LIGGGHTS Reference Card

(c) 2015 Siddharth Kanungo <siddharth.soka@gmail.com>
http://www.mendax-grip.github.io

1 Input File

A LIGGGHTS input script has four parts:

- **Initialisation** Set the parameters that need to be defined before particles are created
- **Setup** Define the material properties, particles, geometry and particle generation
- **Detailed Settings** Define some settings that correspond to speed and memory utilisation, output options etc
- **Execution** The actual *run* command that executes the simulation

There are two types of statements in the LIGGGHTS input deck:

Type of Commands Individual Commands It establish basic settings for the simulation

Type of Commands Fixes To set particular aspects of the simulation

Generally, fixes and some particular commands follow common structure:

```
fix ID group-ID style args
```

- ID ūser-assigned name for the fix
- Group-ID ĪD of the group to which the fix is applied
- style t̄ype of fix being applied
- args ārguements used by a particular style; often consists of a keyword and particular value

2 Initialisation

2.1 Preliminaries

Commands	Comment
`units si`	Gives the Units system to be used
`atom_style granular`	Describes the types of atoms to be used in the simulation
`atom_modify map array`	Modify properties of atom style. Map keyword determines how atom ID Lookup is done for molecular problems
`boundary f f f`	Describes the boundaries of the domain as fixed(f), periodic(p) or movable(m)
`newton off`	Determines whether or not to calculate pairwise interactions on each processor; Best to leave off for DEM
`communicate single vel yes`	Sets the style of inter-processor communication that occurs each timestep as atom coordinates and other properties are exchanged between neighboring processors and stored as properties of ghost atoms
`processors 2 2 3`	Specifies how to decompose domain for parallelization

2.2 Declare domain

`region domain block xlo xhi ylo yhi zlo zhi units box`	Specifies a region called ’domain’ that describes the bounds of the domain
`create_box n domain`	This simulation uses n different material types

2.3 Neighbor Listing

`neighbor 0.003 bin`	Neighbor statements describe how large neighbor lists will be and how often to recalculate. Recommended to be a value Diameter (avoid!)
`neigh_modify keyword values`	Sets parameter that affect the building and use of pairwise neighbor lists

3 Setup

The Setup portion of the input file consists of the use of many fix command.

3.1 Material and Interaction Properties required

The format of the fix is the following:

```
fix ID group-ID style args
```

Command	Value
ID	Name of the fix so as to reference later
group-ID	The atom-types that you want the fix to work on; write **all** for all atoms
style	property/global propertyName
args	peratomtype or peratompair

Hence onewards only the style and args will be shown

List of properties name

- youngsModulus peratomtype value
- poissonsRatio peratomtype value
- coefficientFriction peratompair numberOfAtoms Value11 Value12 .. Value nn
- coefficientRestitution peratompair numberOfAtoms Value11 Value12 .. Value nn
- coefficientRollingFriction peratompair numberOfAtoms Value11 Value12 .. Value nn

3.2 Particle Insertion

Particle insertion consists of the four important stages:

- Defining the particle template
- Defining the particle distribution template
- Defining the region of insertion
- Defining the Insertion method

3.2.1 Particle Template

Value	Command
`particleTemplate/sphere`	style
`atom_type, density, radius`	args

3.2.2 Particle Particle Distribution Template

Value	Command
`particledistribution/discrete`	style
`ID-of the particle template to be used`	args

3.2.3 Region of Insertion

Value	Command
mesh/surface	style
region command	style
type	args

In case of Insertion region, you can either

- Define a mesh as a insertion region by importing it
- or, Define a region as insertion face

3.2.4 Particle Insertion Method

Describe the particle insertion. There are three methods of insertion

- Insert/rate/region
- Insert/pack
- Insert stream

The recommended is to use the rate/region or stream.

Value	Command
insert/rate/region	style
insert/pack	style
insert/stream	style

It is also to be noted that the method of insertion requires how you would like to insert particles ie. on the basis of Mass, Volume or Number of Particles.The distribution template, region of insertion and the velocity at the time insertion are given as arguments.

3.2.5 Importing Mesh From CAD

```
 /* Here the file is imported named as cad1
The style is mesh/surface
The location is give to keyword file.stl
The geometry can be scaled using the scale argument */
 fix cad1 all mesh/surface file file.stl type 2 scale 0.1
```

3.2.6 Use of Imported Mesh as Granular Wall

```
 /* Here the wall is named geometry
The style is wall/gran
The number of meshes is specified in n˙meshes
The ID of the imported cad file is given in meshes */
 fix geometry all wall/gran model hooke tangential history &
 mesh n_meshes 1 meshes cad
```

3.2.7 Creating primitives shapes to use as Walls

Apart from importing stl files, we can also use primitive shapes such as plane, cylinder, sphere to be used as walls.

```
 /* Here the name of the wall is p1
The atom type is 2
The wall is in the XY plane passing through origin */
 fix p1 all wall/gran model hooke tangential history &
 primitive type 2 zplane 0.0
```

3.2.8 Defining the Physics

Pair Coeffeciants statements can be used to model different interactions between different particle types. Suppose modelling interaction between a particle with wall which is more cohesive than a second one.

```
/* This is the pair style to be used when using hooke pair style
 # The second statement assumes same pair˙style for every atoms */
 pair_style gran model hooke tangential history
 pair_coeff * *
```

4 Detailed Settings

4.1 Integrator

Declaration of the integrator to use. It will always be nve/sphere, unless multisphere particles are used.

```
 fix integrate all nve/sphere
```

4.2 Gravity

```
 /* For every particle, we define a property gravity
acts in the direction of the vector specified */
 fix grav all gravity 9.81 vector 0.0 0.0 -1.0
```

4.3 Timestep

```
   /* Define the timestep equal to 0.001 sec.
 The unit depends on the SI unit used.
 It is recommended that the simulation should
 be 20“% or lesser than a Rayleigh TimeStep*/
timestep 0.001
```

4.4 Thermodynamic output settings

For most settings leave this unchanged.

```
 /*Describe quantities to be printed on logfile
and the output screen. The number of interval to the
write the thermodynamic quantities.
Lost ˙Ignore ignore lost particle */
 thermo_style custom step atoms ke cpu
 thermo 10000
 thermo_modify norm no lost ignore
```

4.5 Check, time sttep and Initialising dump file

```
 /* Check the time step and compare it with Rayleigh.
Give error if its greater than 0.01 “% greater.
Initialize dump by running 1 timestep. Is recomended to do so.
Unfix the checking after once. The result is written in log file*/
 fix ctg all check/timestep/gran 1 0.01 0.01
 run 1
 unfix ctg
```

4.6 Create Imaging Information

```
 /*Generates a set of dump files
that contain information for imaging
the system. Give the interval and file type to save.
This generates huge files, therefore it is
recommended to dump properties that are necessary.  */
 dump dumpstl all stl 10000 dump*stl
 dump dmp all custom 10000 dump.1 id type x y z
```

5 Execution and Furthur Settings

5.1 Run

```
 /* run the simulation for partilcular timestep */
 run 15000 upto
```

For a complete reference, see:
⇒ LIGGGHTS Documentation
http://www.cfdem.com/media/DEM/docu/Manual.html