



MIDWEST INTEGRATED CENTER FOR COMPUTATIONAL MATERIALS

<http://miccom-center.org>

Topic: COPSS Hands-on

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COPSS-Polarization, Step 1

Log into Midway1

Get copies of today's slides

```
/project2/micom-school/copss/slides/copss-hands-on.pdf  
(copy this to your local computer)
```

Request sinteractive node

```
$ cp /project2/micom-school/copss/interactive_request.sh ~/
```

Copy COPSS examples to your home directory

```
$ cp -r /project2/micom-school/copss/polarization_ex1 ~/  
$ cp -r /project2/micom-school/copss/copss-polarization-  
public/examples ~/polarization_ex2
```



Install Paraview locally

- **Download:** <https://www.paraview.org/download/>
- **Version:** v5.4
- **Operation system:** Mac OS X or Windows or Linux
- **Install:** Just click the download program



COPSS-Polarization, Step 3

Example 1

```
$ cd polarization_ex1
```

Submit job

```
$ sbatch polarization_dynamics.sbatch
```

Polarization files

```
control.in
```

```
interfaces.in
```

```
mesh.e
```

Lammps files

```
data.particles
```

```
lammps.in
```



COPSS-Polarization, Step 3

lammps.sandia.gov/doc/Section_start.html#start-4

2.3. Making LAMMPS with optional packages
 2.4. Building LAMMPS as a library
 2.5. Running LAMMPS
 2.6. Command-line options
 2.7. LAMMPS screen output
 2.8. Tips for users of previous LAMMPS versions

2.4. Building LAMMPS as a library

LAMMPS can be built as either a static or shared library, which can then be called from another application or a scripting language. See [this section](#) for more info on coupling LAMMPS to other codes. See [this section](#) for more info on wrapping and running LAMMPS from Python.

2.4.1. Static library

To build LAMMPS as a static library (*.a file on Linux), type

```
make foo mode=lib
```

where foo is the machine name. This kind of library is typically used to statically link a driver application to LAMMPS, so that you can insure all dependencies are satisfied at compile time. This will use the ARCHIVE and ARFLAGS settings in src/MAKE/Makefile.foo. The build will create the file liblammps_foo.a which another application can link to. It will also create a soft link liblammps.a, which will point to the most recently built static library.

2.4.2. Shared library

To build LAMMPS as a shared library (*.so file on Linux), which can be dynamically loaded, e.g. from Python, type

```
make foo mode=shlib
```

```
[xikai@midway-login2 examples]$ ls
accelerate  comb      DIFFUSE    ellipse    hugoniosat  melt      neb        prd
ASPHERE    controller dipole     flow       indent      micelled  inemd     python
balance    coreshell dreiding   friction   KAPPA      min       obstacle   qeg
body       COUPLE    eim        gcmc       kim         mscg     peptide    README
cmap       crack     ELASTIC   granregion MC          msst     peri       reax
colloid    deposit   ELASTIC_T HEAT       meam       nb3b     pour       rigid
[xikai@midway-login2 examples]$ cd COUPLE/
[xikai@midway-login2 COUPLE]$ ls
fortran  fortran2  lammps_quest  lammps_spparks  library  multiple  README  simple
```



COPSS-Polarization, Step 4

Start interactive session

```
cd ~/
interactive_request.sh
```

Example 2

```
cd polarization_ex2
cd sphere
cd 2_spheres
```

Run simulations by scanning center-to-center distance

```
./scan_distance.sh
```

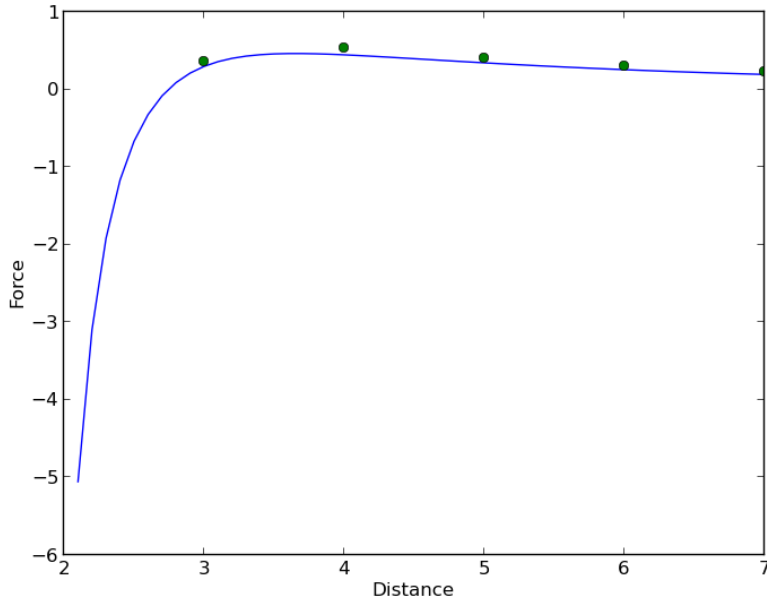
Generate plot

```
python plot_forces.py
```

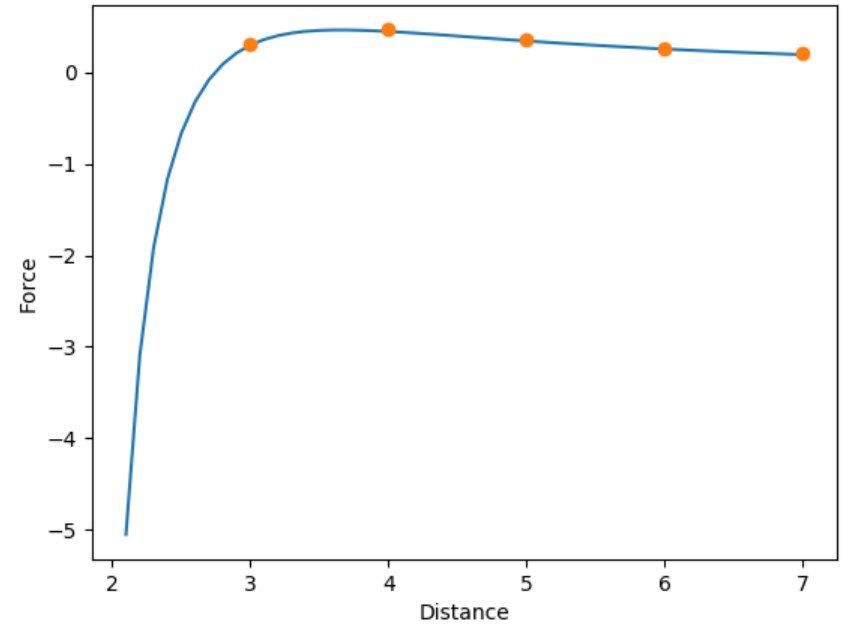
View forces in `compare_forces.png`



COPSS-Polarization, Step 4



722 element



2974 element



Change mesh file in the control file



COPSS-Polarization, Step 5

Check how the Example 1 goes
qstat -u username

After ~1 hour, back to Example 1
cd ~/polarization_ex1

Look at the folder
ls

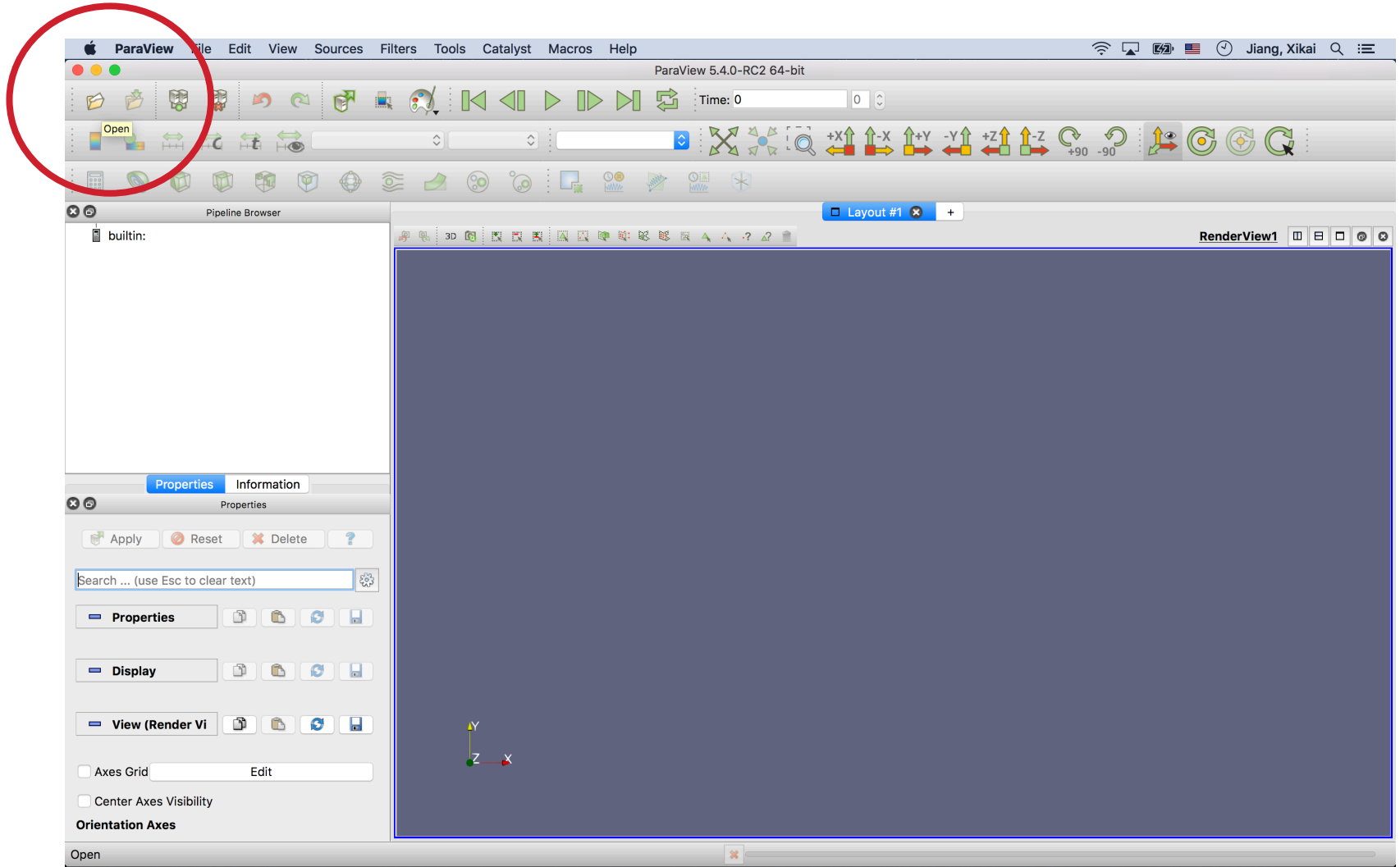
Visualize the particles' trajectory
if you can use Paraview on Midway
sinteractive.sh
paraview

if you can't use Paraview on Midway
On you laptop
sftp username@midway1.rcc.uchicago.edu
cd ~/polarization_ex1
get out.*

Open Paraview on your laptop



COPSS-Polarization, Step 6





COPSS-Polarization, Step 6

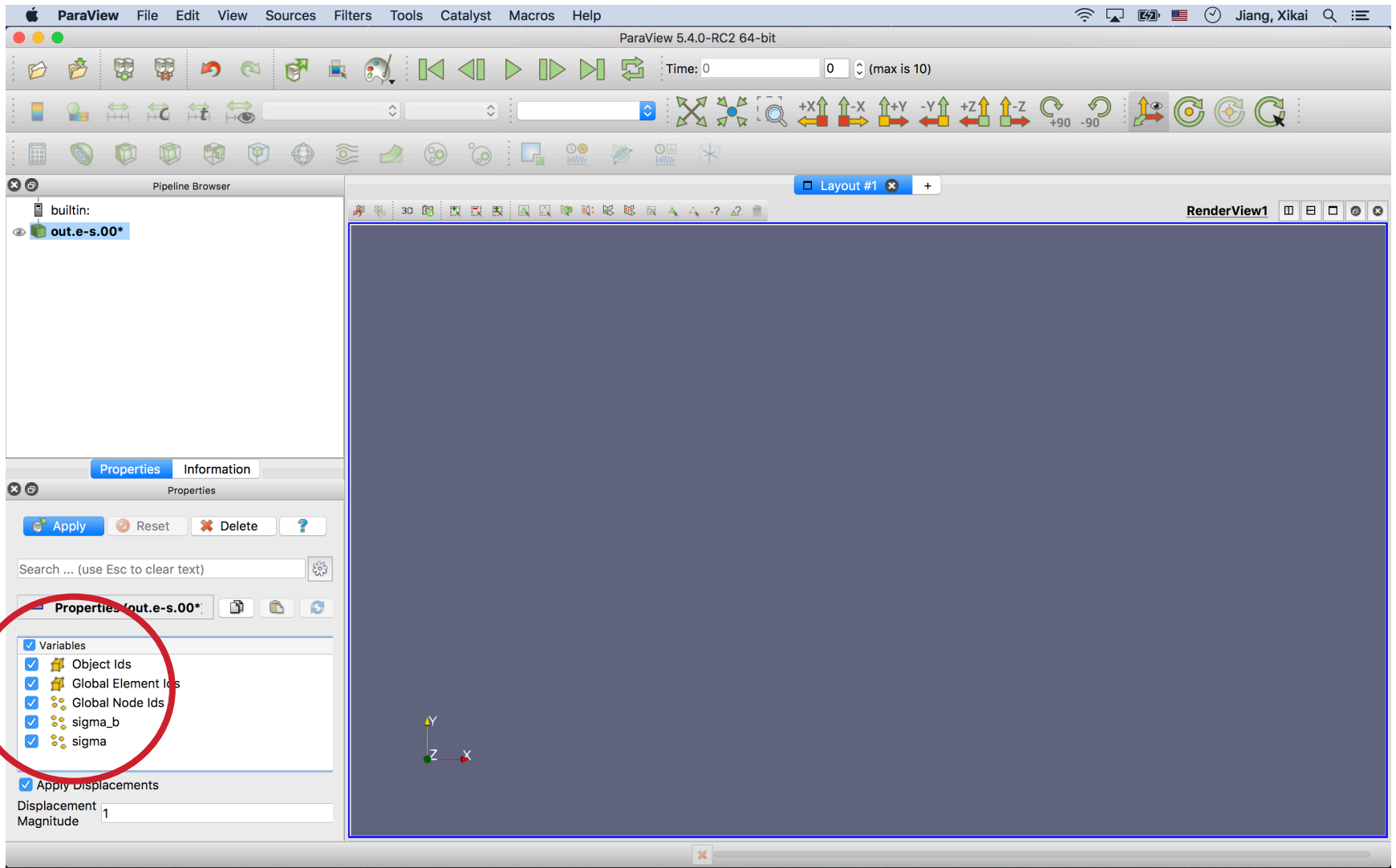
The screenshot shows the ParaView 5.4.0-RC2 64-bit interface. The main window is titled 'RenderView1' and displays a 3D view of a mesh. An 'Open File' dialog box is open, showing the file system structure. The 'Look in' field is set to '/Users/xikai/'. The file list shows the following entries:

Filename	Type	Size	Date Modified
Library	Folder		6/1/17 3:18 PM
finite-size-1000step	Folder		2/16/17 10:08 AM
ex03_cylinders_s...s_different_size	Folder		2/7/17 4:11 PM
Downloads	Folder		7/18/17 12:38 PM
Documents	Folder		7/15/17 3:38 PM
Desktop	Folder		7/18/17 10:02 PM
copss-polarization-public	Folder		7/17/17 5:05 PM
Box Sync	Folder		10/20/16 8:18 PM
Applications	Folder		5/25/17 11:51 AM
anaconda2	Folder		3/13/17 1:30 PM
▶ out.e-s	Group		
mesh.e	File	24.4 KB	7/18/17 8:27 PM

The 'out.e-s' folder is highlighted in blue, and a red circle is drawn around it. The 'File name' field contains 'out.e-s'. The 'Files of type' dropdown is set to 'Supported Files (*.inp *.cosmo *.cgns *.cml *.csv *.txt *.CSV *.TXT *...)'.

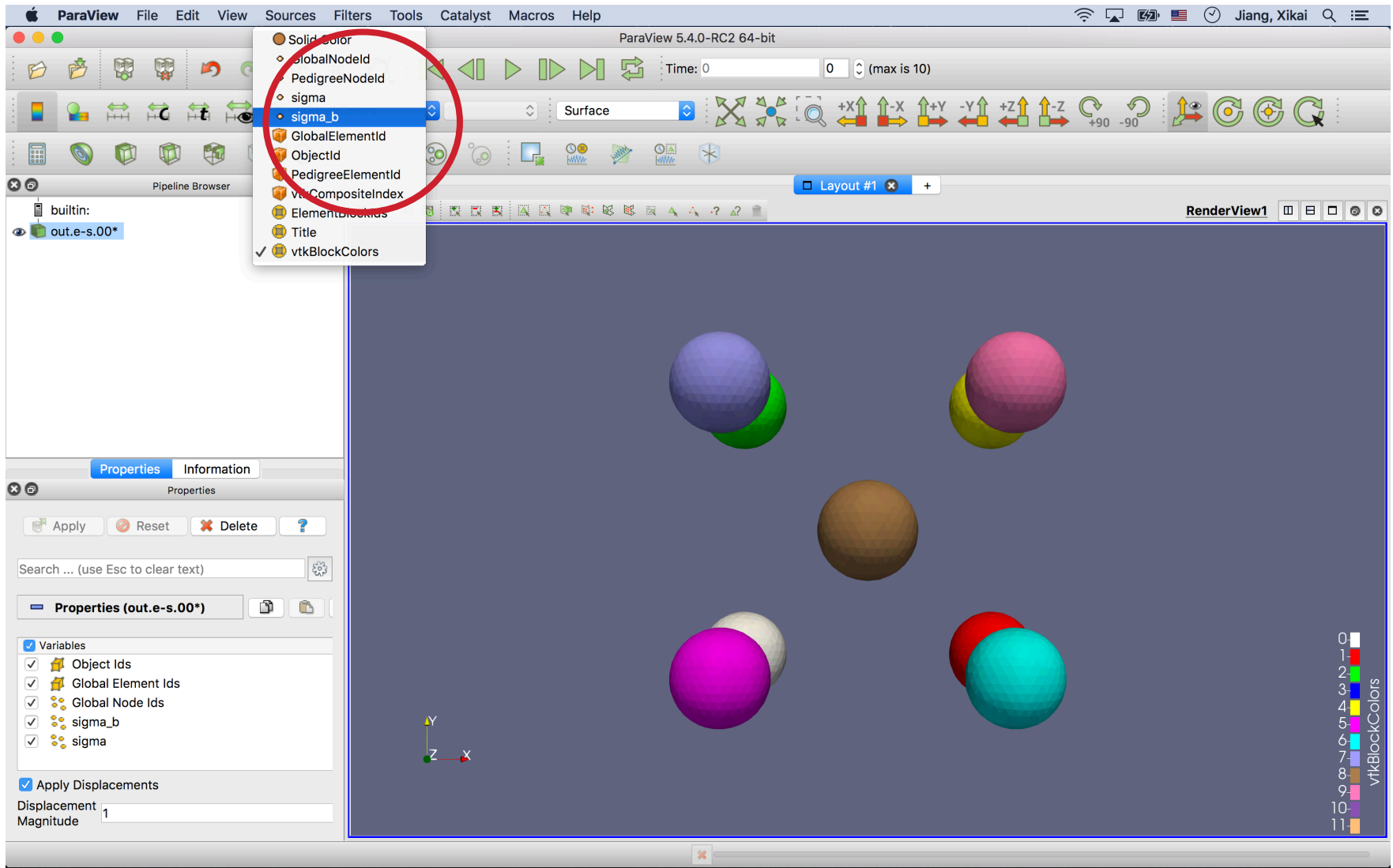


COPSS-Polarization, Step 6



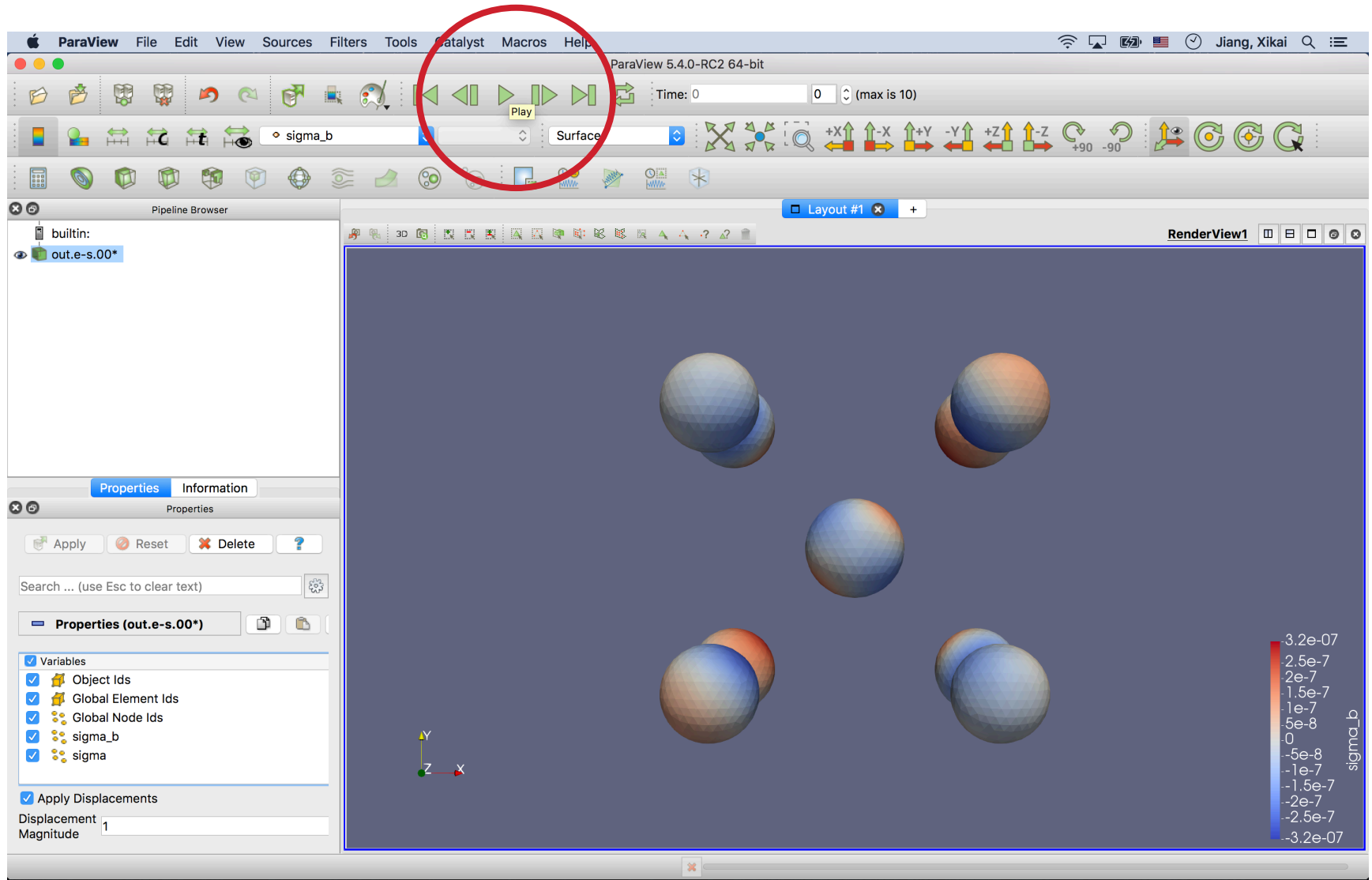


COPSS-Polarization, Step 6



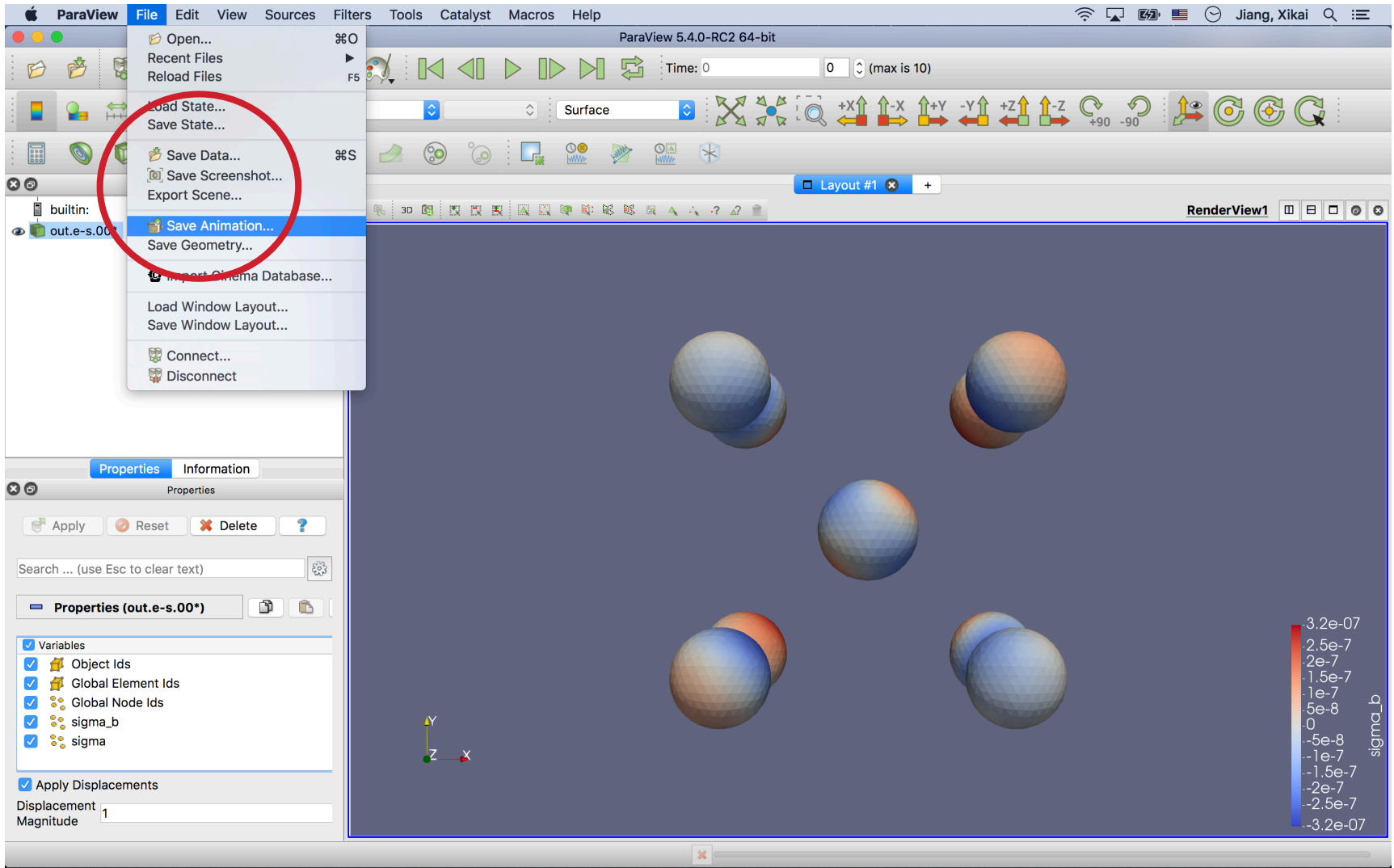


COPSS-Polarization, Step 6





COPSS-Polarization, Step 6





COPSS-Polarization, Step 6

The screenshot displays the ParaView 5.4.0-RC2 64-bit interface. The main window shows a 3D visualization of several spheres. A dialog box titled "Save Animation Options" is open in the center, with the "OK" button circled in red. The dialog box contains the following fields and options:

- Search ... (use Esc to clear text)
- Size and Scaling**
 - Image Resolution: 1075 x 634
- Coloring**
 - Override Color Palette: No change
 - Transparent Background
- Buttons: Cancel, OK

The background interface includes the Pipeline Browser on the left with "out.e-s.00*" selected, the Properties panel with "Properties (out.e-s.00*)" active, and a color scale for "sigma_b" on the right ranging from -3.2e-07 to 3.2e-07.



COPSS-Polarization, Step 6

ParaView 5.4.0-RC2 64-bit

Time: 0 (max is 10)

sigma_b Surface

Layout #1

RenderView1

Save Animation Options

Search ... (use Esc to clear text)

Size and Scaling

Image Resolution 1075 x 634 x2 /2

Coloring

Override Color Palette

- No change
- Black Background
- Default Background
- Gradient Background
- Gray Background
- Print Background
- White Background

Cancel OK

Properties (out.e-s.00*)

- Variables
 - Object Ids
 - Global Element Ids
 - Global Node Ids
 - sigma_b
 - sigma
- Apply Displacements
 - Displacement 1
 - Magnitude 1

sigma_b

3.2e-07

2.5e-7

2e-7

1.5e-7

1e-7

5e-8

0

-5e-8

-1e-7

-1.5e-7

-2e-7

-2.5e-7

-3.2e-07



COPSS-Polarization, Step 6

ParaView 5.4.0-RC2 64-bit

Time: 0 (max is 10)

sigma_b Surface

RenderView1

Save Animation

Look in: /

Filename	Type	Size	Date Modified
Volumes	Folder		7/18/17 6:58 PM
var	Folder		6/1/17 12:28 PM
usr	Folder		7/12/17 3:33 PM
Users	Folder		6/1/17 12:22 PM
tmp	Folder		7/18/17 10:03 PM
System	Folder		6/1/17 12:18 PM
sbin	Folder		6/1/17 12:21 PM
private	Folder		6/1/17 12:22 PM
OS X Install Data	Folder		5/25/17 2:59 PM
opt	Folder		12/23/15 8:09 AM
Network	Folder		7/10/17 8:59 PM
net	Folder		7/18/17 7:05 PM

File name: polarizableMovie

Files of type: AVI files (*.avi) Ogg/Theora files (*.ogv) PNG images (*.png) JPEG images (*.jpg) TIFF images (*.tif) BMP images (*.bmp) PPM images (*.ppm)

OK Cancel

sigma_b

3.2e-07
2.5e-7
2e-7
1.5e-7
1e-7
5e-8
0
-5e-8
-1e-7
-1.5e-7
-2e-7
-2.5e-7
-3.2e-07



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Topic: COPSS-Hydrodynamics

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Outline

- Launch the code
- Run a few examples
- Data visualization using Paraview



Launch the code on Midway

- SSH to Midway
- Make a copy of COPSS-Hydrodynamics-Public codes

```
$ cp -r /project2/miccom-school/copss/copss-hydrodynamics-public ~/
```

- Compile the code

```
$ cd ~/copss-hydrodynamics-public/src/
```

```
$ bash compile.sh      (takes about a minute)
```



Run an example

- Go to example folder

```
$ cd ~/copss-hydrodynamics-public/examples/general_point_particle/polymer_chain
```

```
$ ls
```

- Take a look at the job submission file

```
$ vi rcc_sbatch.sh
```

- Submit a job using sbatch

```
$ sbatch rcc_sbatch.sh
```

(takes around 20 seconds)

- Take a look at output file

```
$ vi copss_demo
```

- Plot mean square displacement

```
$ module load python/2.7
```

```
$ python msd_plot.py
```



Data visualization

- Make a copy of the data to local laptop (**open a new terminal tab**)

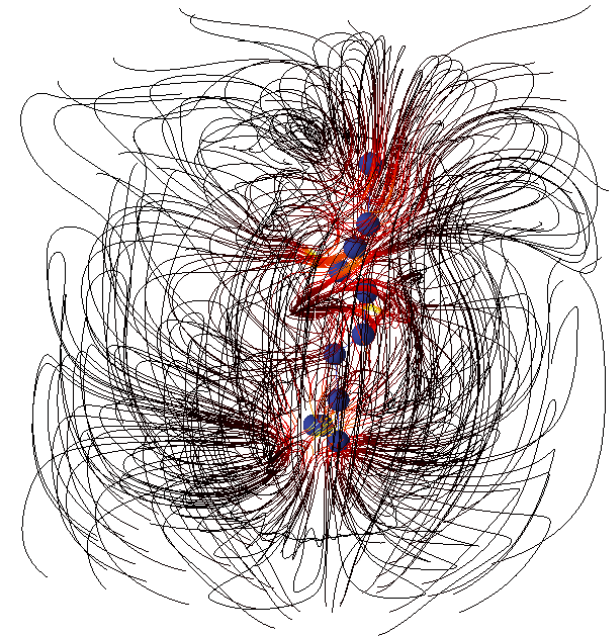
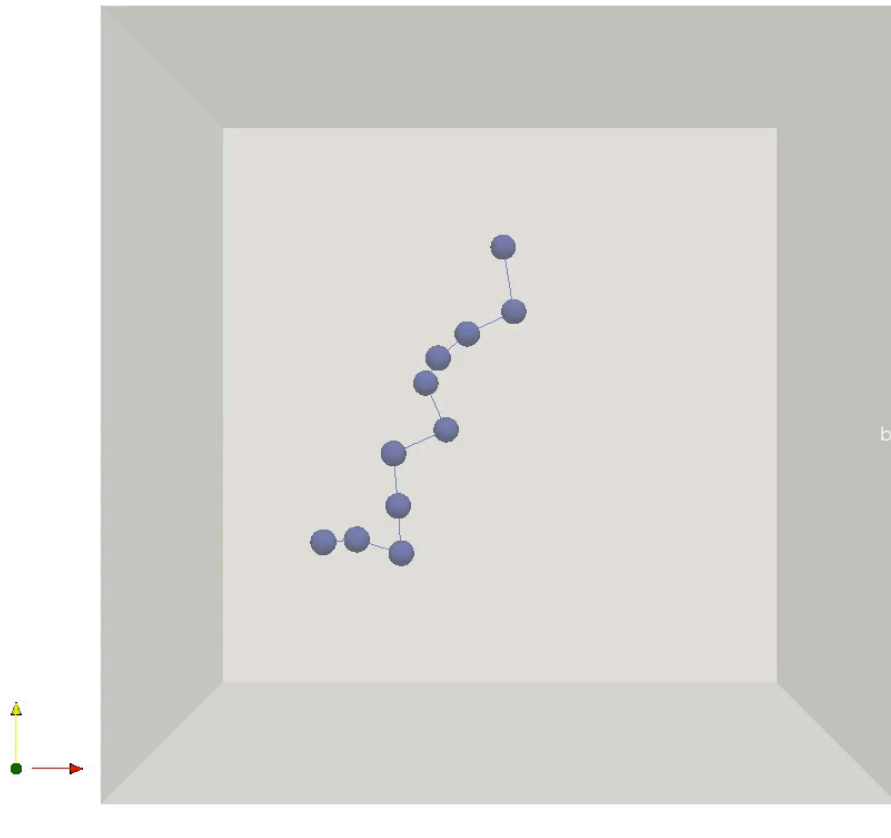
```
$ scp -r midway.rcc.uchicago.edu: ~/copss_hydrodynamics_public/  
examples/general_point_particle/polymer_chain ~/Desktop
```

- Take a look msd plot
(**Meaning MSD usually takes long simulation time**)
- Visualize polymer and fluid using Paraview

Follow me :)



Data Visualization using Paraview



Thanks for your attention.

Q & A.

Safe Travels.