Building a reusable LAMMPS script library

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overview

motivation

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

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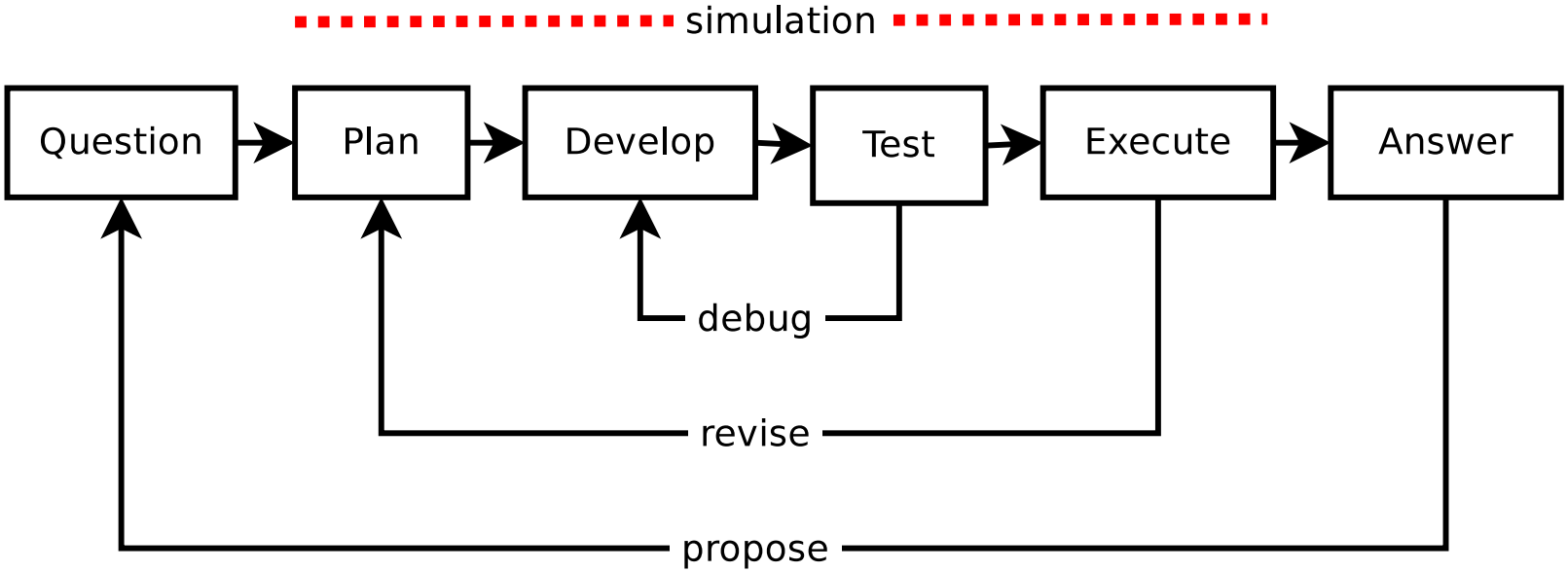
Research workflow:



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 implemention
- clear connection between job and script

Cons:

- scattered script collection
- no clear evolutionary record
- frequent reinvention and regression

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”)

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

simulation strategy v0.2.1

Model: one script per job *type*

- general-purpose scripts stored in central location

simulation strategy v0.2.1

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

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)

implementation details

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

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")

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
```

help example 1

```
$ 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] [--variab
```

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_fil
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
```

help example 2 cont'd

```
# dump_freq: output basic dump snapshots at specified inter
variable dump_freq index 100000
# traj_freq: output detailed trajectory info at specified i
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] [--variabl
```

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.lammp
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
```

closing

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`