
http://miccom-center.org

Topic: COPSS Hands-on

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de Pablo group, The University of Chicago

# COPSS-Polarization, Step 1

Log into Midway1

Get copies of today's slides

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

Request sinteractive node

**$ cp /project2/miccom-school/copss/interactive_request.sh ~/**

Copy COPSS examples to your home directory

**$ cp -r /project2/miccom-school/copss/polarization_ex1 ~/**

**$ cp -r /project2/miccom-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**

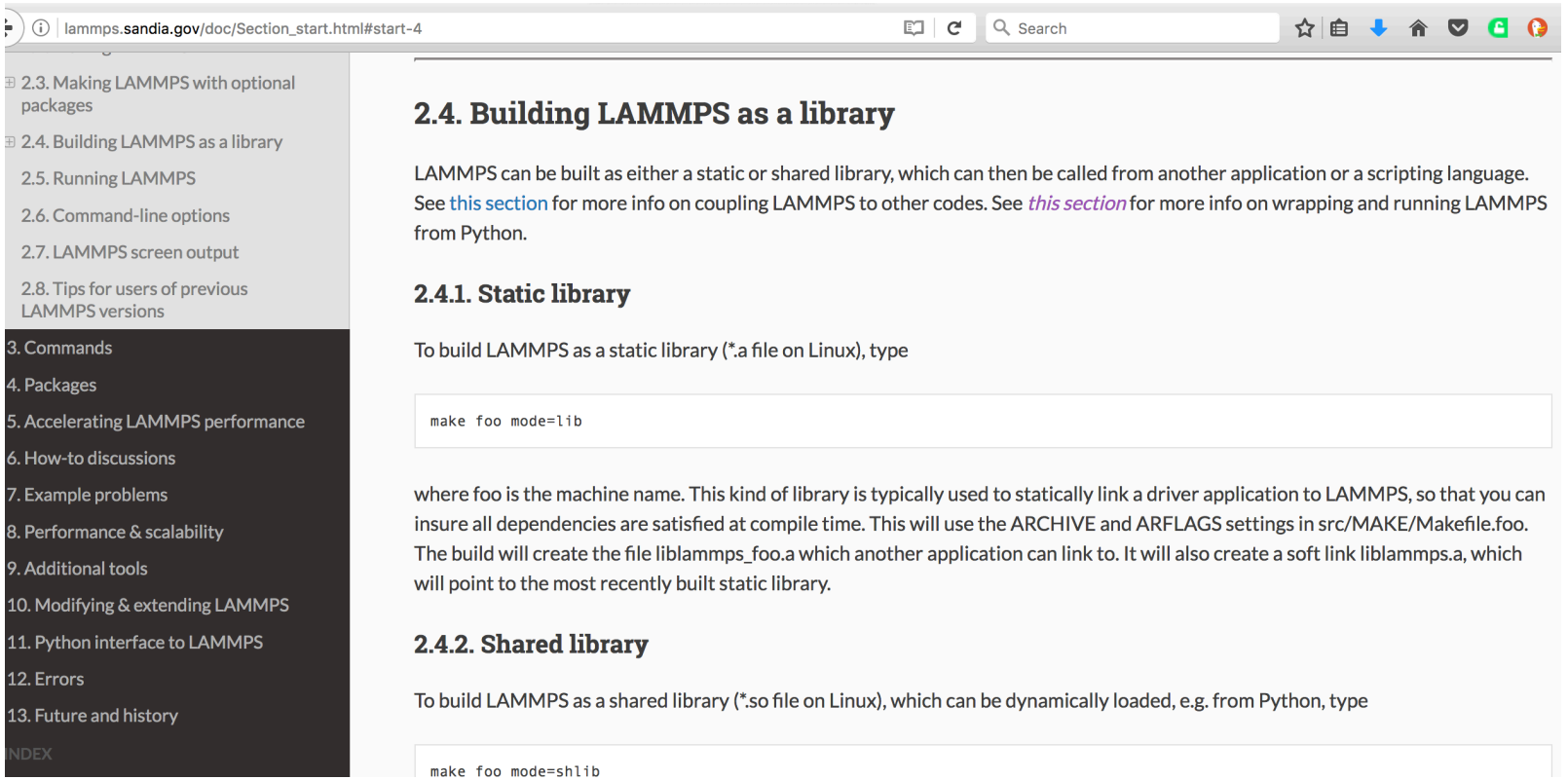
Polarization files

*control.in*
*interfaces.in*
*mesh.e*

Lammps files

*data.particles*
*lammps.in*

# COPSS-Polarization, Step 3




```
[xikai@midway-login2 examples]$ ls
accelerate  comb        DIFFUSE    ellipse     hugoniostat  melt      neb       prd
ASPHERE     controller  dipole     flow        indent       micelle   nemd      python
balance     coreshell   dreiding   friction    KAPPA        min       obstacle  qeq
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

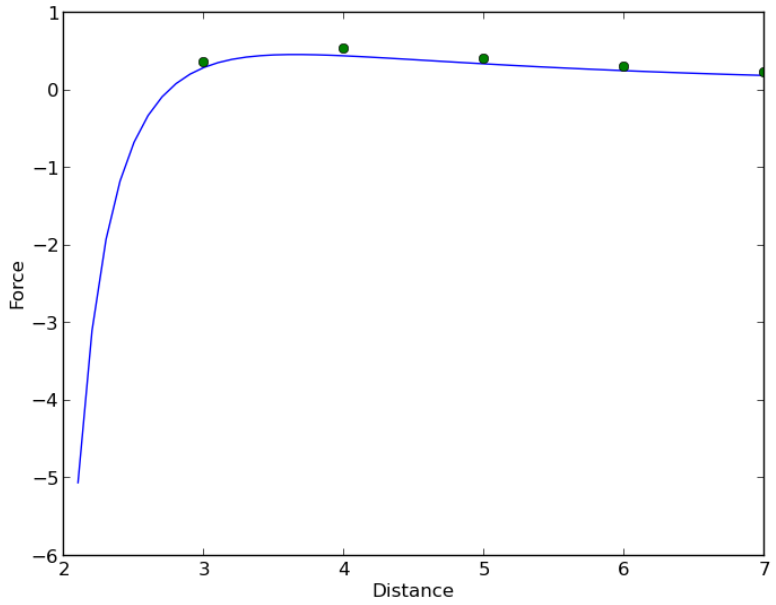
**./scan_distance.sh**

Generate plot

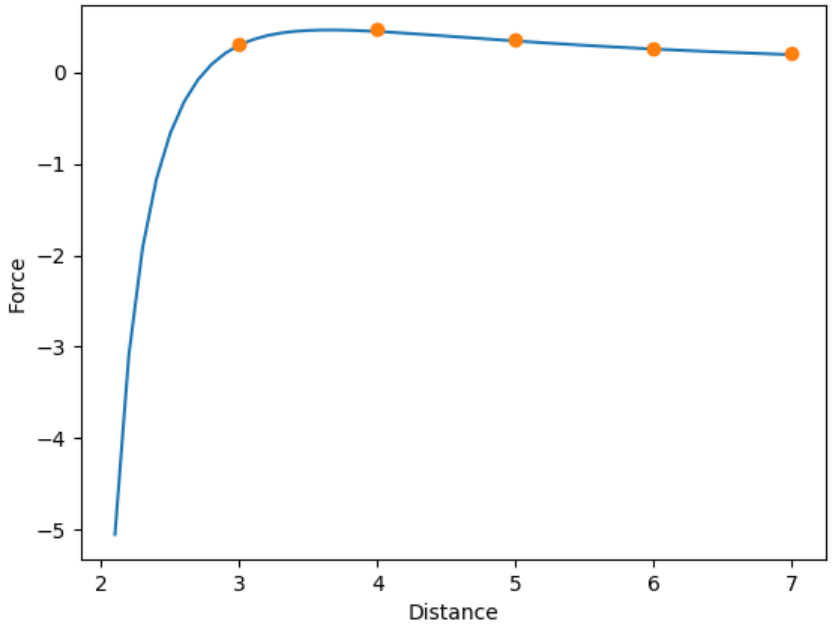
**python plot_forces.py**

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



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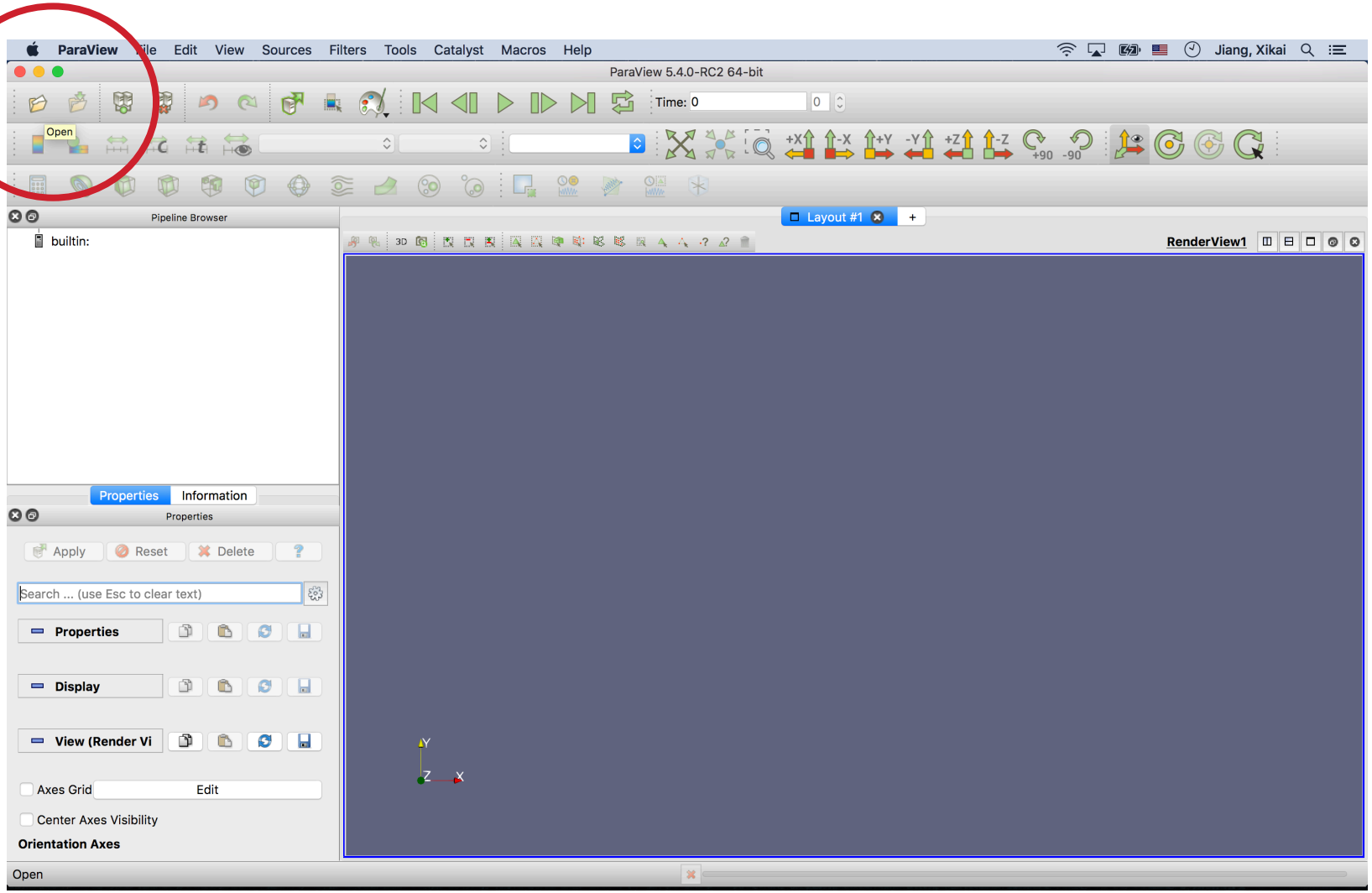
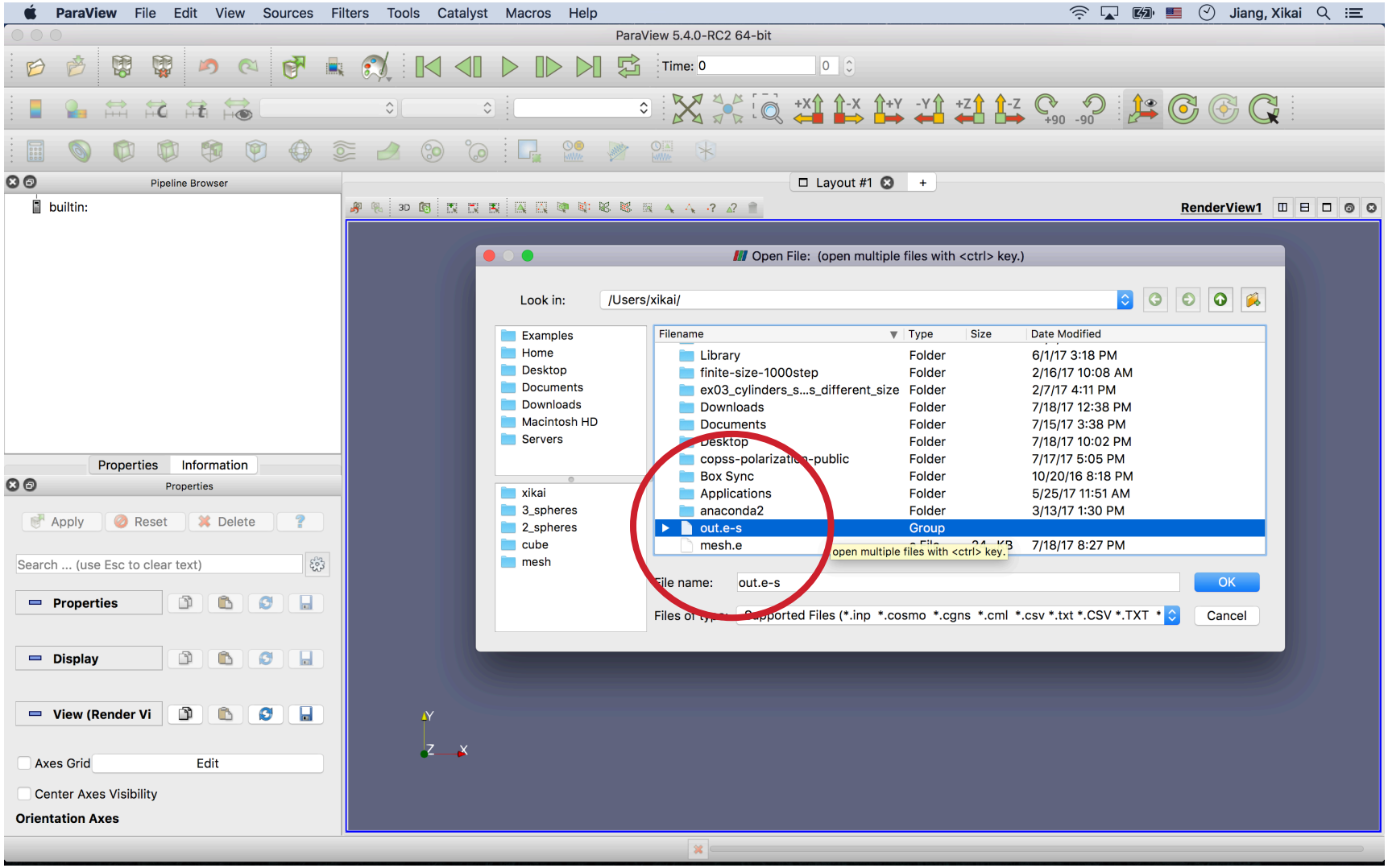
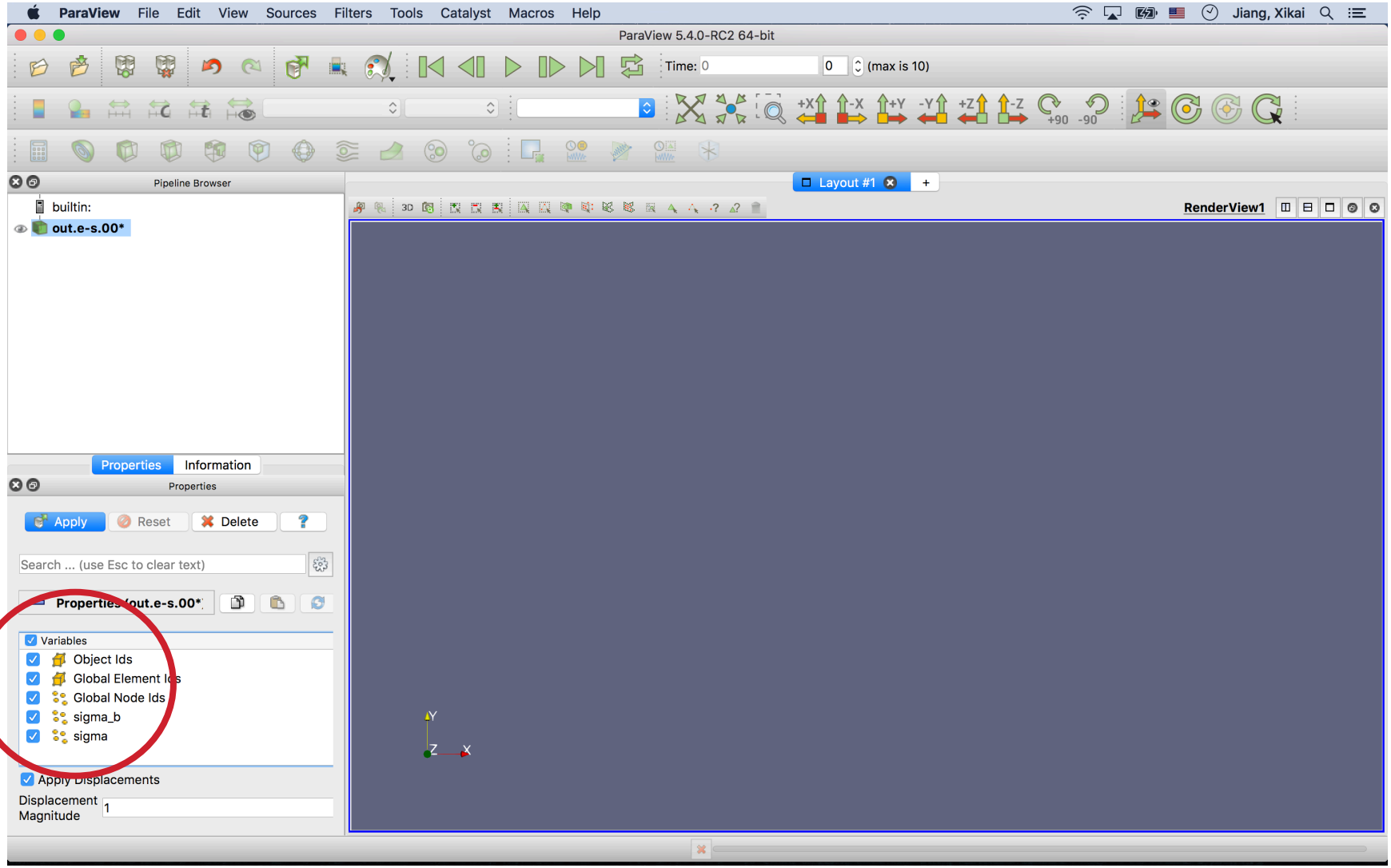
# COPSS-Polarization, Step 6



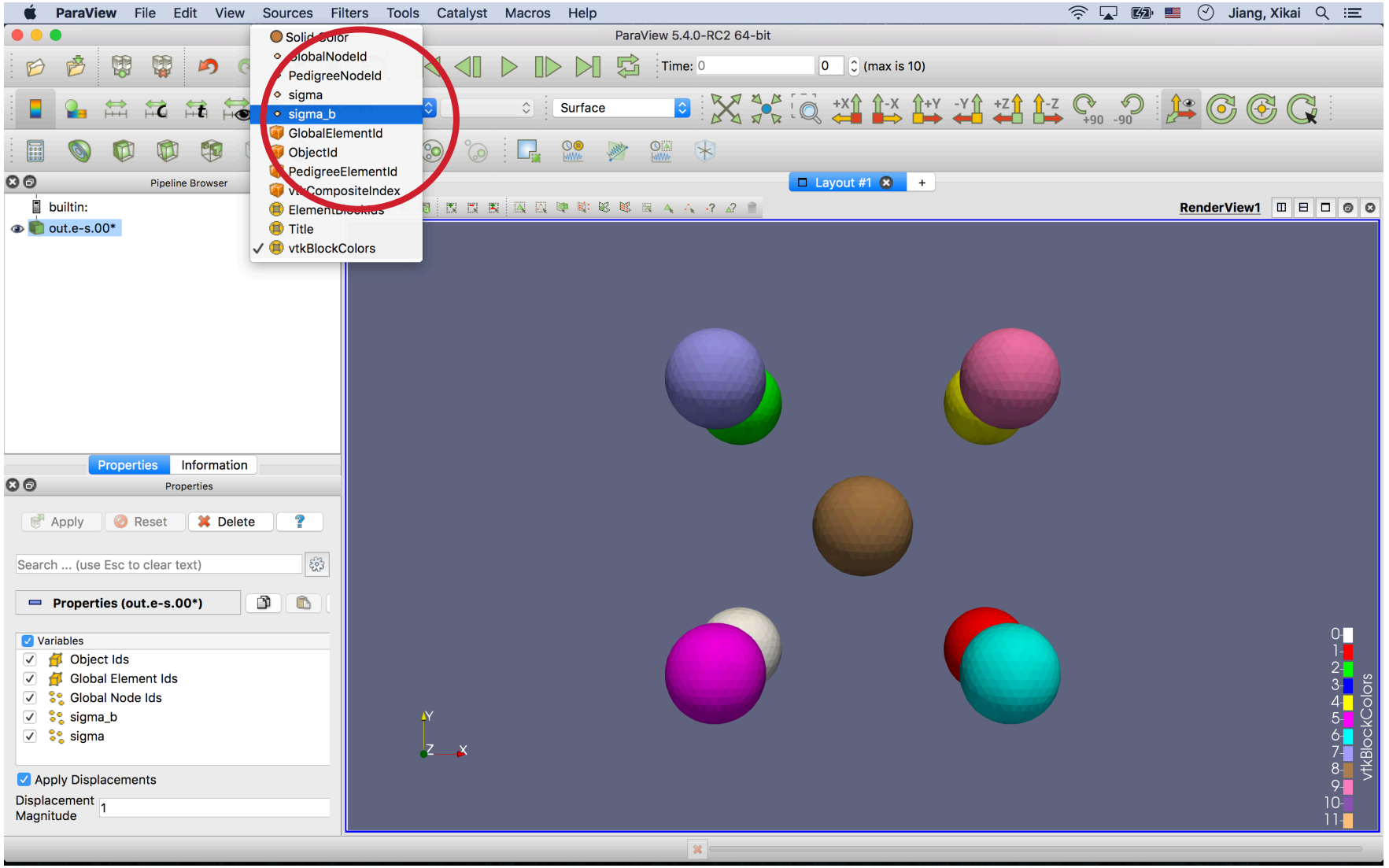
# COPSS-Polarization, Step 6



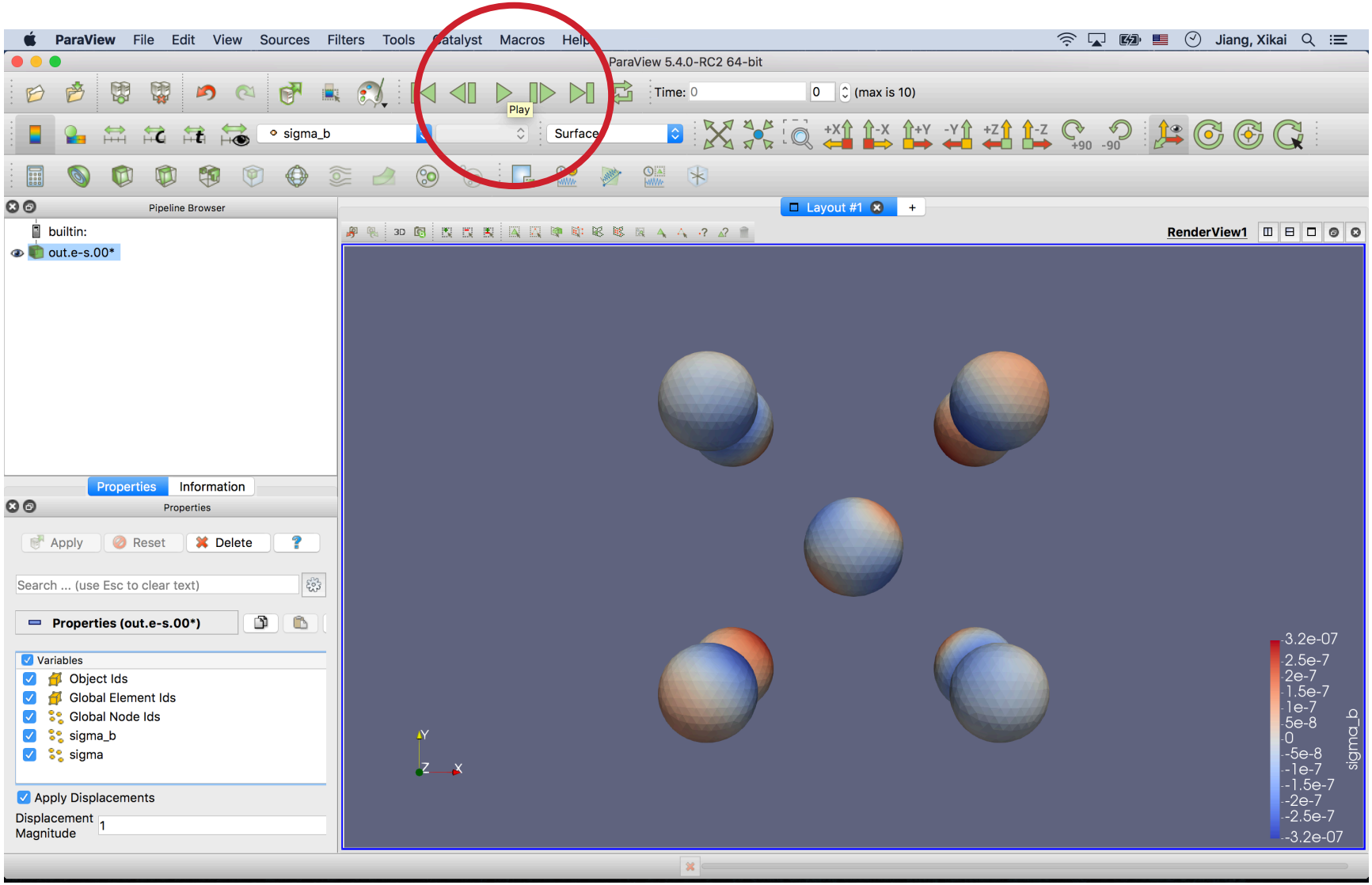
# COPSS-Polarization, Step 6



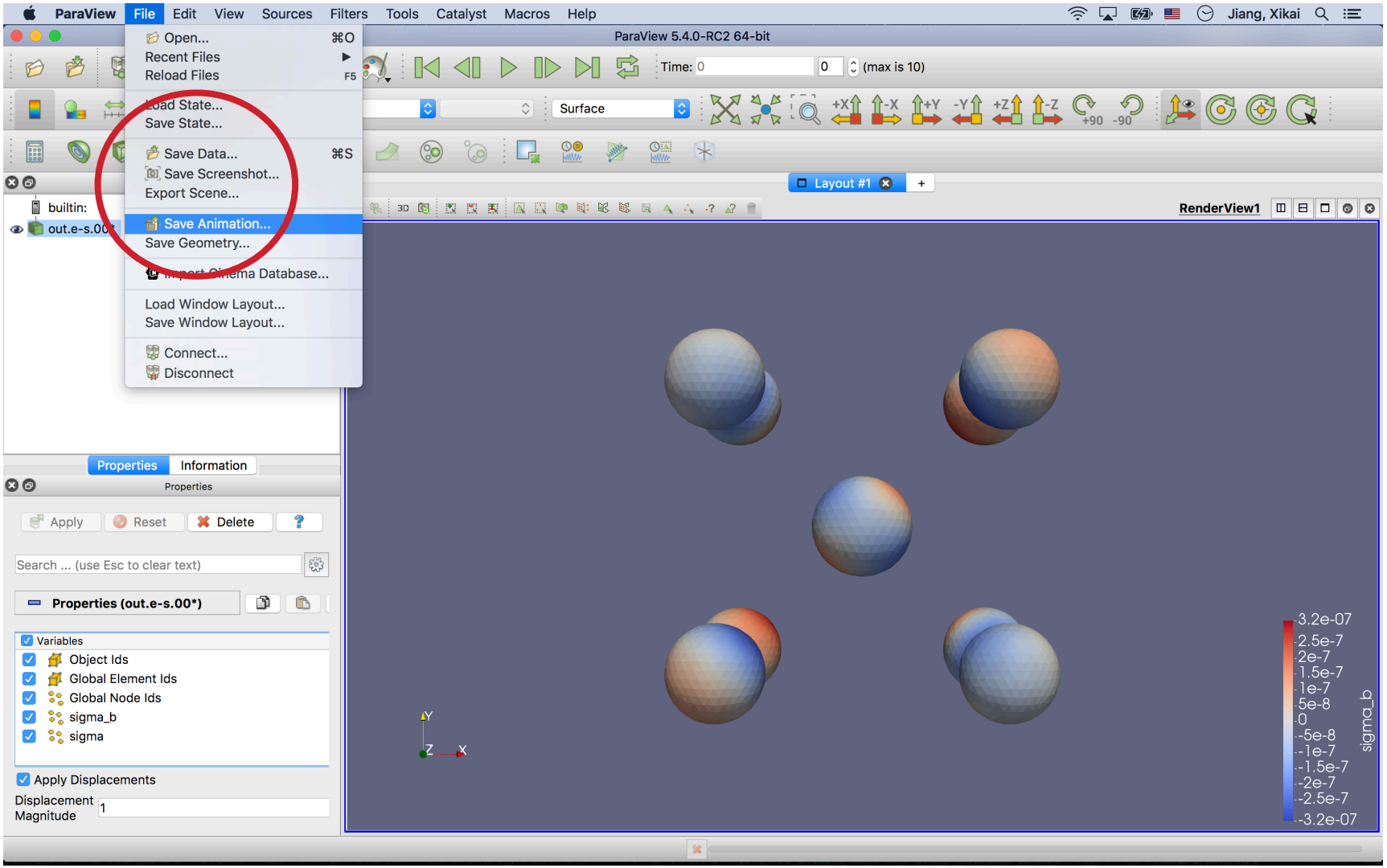
# COPSS-Polarization, Step 6



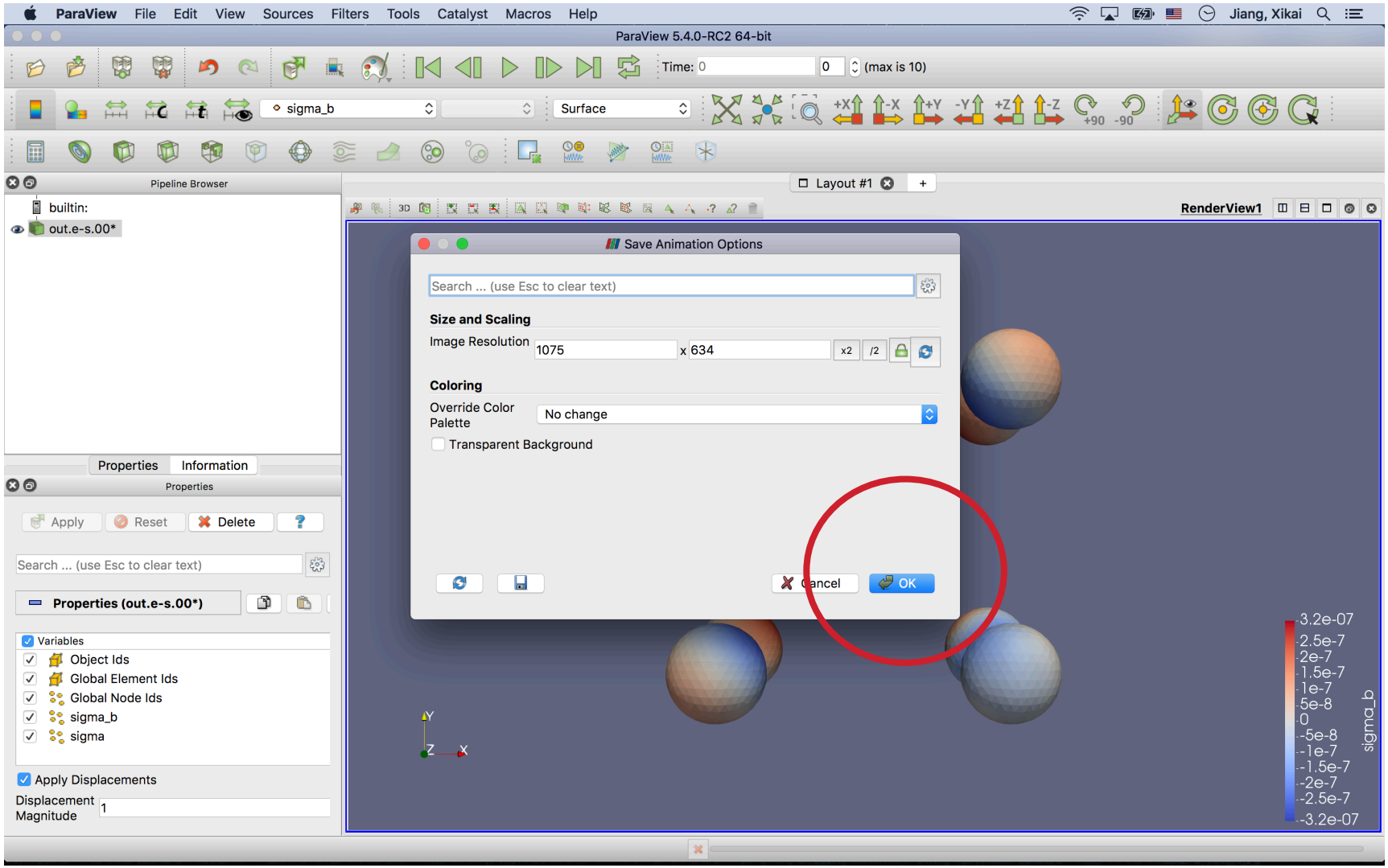
# COPSS-Polarization, Step 6



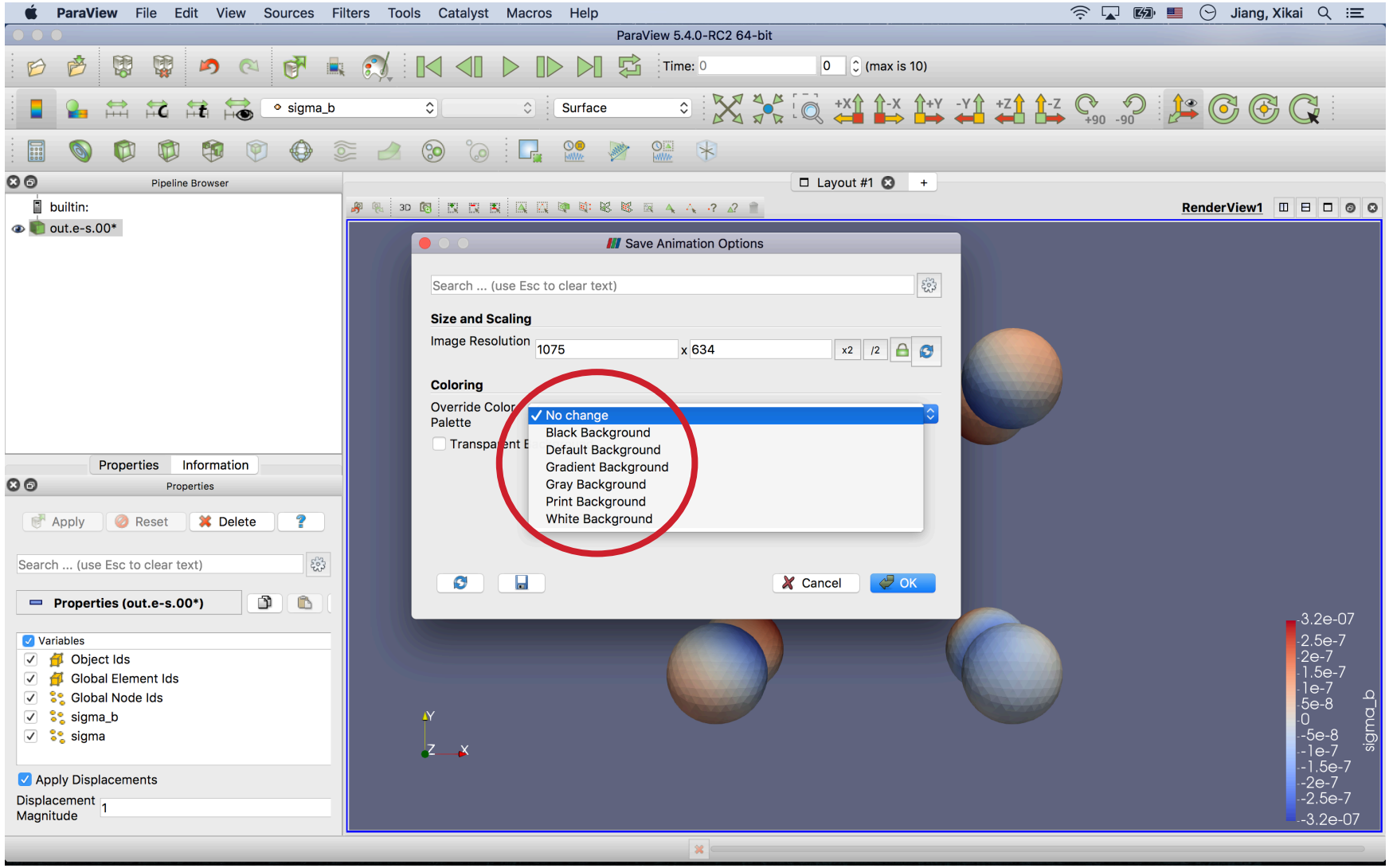
# COPSS-Polarization, Step 6



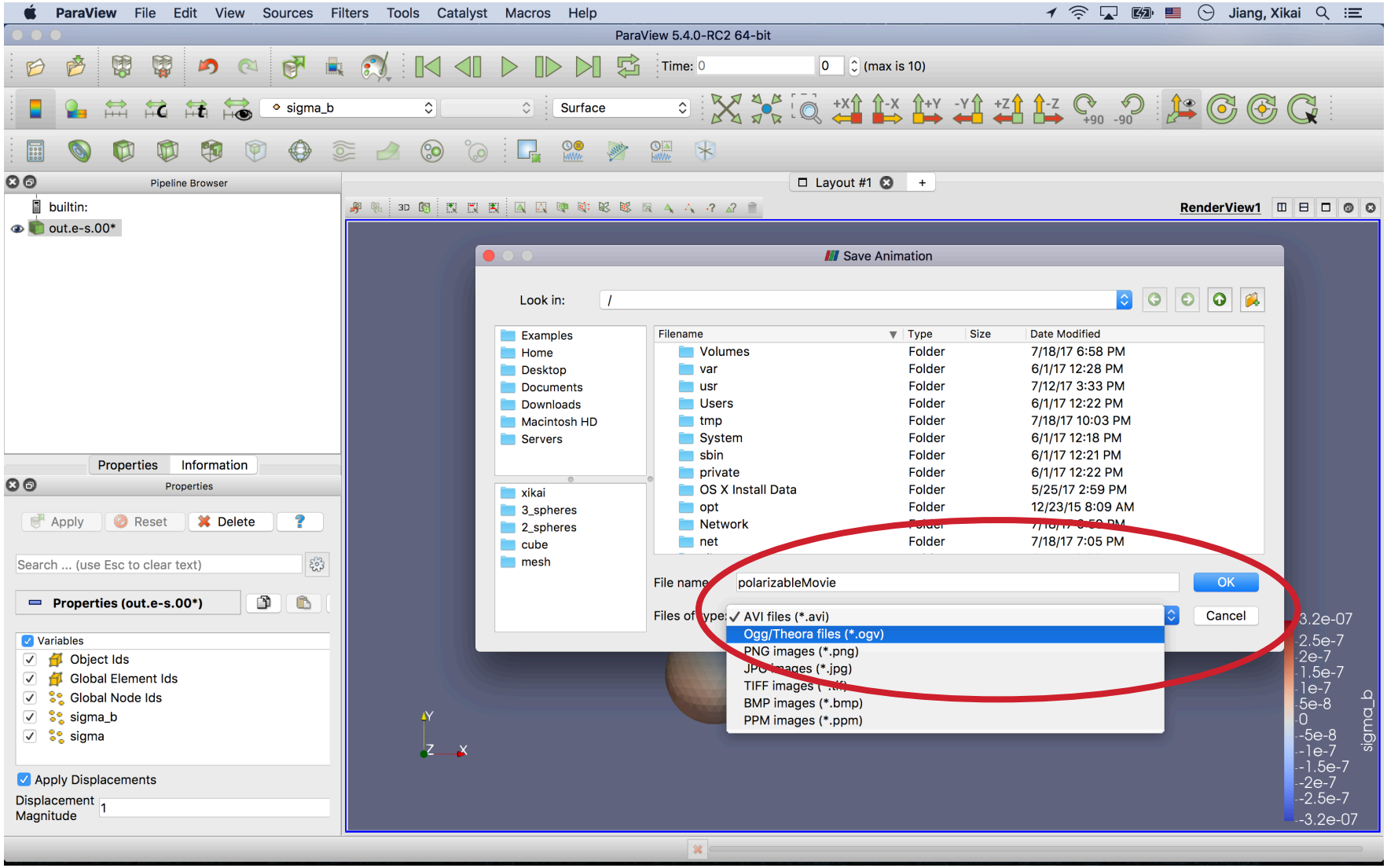
# COPSS-Polarization, Step 6



# COPSS-Polarization, Step 6



# COPSS-Polarization, Step 6

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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**



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# Data visualization

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

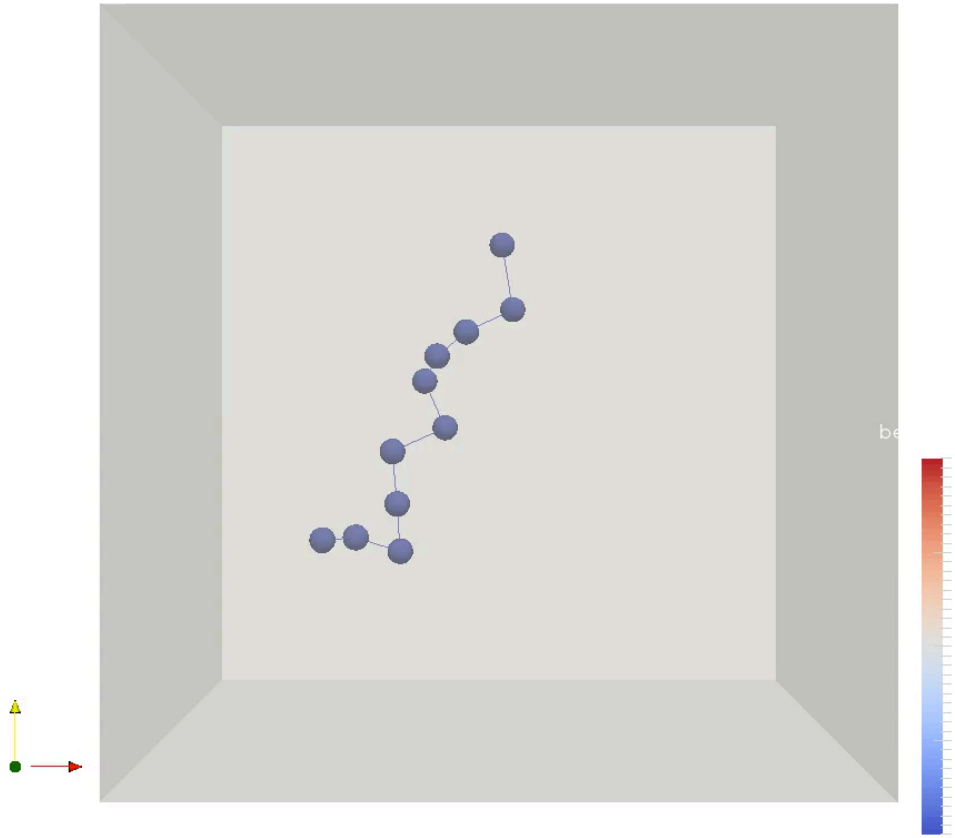
  **$ scp –r midway.rcc.uchicago.edu: ~/copss_hydrodynamics_public/examples/general_point_particle/polymer_chain ~/Desktop**

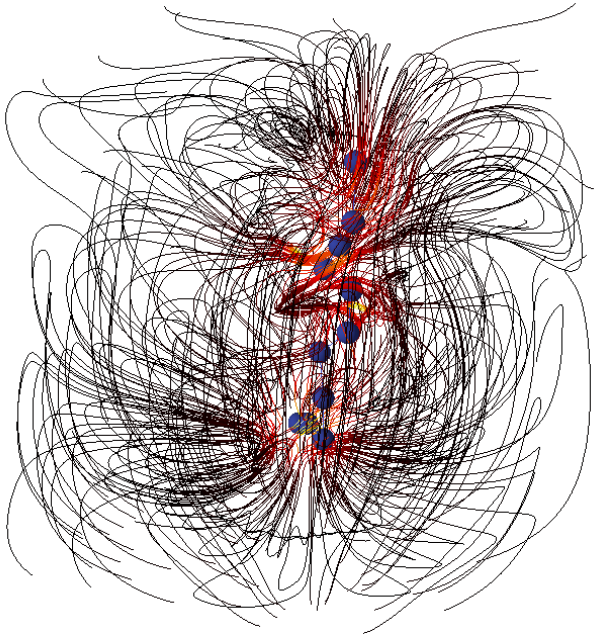
- Take a look msd plot
  **(Meaning MSD usually takes long simulation time)**

- Visualize polymer and fluid using Paraview

  **Follow me :)**

# Data Visualization using Paraview





Thanks for your attention.

Q & A.

Safe Travels.

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