# Ins and Outs of LAMMPS input scripts

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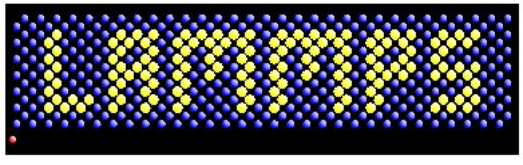




# Goals for this lecture

Teach you how to ...

- Read and understand an existing input script
- Edit an existing input script
- Write a new input script
- Debug an input script

# What is a LAMMPS input script

- Text file containing a sequence of LAMMPS commands
- LAMMPS reads file, executes commands one at a time
  - NOT: run one simulation after entire file is read
  - RATHER: run a simulation whenever run command appears
- One script can run one or many LAMMPS simulations
- Some commands read other flavors of LAMMPS input files
  - data files: read_data data.micelle
  - restart files: read_restart surface.restart.100000
  - molecule files: molecule ID co2.txt h2o.txt
- When last command in file completes, LAMMPS exits
  - earlier commands can also trigger exit

# Input script is parsed into individual commands

See Section 5.2 of User Guide for full details

1. Blank lines are skipped
2. Comments are removed: start with # character
3. Lines ending with & character are concatenated
4. Now have a single line ⇒ single command
5. Single line is split into words by white space
6. Quotes allow one word to contain spaces
   - two words: print "Reached end of equilibration"
7. Within each word, variable names replaced with value
   - variable f string data.micelle
   - read_data $f ⇒ read_data data.micelle
   - variable temp equal 273.0
   - fix ID all nvt temp ${temp} ${temp} 0.01
8. First word = command name, all others are arguments

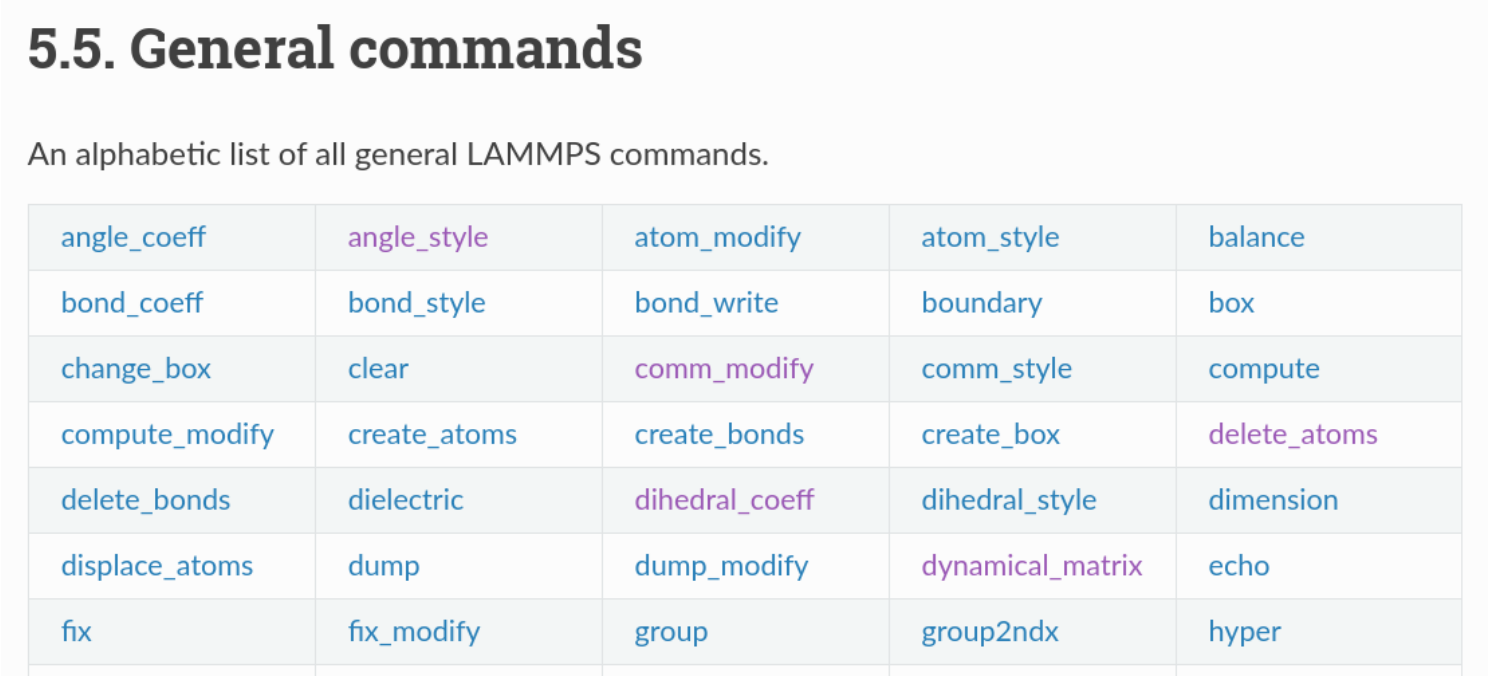
# Every command has its own doc page

IMPORTANT:

The only way to edit/compose your own input scripts and learn how to use LAMMPS well, is to read those doc pages

Click on Commands entry in LAMMPS webpage table

Alternatively, bookmark Section 5.5 of User Guide



## 5.5. General commands

An alphabetic list of all general LAMMPS commands.

| | | | | |
|---|---|---|---|---|
| angle_coeff | angle_style | atom_modify | atom_style | balance |
| bond_coeff | bond_style | bond_write | boundary | box |
| change_box | clear | comm_modify | comm_style | compute |
| compute_modify | create_atoms | create_bonds | create_box | delete_atoms |
| delete_bonds | dielectric | dihedral_coeff | dihedral_style | dimension |
| displace_atoms | dump | dump_modify | dynamical_matrix | echo |
| fix | fix_modify | group | group2ndx | hyper |

and many more (110 commands in current version)

# Most style commands are actually many commands

Table at very top of Commands webpage has style commands

| | | |
|---|---|---|
| General commands | Fix styles | Compute styles |
| Pair styles | Bond styles | Angle styles |
| Dihedral styles | Improper styles | KSpace styles |

Fix styles expands to ∼250 entries, each with own doc page:

## 5.6. Fix commands

An alphabetic list of all LAMMPS fix commands. Some styles have accelerated versions. This is indicated by additional letters in parenthesis: g = GPU, i = INTEL, k = KOKKOS, o = OPENMP, t = OPT.

| | | | | |
|---|---|---|---|---|
| accelerate/cos | adapt | adapt/fep | addforce | addtorque |
| append/atoms | atc | atom/swap | ave/atom | ave/chunk |
| ave/correlate | ave/correlate/long | ave/histo | ave/histo/weight | ave/time |
| aveforce | balance | brownian | brownian/asphere | brownian/sphere |
| bocs | bond/break | bond/create | bond/create/angle | bond/react |
| bond/swap | box/relax | charge/regulation | client/md | cmap |

A command like: fix ID all aveforce ...

may be called a fix command or fix aveforce command

# Structure of a typical input script

1. Global settings
   - units, dimension, atom_style, boundary commands
   - all have default values
2. Create simulation box and atoms
   - region, create_box, create_atoms, lattice commands
   - read_data or read_restart commands
3. Define groups of atoms
   - one atom can be assigned to multiple groups
4. Set atom attributes if needed: velocity, mass
5. Pair_style command for atom interactions
6. Fix commands for time integration and constraints
7. Compute commands for diagnostics
8. Output commands: thermo, dump, restart
9. Action command: run or minimize
10. Rinse and repeat as needed

# Section 1 of examples/friction/in.friction input script

NOTE: There are ~500 input scripts in lammps/examples
See lammps/examples/README to find ones of interest to you

Global settings:

```
dimension 2
boundary p s p
atom_style atomic
neighbor 0.3 bin
neigh_modify delay 5
timestep 0.0025
```

# Section 2 of in.friction input script

Create box and atoms:

```
lattice hex 0.9
region box block 0 50 0 22 -0.25 0.25
create_box 4 box

region lo-fixed block INF INF INF 1.1 INF INF
region lo-slab block INF INF INF 7 INF INF
region above-lo block INF INF INF 7 INF INF side out
region hi-fixed block INF INF 20.9 INF INF INF
region hi-slab block INF INF 15 INF INF INF
region below-hi block INF INF 15 INF INF INF side out

create_atoms 1 region lo-slab
create_atoms 1 region hi-slab
```

# Section 3 of in.friction input script

Define groups: (optional)

```
group lo region lo-slab
group lo type 2
group hi region hi-slab
group hi type 3
group lo-fixed region lo-fixed
group hi-fixed region hi-fixed
group boundary union lo-fixed hi-fixed
group mobile subtract all boundary
```

# Section 4 of in.friction input script

Set atom attributes:

```
set group lo-fixed type 4
set group hi-fixed type 4

mass * 1.0
velocity mobile create 0.1 482748 temp ydim
velocity hi set 1.0 0.0 0.0 sum yes
```

# Section 5 of in.friction input script

Pair_style:

```
pair_style lj/cut 2.5
pair_coeff * * 1.0 1.0 2.5
```

# Section 6 of in.friction input script

Fixes:

```
fix 1 all nve
fix 2 boundary setforce 0.0 0.0 0.0
fix 3 mobile temp/rescale 200 0.1 0.1 0.02 1.0
fix_modify 3 temp ydim
fix 4 all enforce2d
```

# Section 7 of in.friction input script

Computes: (optional)

```
compute ydim mobile temp/partial 0 1 0
```

# Section 8 of in.friction input script

Output:

```
thermo 1000
thermo_modify temp ydim

dump 2 all image 500 image.*.jpg type type &
      zoom 1.6 adiam 1.5
dump_modify 2 pad 5

dump 3 all movie 500 movie.mpg type type &
      zoom 1.6 adiam 1.5
dump_modify 3 pad 5
```

# Section 9 of in.friction input script

Action:

```
run 20000
```

# Log file output = log.lammps

See Section 4.3 of User Guide for full details

- Similar to screen output but some additional info
  - echoes every command including variable substitutions
- Contains warning and error messages
- Some input script commands produce useful output
  - group command prints # of atoms in group
  - delete_atoms command prints # of atoms deleted
- Pre-run info: neighbor lists, memory usage
- Columns of numeric thermodynamic output every N steps
  - state of simulation at that timestep
  - thermo_style command defines what info is output
  - useful to eyeball or plot
- Post-run info:
  - CPU timing and breakdown (pair, neighbor, comm, etc)
  - per-processor stats on counts/timings for atoms & neighbors
  - useful to eyeball for performance issues

# Dump file output

- Dump file = one snapshot of per-atom info every N steps
- File format depends on dump style: text, binary, image, etc
- Input script can specify multiple dump commands
- Choose which atoms and what info to output
- Many fix, compute, variable commands ⇒ per-atom values
- Can also output per-pair or per-bond info
- Useful for post-processing analyses and viz

Fix time-averaging commands can also produce output files:

- fix ave/time - scalar or vector quantities
- fix ave/histo - histograms of per-atom data
- fix ave/correlate - correlation coeffs of scalars or vectors

# (1) Tips for writing and debugging an input script

- Same as writing a computer program
  - albeit in a simple input-script language
- Start as simple as possible
- Add complexity to your script one command at a time
- Check thermo output (plot) and/or viz at every stage

- Two kinds of errors: syntax and run-time
- LAMMPS flags syntax errors, tells you which command
  - common: LAMMPS not built with needed package
  - if error not obvious, read the command doc page
  - NOTE: website doc pages are for current feature release
- PAY ATTENTION to screen/logfile WARNING messages

# (2) Tips for writing and debugging an input script

- Debug ideas for run-time errors:
  - read pre-run portion of log file to insure all-is-well
  - add print commands with variables to examine values
  - run with thermo output every timestep
  - run small problem before big problem
  - run in serial before in parallel
  - plot thermo output, viz snapshots to verify all-is-well
- Four flavors of run-time errors, from easy to hard
  1. Simulation triggers an error messsage:
     - common: lost or out-of-range atoms
     - cause: overlapping atoms or bad model params
  2. Simulation thermodynamics blow up
     - common: bad model or time integration params
  3. Simulation crashes with no error message or blow-up
     - if thermo output looks good, report it
  4. See next slide ...

# Hardest run-time error to debug

(4) Simulation runs, answer is wrong

- How do you know what is right versus what is wrong ?
- Could be normal statistical variation
- Could be LAMMPS did what you asked, your model is wrong
- Could be a bug or problem with LAMMPS
- Hard to deduce without some MD expertise

When all else fails ...

- Ask a local LAMMPS or MD expert (your advisor ?)
- Post a message to LAMMPS discussion forum
- See MatSci forum link on website for details