▶ copy and tweak existing scripts when possible
simulation strategy v0.1

Model: one script per job
  ▶ create new script when needed
  ▶ copy and tweak existing scripts when possible

Pros:
  ▶ easiest implementation
  ▶ clear connection between job and script

Cons:
  ▶ scattered script collection
  ▶ no clear evolutionary record
  ▶ frequent reinvention and regression
Model: one script for many jobs

- simulation parameters are script variables
- variables are passed from command line
  (e.g. “lammmps -var name value -in myscript”)
simulation strategy v0.2

Model: one script for many jobs
- simulation parameters are script variables
- variables are passed from command line (e.g. "lammps -var name value -in myscript")

Pros:
- improved code re-use
- fairly easy implementation

Cons:
- weaker connection between job and script
- interactive and batch jobs handled differently
Model: one script per job type

- general-purpose scripts stored in central location

Pros:

- script evolution tracked via version control
- much improved code re-use

Cons:

- much weaker connection between job and script
Model: one script per job type
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current simulation strategy v0.3

Model: one script *template* per job type

- create custom script from general-purpose template (similar to building web pages dynamically)
- run LAMMPS with custom script
current simulation strategy v0.3

Model: one script *template* per job type
  - create custom script from general-purpose template
    (similar to building web pages dynamically)
  - run LAMMPS with custom script

Pros:
  - clear connection between job and script

Cons:
  - requires specialized front-end
implementation details

two primary components

- library of LAMMPS template scripts (simulation setup, modification, and production tasks)
- front-end for script manipulation and submission (bourne shell script)
template = script with parameters set via “index” variables
  ▶ variables should have safe-ish default values
  ▶ runtime script is template copy with new variable values
    (e.g. “variable myvar index 0” in template
     becomes “variable myvar index 100”)

implementation details
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  ▶ variables should have safe-ish default values
  ▶ runtime script is template copy with new variable values
    (e.g. “variable myvar index 0” in template becomes “variable myvar index 100”)

template library
  ▶ for generality, most templates expect restart file as input
  ▶ forcefield-specific setup templates use data files
  ▶ template can include special “help” comment section
implementation details

front-end

▶ provide “help” framework
▶ collect parameter variables from command line
▶ create custom script from specified template
▶ configure runtime environment
▶ start interactive (test) or batch (production) job
help example 1

$ sub.lammps
$ sub.lammps

Available scripts:
in.lammps.alter
in.lammps.data2restart
in.lammps.npt
in.lammps.nv
in.lammps.rnemd
in.lammps.setup-bulk
in.lammps.setup-droplet
in.lammps.sllod
in.lammps.therm_cond

Usage: sub.lammps lammps_script [--outname=NAME] [--variable=VALUE] ...
help example 2

$ sub.lammps in.lammps.npt
help example 2

$ sub.lammps in.lammps.npt

# NPT simulation of periodic (bulk) system

# these variables must be set from the command line:
variable outname index basename_of_all_output_files
variable infile index full_name_of_read_data_or_restart_file
variable numsteps index 0
# initial and final thermostat setpoints
variable beg_temp index 300
variable end_temp index $beg_temp
# initial and final barostat setpoints
variable beg_press index 1
variable end_press index $beg_press

# options:
# snap_freq: output thermo snapshots at specified interval
variable snap_freq index 10000
# dump_freq: output basic dump snapshots at specified interval
variable dump_freq index 100000

# traj_freq: output detailed trajectory info at specified interval
variable traj_freq index 0

# these variables have generally conservative defaults:
# kspace != 0: turn on kspace_style
variable kspace index 1

# restart_freq: output restart files at specified interval
variable restart_freq index 1000000

# new_step >= 0: reset current step to new_step
variable new_step index -1

# ___end command line variable section___

Usage: sub.lammps lammps_script [--outname=NAME] [--variable=VALUE] ...
job submission example

$ sub.lammps in.lammps.npt --outname=mysimulation \ 
   --infile=myrestart.0 --numsteps=10000 --beg_temp=300
job submission example

$ sub.lammps in.lammps.npt --outname=mysimulation \
   --infile=myrestart.0 --numsteps=10000 --beg_temp=300

Building custom LAMMPS input script from provided variables:
template: /home/ctenney/Private/src/lammps/scripts/in.lammps.npt
replacing variable outname in mysimulation.in
replacing variable infile in mysimulation.in
replacing variable numsteps in mysimulation.in
replacing variable beg_temp in mysimulation.in

LAMMPS command:
/home/ctenney/Private/bin/lmp_serial -in mysimulation.in

LAMMPS (15 Jan 2010)
Reading restart file ...
WARNING: Restart file version does not match LAMMPS version
   restart file = 7 Jul 2009, LAMMPS = 15 Jan 2010
   orthogonal box = (-11.2178 -11.2178 -11.2178) to (100.96 100.96 100.96)
LAMMPS script library implementation
  ▶ template scripts
    ▶ bulk and droplet simulation setup and modification
    ▶ NPT, NVT, NVE, and various flavors of NEMD
  ▶ front-end
    ▶ provides pseudo “man” pages
    ▶ creates archivable LAMMPS scripts from templates
    ▶ handles environment setup and job submission

more info on Maginn group wiki:
http://puccini.cheg.nd.edu