CL 708: Granular Mechanics
Final Presentation

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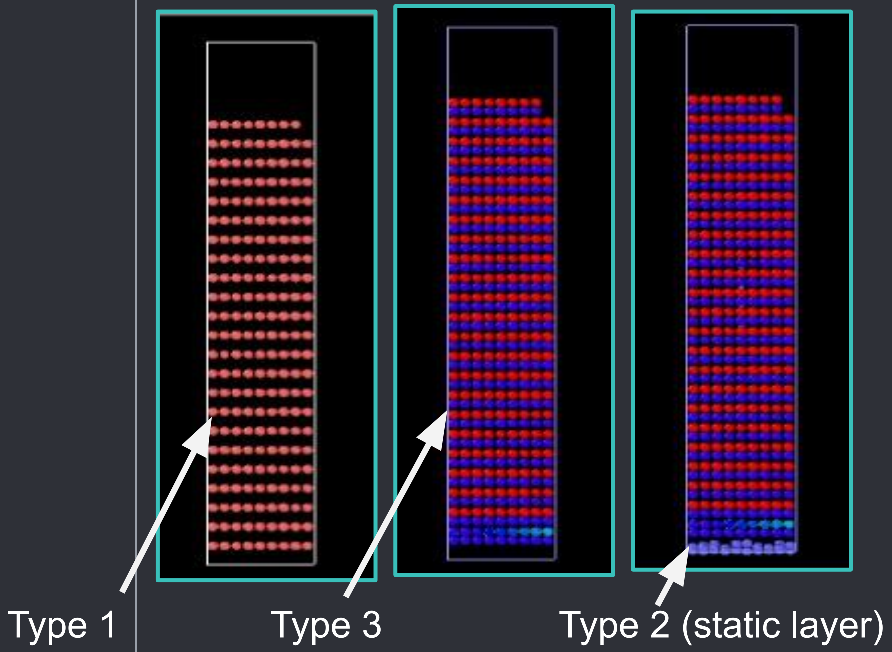
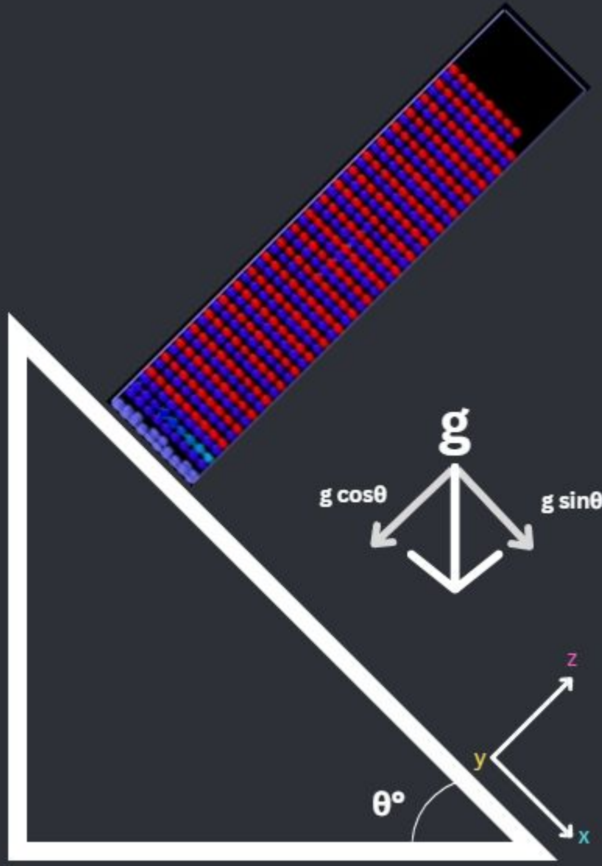
Problem Statement, Parameters
&
Scripts

Problem Statement

- Segregation of a granular mixture of particles of **two species** with **different diameters** flowing due to gravity on a **rough inclined plane**, with **periodic boundary conditions** in the **flow** and **neutral** directions.



Schematic Diagram



Particle Parameters

2 species of diameter	0.1 cm 0.08 cm
Number of particles	1600 of each species
Particle density	2.5 g/cc
Inclination of plane	24°
Coefficient of friction (inclined plane surface)	0.5
Coefficient of restitution	0.9
Lx, Ly, Lz	1.5 cm, 1 cm, 6 cm
Kn, Kt	2568000 dyne/cm, 0 dyne/cm
Gn, Gt	4952 s^{-1} , 0 s^{-1}
dampflag	0

Approach & LAMMPS Script

Starting Point: Example 3 from the LAMMPS examples discussed in class

Method Used:

1. Arrange the two different groups of particles in alternate rows to simulate random arrangement, while maintaining the static layer
2. Create an array named **xv2** similar to **xv**, which contains the initial positions and velocities of the second type of particles.
3. This is accomplished by increasing the spacing between two layers of the same type of particles
4. Find the number fractions of the particles relative to bin height to analyse the segregation taking place as a result of the size difference
5. Analyse the velocity profiles at different inclinations of the inclined plane

```
sp=d0+deld;
x[1][1]=sp/2;
x[1][2]=sp/2;
x[1][3]=sp/2+1.5*d0+db+deld;
for (i=2;i<=Nparts;++i) {
    x[i][1]=x[i-1][1]+sp;
    x[i][2]=x[i-1][2];
    x[i][3]=x[i-1][3];
    if (x[i][1]>(Lx-sp/2+eps))
    {
        x[i][1]=sp/2;
        x[i][2]=x[i-1][2]+sp;
        if (x[i][2]>(Ly-sp/2)){
            x[i][1]=sp/2;
            x[i][2]=sp/2;
            x[i][3]=x[i-1][3]+2*sp;
        }
    }
}

x2[1][1]=sp/2;
x2[1][2]=sp/2;
x2[1][3]=sp/2+2.5*d0+db+deld;
for (i=2;i<=Nparts;++i) {
    x2[i][1]=x2[i-1][1]+sp;
    x2[i][2]=x2[i-1][2];
    x2[i][3]=x2[i-1][3];
    if (x2[i][1]>(Lx-sp/2+eps))
    {
        x2[i][1]=sp/2;
        x2[i][2]=x2[i-1][2]+sp;
        if (x2[i][2]>(Ly-sp/2)){
            x2[i][1]=sp/2;
            x2[i][2]=sp/2;
            x2[i][3]=x2[i-1][3]+2*sp;
        }
```

0ip

```
units cgs
atom_style sphere

boundary p p f
region box block 0 1.5 0 1 0 6
create_box 3 box

read_data st.data add append
read_data xv.data add append
read_data xv2.data add append

set atom 1 diameter 0.1
set atom 2 diameter 0.08
set atom 3 diameter 0.08

group mb type 1
group mb2 type 3
group st type 2


variable th file th
variable nwr equal 2
variable dn equal 1000
variable nstp equal ${nwr}*${dn}
variable gx equal sin(${th}*PI/180)
variable gz equal -cos(${th}*PI/180)
```

```
pair_style gran/hooke/history 2568000.0 NULL 4952.0 0 0.5 0
pair_coeff * *
comm_modify vel yes

timestep 1e-5

fix 1 all wall/reflect zlo EDGE zhi EDGE
fix 2 all gravity  981 vector ${gx} 0 ${gz}
fix 3 mb nve/sphere
fix 4 mb2 nve/sphere

dump 1 all custom ${dn} ip0.dump type radius x y z vx vy vz
thermo ${dn}
thermo_style custom step ke

run_style verlet
run ${nstp}

write_data ip.data
write_restart rsip.inp
```

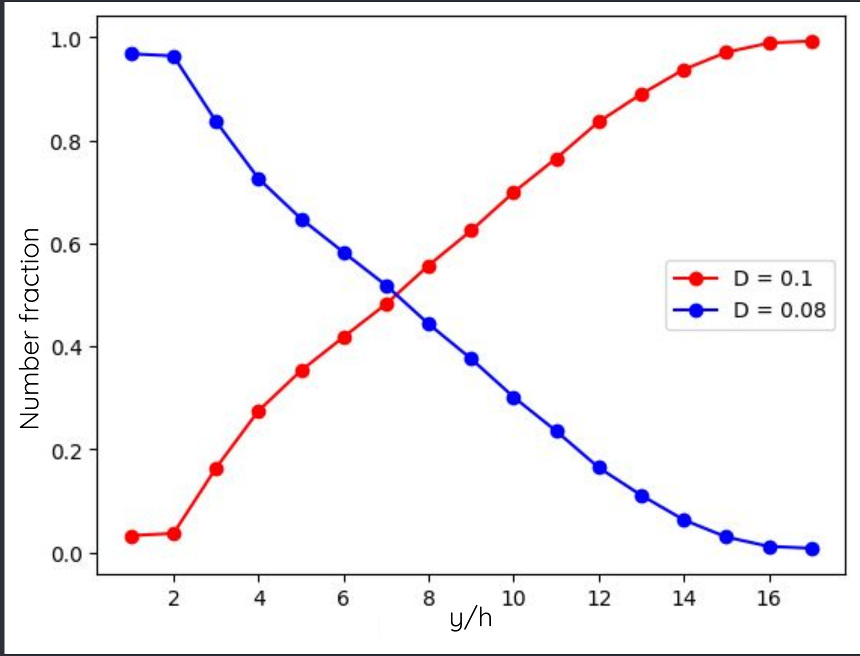
1ip

```
read_restart rsip.inp

group mb type 1
group st type 2
group mb2 type 3

variable th file th
variable nwr equal 4000
variable dn equal 1000
variable nstp equal ${nwr}*${dn}
variable gx equal sin(${th}*PI/180)
variable gz equal -cos(${th}*PI/180)
variable mdot atom mass*vx/0.5

pair_style gran/hooke/history 2568000.0 NULL 4952.0 0 0.5 0
pair_coeff * *
comm_modify vel yes

timestep 1e-5

region mbox block 0.5 1 0 1 0 6
compute s mb stress/atom NULL pair
compute s2 mb2 stress/atom NULL pair
compute md mb chunk/atom type region mbox
compute md2 mb2 chunk/atom type region mbox
compute ch mb chunk/atom bin/1d z lower 0.1
compute ch2 mb2 chunk/atom bin/1d z lower 0.1
compute np mb property/chunk ch count
compute np2 mb2 property/chunk ch2 count
```

```
fix 1 all wall/reflect zlo EDGE zhi EDGE
fix 2 all gravity  981 vector ${gx} 0 ${gz}
fix 3 mb nve/sphere
fix 4 mb2 nve/sphere
fix av mb ave/chunk 2 50 100 ch density/mass vx c_s[3] c_s[5] ave running file fvs.dat overwrite
fix avmd mb ave/chunk 10 10 100 md v_mdot ave running file md.dat overwrite
fix av2 mb2 ave/chunk 2 50 100 ch2 density/mass vx c_s2[3] c_s2[5] ave running file fvs2.dat overwrite
fix avmd2 mb2 ave/chunk 10 10 100 md2 v_mdot ave running file md2.dat overwrite
fix 5 mb ave/time 2 50 10000  c_np[1] c_np[2] c_np[3] c_np[4] c_np[5] c_np[6] c_np[7] c_np[8] c_np[9] c_np[10] c_np[11] c_np[12] c_np[13] c_np[14] c_np[15]
c_np[16] c_np[17] c_np[18] ave running file np.dat
fix 6 mb2 ave/time 2 50 10000 c_np2[1] c_np2[2] c_np2[3] c_np2[4] c_np2[5] c_np2[6] c_np2[7] c_np2[8] c_np2[9] c_np2[10] c_np2[11] c_np2[12] c_np2[13] c_np2[14]
c_np2[15] c_np2[16] c_np2[17] c_np2[18] ave running file np2.dat

dump 1 all custom ${dn} ip.dump type radius x y z vx vy vz

thermo ${dn}
thermo_style custom step ke

run_style verlet
run ${nstp}
write_data ip.data
write_restart rsip.inp
```

Segregation Results

- We have 2 types of particles with diameters 0.1 and 0.08 cm
- The domain has been divided into chunks of h = 0.1 cm along the z-axis
- Number fraction is defined as the fraction of each type of particle in a chunk
- The number fraction of the smaller particles drop as y increases. Conversely, the number fraction of the larger particles increase with increase in y



Size Ratio Analysis

Size Ratio Analysis

- We define $\mathbf{R = D_1/D_2}$: The ratio of the bigger particle radius to the smaller
- A dynamic analysis of the segregation can be performed by plotting the number fraction for the larger particles against the chunk index for different time steps.
  - This analysis has been shown in Figures **1** to **3** on the next slide
  - The common point of intersection of the trajectories plotted at each time step indicate the chunk index of the interface.
  - Note that **increasing R** while keeping $\mathbf{D_1}$ **constant** results in interface to shift downwards along the z-axis because smaller particles will occupy less volume than before.
  - A comparison between the trajectories at the same time step and different R show that **higher is the size ratio, faster is the segregation**

Results : Size Ratio Analysis

Figure 1.

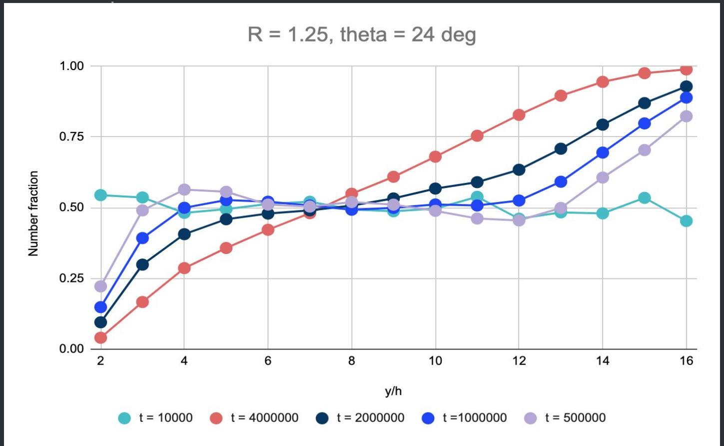


Figure 2.

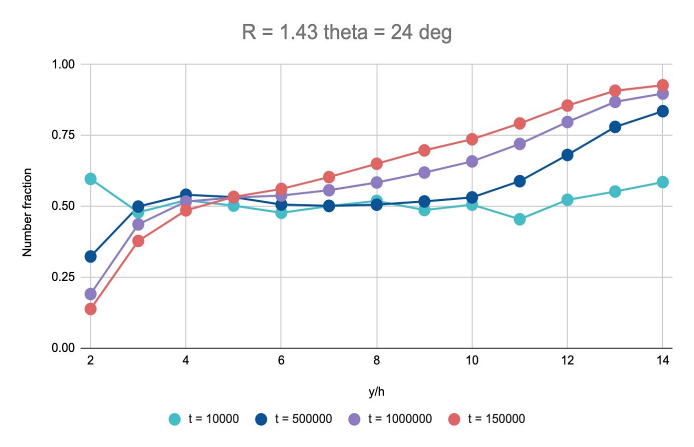
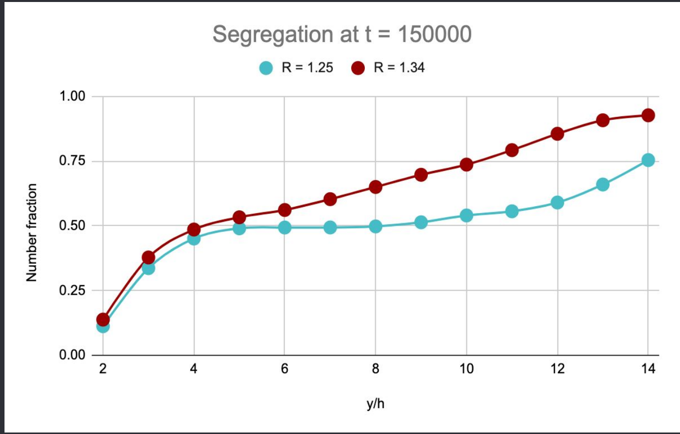


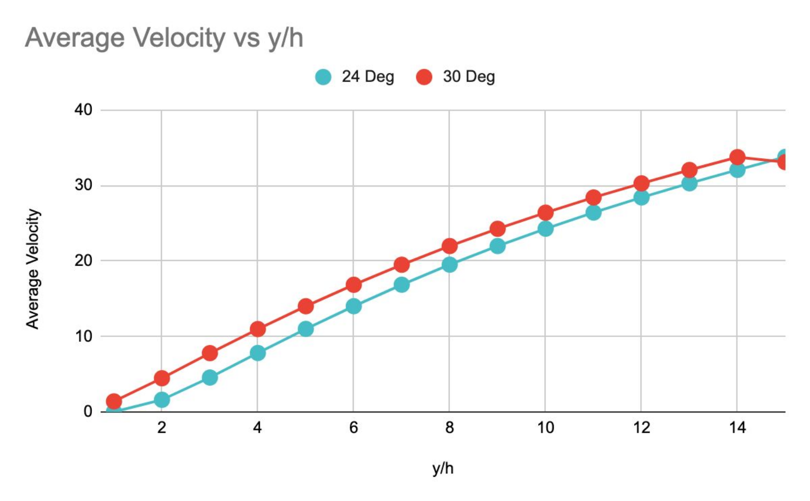
Figure 3.



Inclination Analysis

Inclination Analysis

- Plotting the average velocity of the bulk flow along the inclined plane against chunk index at different inclinations gives the following results :



- As per expectation, an increased inclination increases the acceleration along the inclined plane thereby increasing the velocity

References

- Anurag Tripathi, Alok Kumar, Mohit Nema, and D. V. Khakhar, *“Theory for size segregation in flowing granular mixtures based on computation of forces on a single large particle”*, Phys. Rev. E 103, L031301

Thank You!