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## Example 4: move an intruder in a 2D granular material
#  New tricks:  use grains as a boundary, 2D simulation, use group to control particles separately
#  Commands that appears in previous examples will not be repeatedly explained.
#  More command details in the documentation https://lammps.sandia.gov/doc/Commands.html
#  LAMMPS version: LAMMPS (7 Aug 2019) on linux

# change the default dimension to 2
dimension       2
atom_style      sphere
boundary        p p p
newton          off
comm_modify     vel yes

region          reg block -5 5 -5 5 -0.5 0.5 units box
# define a simulation region with 2 particle types
create_box      2 reg

# In the data file, we have randomly positioned particles, which means that they can highly overlap,
# and two intruders of diameter 3.0, one of them is the 32th particle, the other is the 76th particle.
# All the rest are smaller particles (of diameter 1.0 or 1.4) that form the packing.
# their density is 1.0.
# the intruders are of type=2, the rest particles are of type=1
read_data       data add merge

# To separately manipulate particles, we define different groups according to their attributes
# define a group of particles named ‘intruder1’, which contains a particle with ID==32
group           intruder1 id == 32
# define a group of particles named ‘intruder2’, which contains a particle with ID==76
group           intruder2 id == 76
# define a group of particles named ‘packing’, which contains particles with particle type<=1
group           packing type <= 1

fix             1 packing nve/sphere
fix             11 intruder1 nve/sphere
fix             12 intruder2 nve/sphere

neighbor        0.2 bin
neigh_modify    delay 0

pair_style      gran/hooke/history 400.0 NULL 10.0 NULL 0.75 1
pair_coeff      * *

timestep        0.001

# just zero out the z-dimension velocity and force on all atoms
fix         2 all enforce2d

compute             ke all ke
compute             re all erotate/sphere
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thermo_style   custom step atoms c_ke c_re
thermo         100
thermo_modify          lost warn norm no

dump           2 all image 100 *.jpg type diameter zoom 1.6 view 0 0
dump_modify 2 pad 5

# the first run relax the initial random positioning of the particles,
# so it looks like a packing in the end of this run
run 5000

# exclude interactions between the two intruders
neigh_modify exclude group intruder1 intruder2

# we remove the effect of the fix command named '12'
# the position and velocity of intruder2 will not be updated according to F=ma (i.e. nve)
# That is, intruder2 will no longer move, but used as a fixed boundary
unfix          12

# Add a position-controlled fix to intruder1, so that its velocity is fixed to vx=0.0, vy=0.7,
# and the z direction is not influenced (NULL).
# That is, intruder1's motion is position-controlled, and the force on it will fluctuates.
fix            hxFix intruder1 move linear 0.0 0.7 NULL
# need to remove the F=ma integration on intruder1, because the two fixes will make the intruder move
# twice during simulations.
unfix          11

# the second run stirs the packing by moving one intruder and fixing the other.
run 10000
```