Creating a Simple Simulation

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Creating a New Simulation

- Using the shortcut you previously created, navigate to the tutorial shortcut -> LIGGGHTS_Flexible_Fibers -> examples -> BondPackage -> Tutorials -> Single_Tests
- Make a new folder by
  mkdir simple_sim
- Change to the new directory
  cd simple_sim
- Create a new file
  touch in.liggghts
- Open this file in a txt editor

Starting the Script

- Defining the type of atoms
  atom_style hybrid granular bond/gran n_bondtypes 1 bonds_per_atom 6
  atom_modify map arrayhard_particles yes # For high young's modulus
- Turn off newton's 3rd law
  newton off
  communicate single vel yes
- Set boundaries as fixed
  boundary f f f
- Set units to si
  units si
- Create the simulation domain and state there is one type of atom
  region domain block 0.0 0.125 0.0 0.125 -0.01 0.10
  create_box 1 domain

Adding Physics

- Give the contact model
  pair_style gran model hertz tangential history
- Give the bond model
  bond_style gran
- Set the bin size
  neighbor 0.001 bin
- Tell liggghts to update the neighbor list every time step
  neigh_modify delay 0
- Set contact coefficients
  pair_coeff * * # contact physics do not need coefficients
- Set bond coefficients
  bond_coeff 1 1.0 0.0 4.0e9 2.0e8 1 0.01 1 1.0e16 1.0e16

Setting Material Properties, Adding a Wall, Add Gravity, and Set the Integration Scheme

- Setting properties
  fix m1 all property/global youngsModulus peratomtype 4.0e9
  fix m2 all property/global poissonsRatio peratomtype 0.3
  fix m3 all property/global coefficientRestitution peratomtypepair 1 0.5
  fix m4 all property/global coefficientFriction peratomtypepair 1 0.1

- Place the floor for the simulation
  fix floor all wall/gran model hertz tangential history primitive type 1 zplane 0.0

- Add gravity in the z-direction
  fix grav all gravity 9.81 vector 0.0 0.0 -1.0

- Use velocity verlet to update the simulation
  fix integr all nve/sphere

- Set the time step
  timestep 1.0e-6

Build Particle Template and Set Particle Insertion

- Set the fiber template

```
fix pts all particletemplate/multiplespheres 15485863 atom_type 1 density constant 2500 &
        nspheres 5 ntry 50000 spheres &
        0.000 0.0 0.0 0.001 &
        0.002 0.0 0.0 0.001 &
        0.004 0.0 0.0 0.001 &
        0.006 0.0 0.0 0.001 &
        0.008 0.0 0.0 0.001 &
        bonded yes
```

- Set particle distribution

```
fix pdd1 all particledistribution/discrete 32452843 1 pts1 1.0
```

- Create insertion region

```
region fill_box block 0.0 0.125 0.0 0.125 0.0065 0.07 units box
```

- Give insertion information

```
fix ins all insert/pack seed 32452867 distributiontemplate pdd1 maxattempt 500 insert_every once &
overlapcheck yes orientation random all_in yes vel constant 0.0 0.0 0.0 &
region fill_box particles_in_region 500 ntry_mc 10000 check_dist_from_subdomain_border no
```

Set Output

- Set output to the screen
  thermo_style custom step atoms numbond cpu cpuremain ke
- Print output every 1000 steps
  thermo 1000
- Ignore atoms that leave the domain and do not normalize output
  thermo_modify lost ignore norm no
- Create post folder for file output
  shell mkdir post
- Set particle dump output for ParaView
  dump dmp all custom 1000 post/damp*.liggghts id type x y z vx vy vz fx fy fz omegax omegay & omegaz radius

Bond the Particles

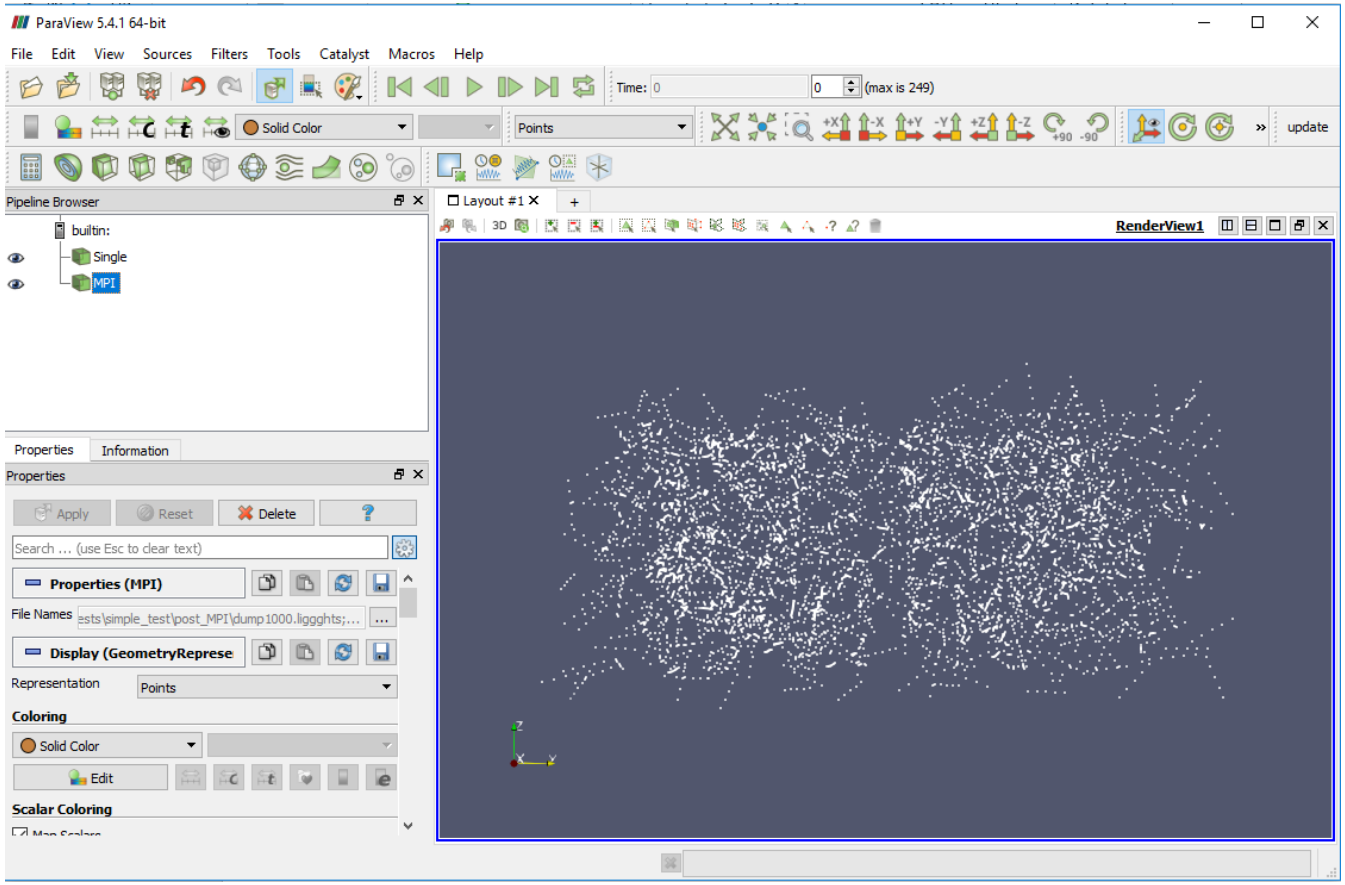
- Run once to insert the atoms
  run 1
- Create fix to bond atoms
  fix bondcr all bond/create/gran 1 1 1 0.002001 1 6
- Bond atoms to make particles
  run 1
- Do not allow any more bonds to form
  fix_modify bondcr every 0
- Run the simulation
  run 250000 upto
- Save script

Run the Simulation

- From the command line, run the script
  liggghts –in in.script
- After the simulation ends, move post to post_single
  mv post post_single
- Now run your script using MPI
  mpirun –n 4 liggghts –in in.script
- After simulation ends, move post to post _MPI
  mv post post_MPI

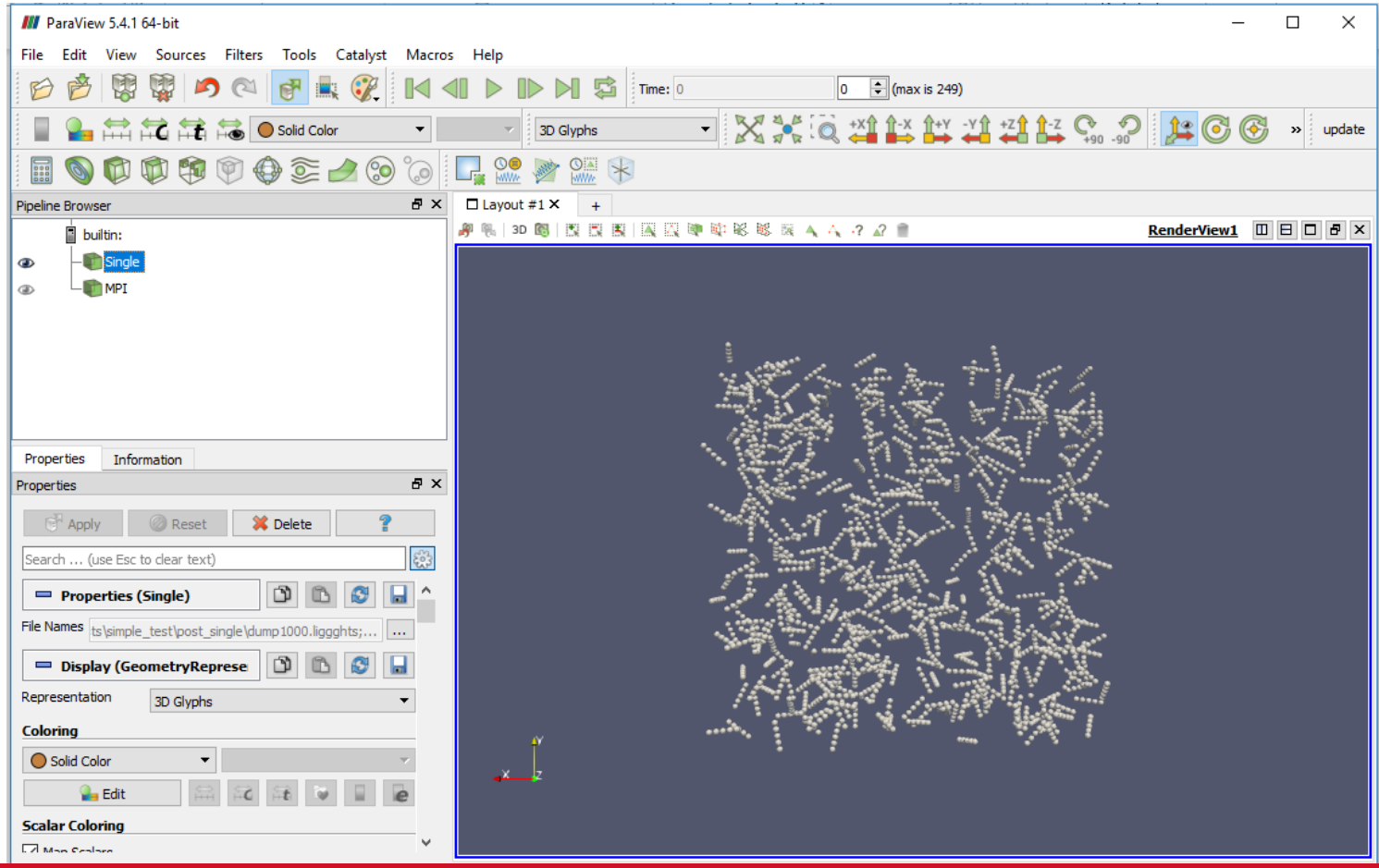
View Simulation in ParaView

- Open ParaView, Import both dump files, and rename them to Signle and MPI



Compare Single Core vs MPI runs

- Single Core – Notice uniformly distributed



Compare Single Core vs MPI runs

- Multicore – Notice the separate packings