```
###################################Header for General
commands##########################################################

atom_style        granular                    #Simulation of particles

boundary          f f f                       #fixed boundaries -> particles will be deleted if
leaving the simulation box

units             si

communicate       single vel yes  #default

newton            off                                  #default



###################################System
variables###############################################################

#Definition of boundaries
variable xmin equal -2.55
variable xmax equal 3

variable ymin equal -2.55
variable ymax equal 3

variable zmin equal -0.05
variable zmax equal 5.0

#Definition of the timestep

variable dt equal 1e-4             #timestep = 0.0001 second; Each iteration step represents
0.0001 seconds.
#variable dt equal 1e-3
#variable dt equal min(1e-3,0.1*rayleigh_time)




###################################Specific variables for current
simulation#########################################

variable natoms equal 2           #1 -> particle #2-> hopper,frame and ground, lid

####variable for material properties####

####Young Modulus####
variable          youngmodulus1   equal   1e8                #N/mm²
variable          youngmodulus2   equal   1e8                #N/mm²

####Poission ratio####
variable          poission1       equal   0.3
variable          poission2       equal   0.3

####variable for contact properties####

####coefficient of restitution####
variable          CoR11   equal   0.6
variable          CoR12   equal   0.6
variable          CoR21   equal   0.6
variable          CoR22   equal   0.6

####sliding friction coefficient####
variable          sf11    equal   0.3
variable          sf12    equal   0.36
variable          sf21    equal   0.36
variable          sf22    equal   0.0
```

```
   ####rolling friction coefficient####
   variable        rf11    equal   0.8
   variable        rf12    equal   0.8
   variable        rf21    equal   0.8
   variable        rf22    equal   0.8




   ####variable for particle####

   #Number of particle radius
   variable        nradii  equal   2

   variable        radius1 equal   0.00200 #m
   variable        radius2 equal   0.00300 #m

   variable        frac1   equal   0.2             #20%
   variable        frac2   equal   0.8             #80%

   variable        density equal   4000    #kg/m³




   ####filling parameters####

   variable        filltime        equal   2               #seconds

   variable        fillmass        equal   0.1             #kg

   variable        fillmassrate    equal   ${fillmass}/${filltime} #kg/s

   variable        fillsteps       equal   ${filltime}/${dt}               #Transform time
   to iteration steps

   ####settle time####

   variable        settletime      equal   1 #second

   variable        settlesteps     equal   ${settletime}/${dt}             #Transform time
   to iteration steps

   ####open parameter of the lid####

   variable        openvel         equal   0.4     #m/s

   variable        opentime        equal   1 #second

   variable        opensteps       equal   ${opentime}/${dt}               #Transform time
   to iteration steps


   ####discharge time#####

   variable        dischargetime   equal   10 #seconds

   variable        dischargesteps  equal   ${dischargetime}/${dt}          #Transform time
   to iteration steps




   ##################################Definition of
   simulationbox####################################################

   region          reg block ${xmin} ${xmax} ${ymin} ${ymax} ${zmin} ${zmax} units box
```

```
create_box        2 reg

neighbor          0.005 bin                    #default

neigh_modify      delay 10 check yes               #default

###############################Definition of the contact
models#########################################################

pair_style gran model hertz tangential history rolling_friction epsd2   #contact model

pair_coeff        * *                              #default

timestep ${dt}

fix               integrator all nve/sphere                            #default

fix               gravi all gravity 9.81 vector 0.0 0.0 -1.0            #gravity of 9.81
m/s² in negative z direction




###############################Definition of Material
properties#####################################################


fix               m1 all property/global youngsModulus peratomtype ${youngmodulus1}
${youngmodulus2}

fix               m2 all property/global poissonsRatio peratomtype ${poission1}
${poission2}

fix               m3 all property/global coefficientRestitution peratomtypepair ${natoms}
0.6 0.6 0.6 0.6

fix               m4 all property/global coefficientFriction peratomtypepair ${natoms}
${sf11} ${sf12} ${sf21} ${sf22}

fix               m5 all property/global coefficientRollingFriction peratomtypepair
${natoms} ${rf11} ${rf12} ${rf21} ${rf22}




###############################Generation and Loading of the Geometry
.stl###################################

#fix         silo    all mesh/surface file 60zip/siloset.stl          type 2  scale
0.001   #load mesh from STL file. Type 2 for geometry. Scale down to transform mm #to
meters

fix          silo    all mesh/surface file 60zip/silo_new.stl          type 2  scale
0.001
fix          lid    all mesh/surface file 60zip/lidset.stl          type 2  scale 0.001
fix          ground  all mesh/surface file 60zip/ground.stl          type 2  scale 0.001
fix          frame   all mesh/surface file 60zip/support.stl         type 2   scale
0.001
fix          nozzle   all mesh/surface file 60zip/nozzleupdated.stl        type 2
scale 0.001

fix          walls    all wall/gran model hertz tangential history rolling_friction
epsd2 mesh n_meshes 5 meshes silo lid ground frame nozzle


###############################Generation and Insertion of the
```

```
particles######################################

fix            pts1 all particletemplate/sphere 10487 atom_type 1 density constant
${density} radius constant ${radius1}

fix            pts2 all particletemplate/sphere 11887 atom_type 1 density constant
${density} radius constant ${radius2}

fix            pdd1 all particledistribution/discrete 32452867 ${nradii} pts1 ${frac1}
pts2 ${frac2}

#Modified insertion to use four nozzles
fix     ins_mesh all mesh/surface/planar file 60zip/insset.stl type 1 scale 0.001

fix             ins all insert/stream seed 86028157 distributiontemplate pdd1 &
        mass ${fillmass} massrate ${fillmassrate} overlapcheck yes all_in yes vel
constant 0.01 0.01 2 &
        insertion_face ins_mesh extrude_length 0.05




################################Dumping of the data for post-processing to
visualize###########################

shell    mkdir post

#Definition of the dumptime

variable dumptime equal 0.1      # Every 0.05 s 1 image

variable dumpstep equal ${dumptime}/${dt}        #Transform to iteration steps


dump     dmpparticle all custom/vtk ${dumpstep} post/particles_*.vtk id type x y z vx vy
vz fx fy fz radius mass
dump     dmpground all mesh/stl ${dumpstep} post/ground*.stl ground
dump     dmpsilo all mesh/stl ${dumpstep} post/siloset*.stl silo
dump     dmpframe all mesh/stl ${dumpstep} post/support*.stl  frame
dump     dmplid all mesh/stl ${dumpstep} post/lidset*.stl lid
dump     dmnozz all mesh/stl ${dumpstep} post/nozzle*.stl nozzle




################################RUN the simulation
filling#######################################################

run       ${fillsteps}

unfix    ins

################################RUN the simulation
settling######################################################

run       ${settlesteps}

################################RUN the simulation Open
Door#####################################################
fix             MoveLid all move/mesh 60zip lidset      linear ${openvel} 0. 0.

run       ${opensteps}

unfix    MoveLid
run       ${dischargesteps}

################################RUN the simulation
```

```
  Outflow###############################################################


  run        ${dischargesteps}
```