

70 YEARS OF CREATING TOMORROW



**Los Alamos**  
NATIONAL LABORATORY

# Visualizing PSI Simulation with ParaView

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Data Science @ Scale Team

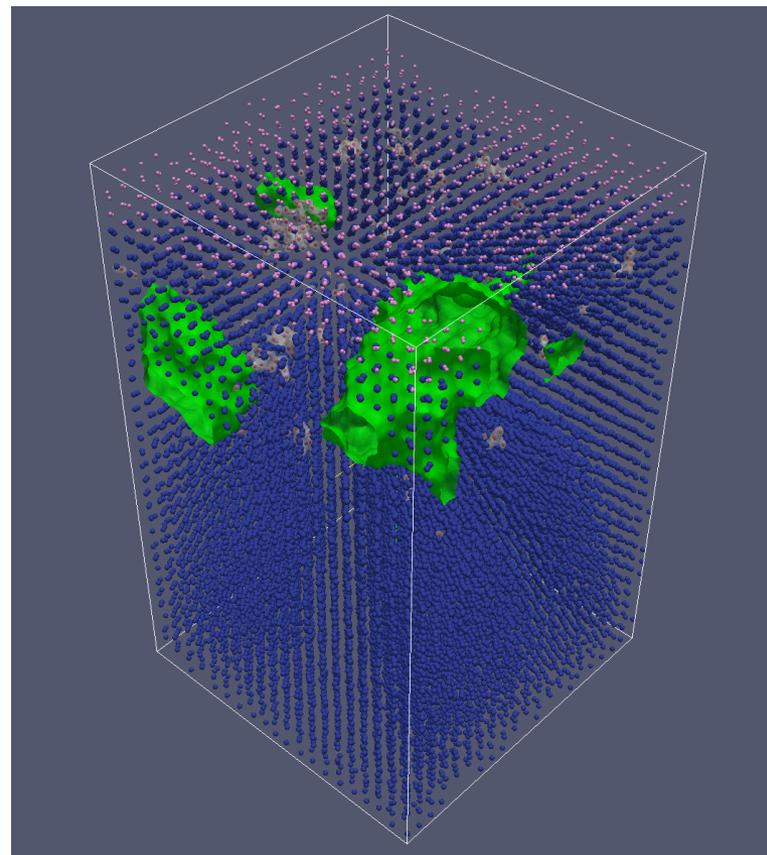
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UNCLASSIFIED



# Goals

- ParaView as *your* visualization tool
- Visualization techniques
- Avoid common pitfalls
- Inspired by *ParaView The Red Blood Cell Tutorial* from Argonne.





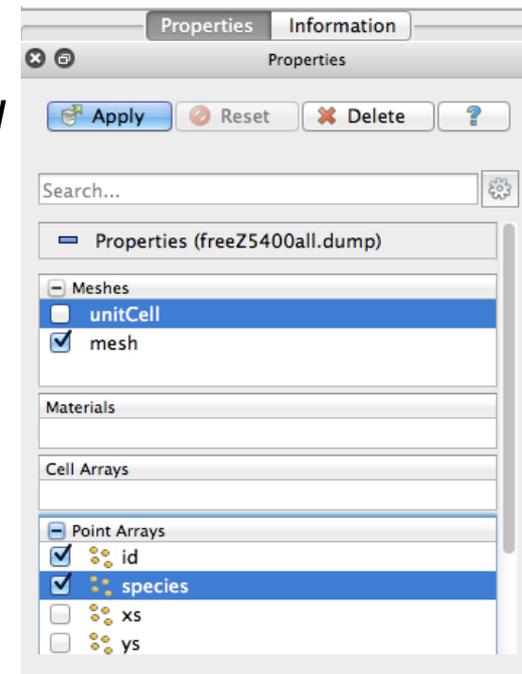
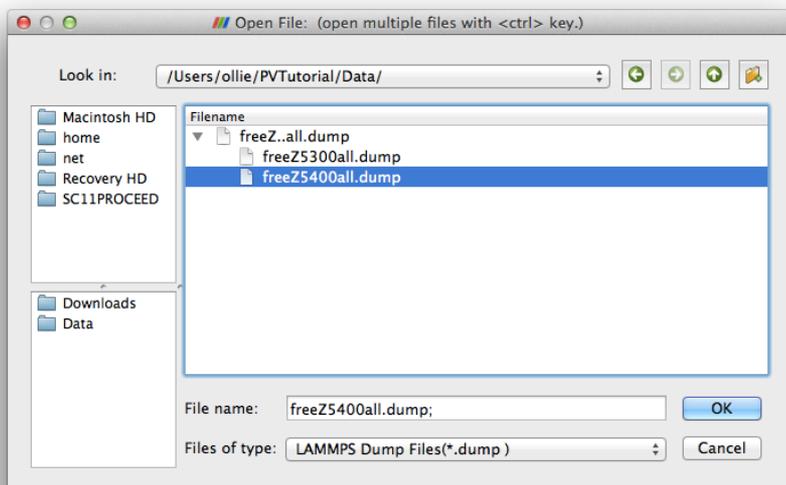
# Data

- LAMMPS simulation of Plasma Surface Interaction
- He injection/He bubble/Bubble burst/Tungsten cavity
- Courtesy of Faiza Sefta



# Load LAMMPS Dump File

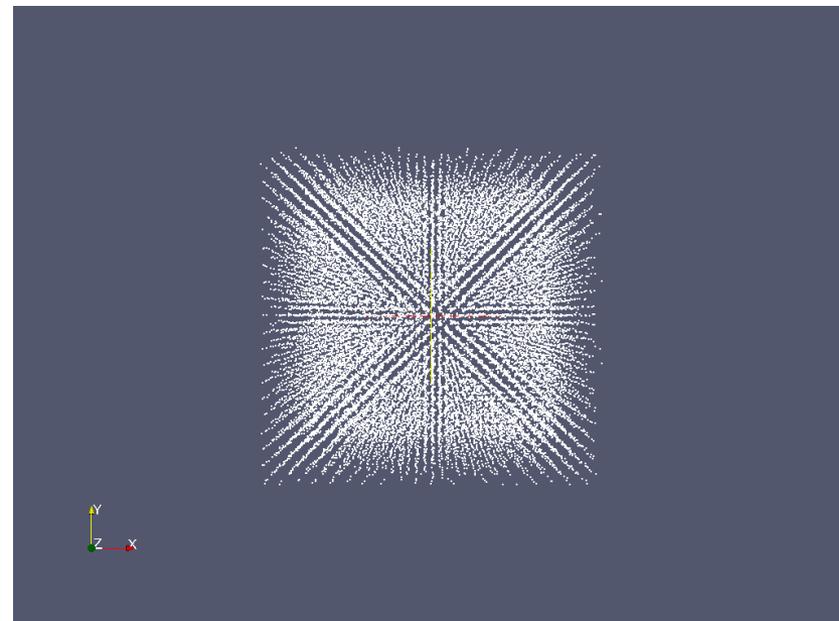
- From File menu:
  - Open
  - Choose LAMMPS Dump Files
- In *Properties* tab:
  - Check *mesh*
  - Uncheck *unitCell*
  - Check *id* and *species*
  - Click *Apply*





# Default View

- Atoms are represented as points
- Single solid white color
- Looking toward -Z





# Data Inspection

- *Information* tab shows:
  - Underlying VTK data type
  - Number of cells/points
  - Bounding box of cells/points
  - Attributes (data arrays) and their ranges

The screenshot shows a software window titled 'Information' with two tabs: 'Properties' and 'Information'. The 'Information' tab is active. The window displays the following information:

**Data Hierarchy**

- Multi-block Dataset (expanded)
- mesh

**Properties**

Filename: freeZ5400all.dump  
Path: /Users/ollie/PVTutorial/Data

**Statistics**

Type: Multi-block Dataset  
Number of Cells: 24712  
Number of Points: 24712  
Memory: 0.87 MB

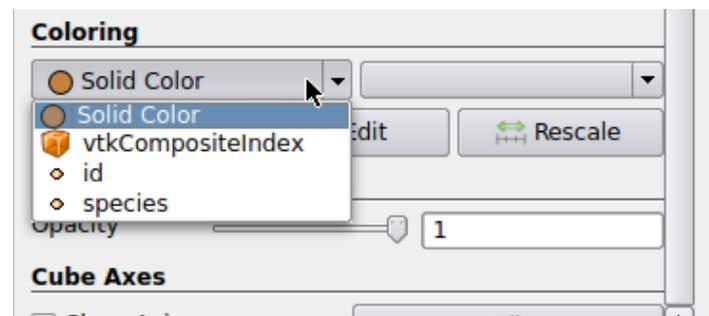
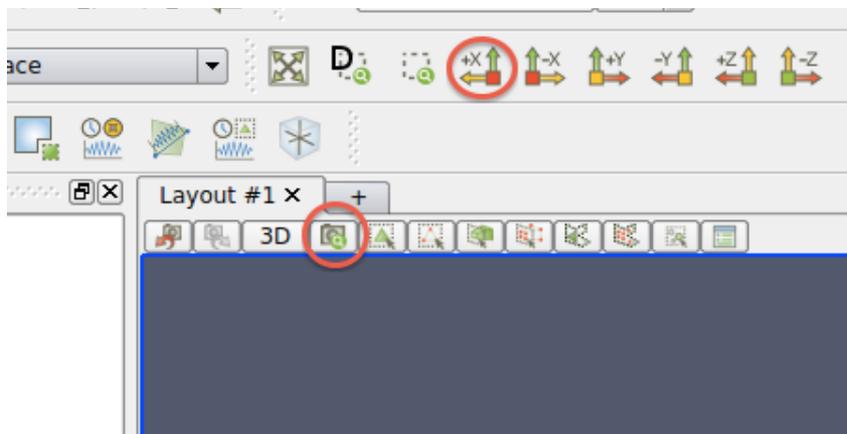
**Data Arrays**

Name	Data Type	Data Ranges
◇ id	int	[1, 29346]
◇ species	int	[0, 1]



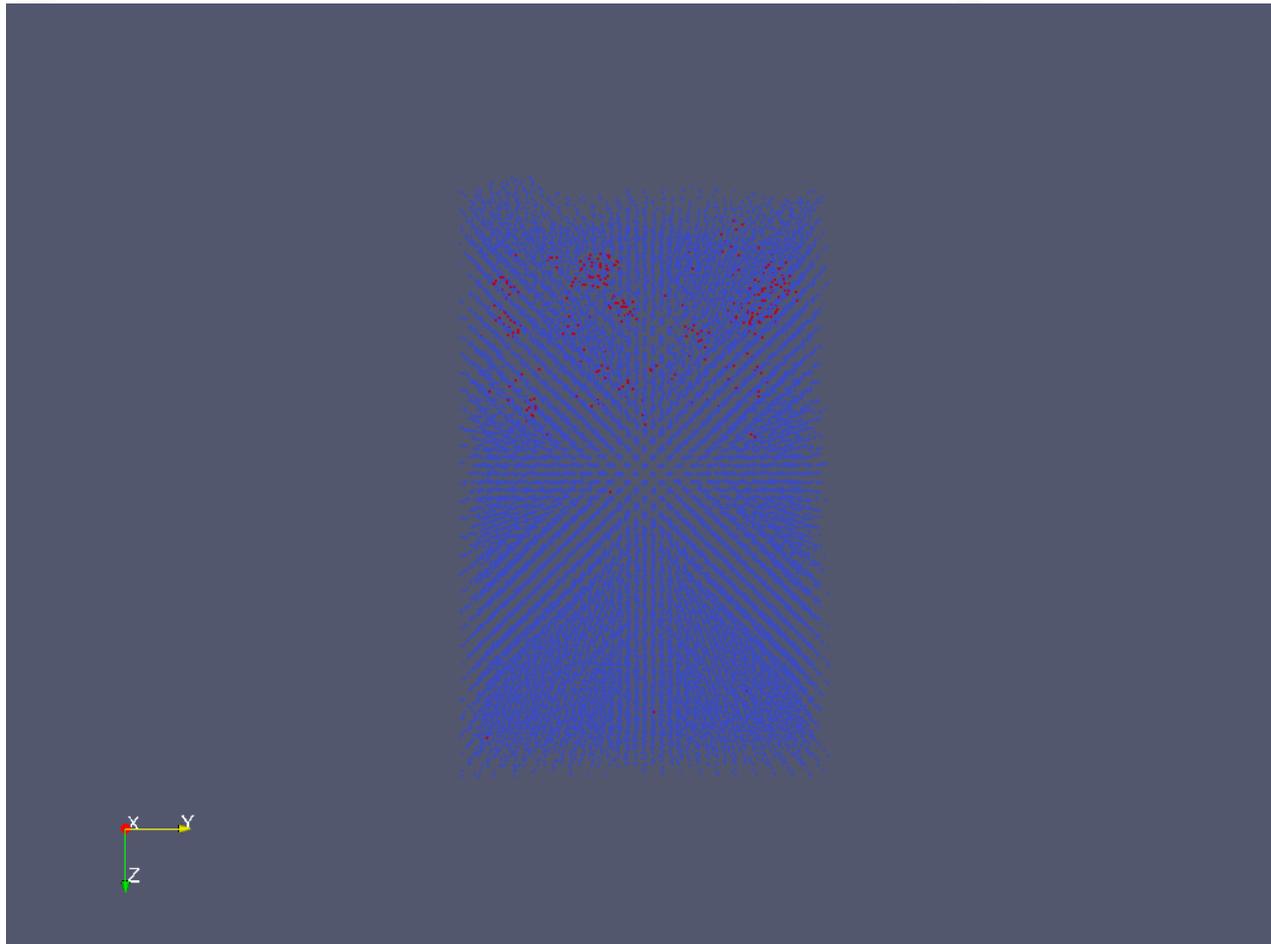
# View and Color Scheme

- Change camera position/orientation
  - Click +X icon
  - Click Adjust Camera
  - Set View Up to 0, 0, -1
- Change color for Helium/Tungsten atoms
  - Select Coloring to species





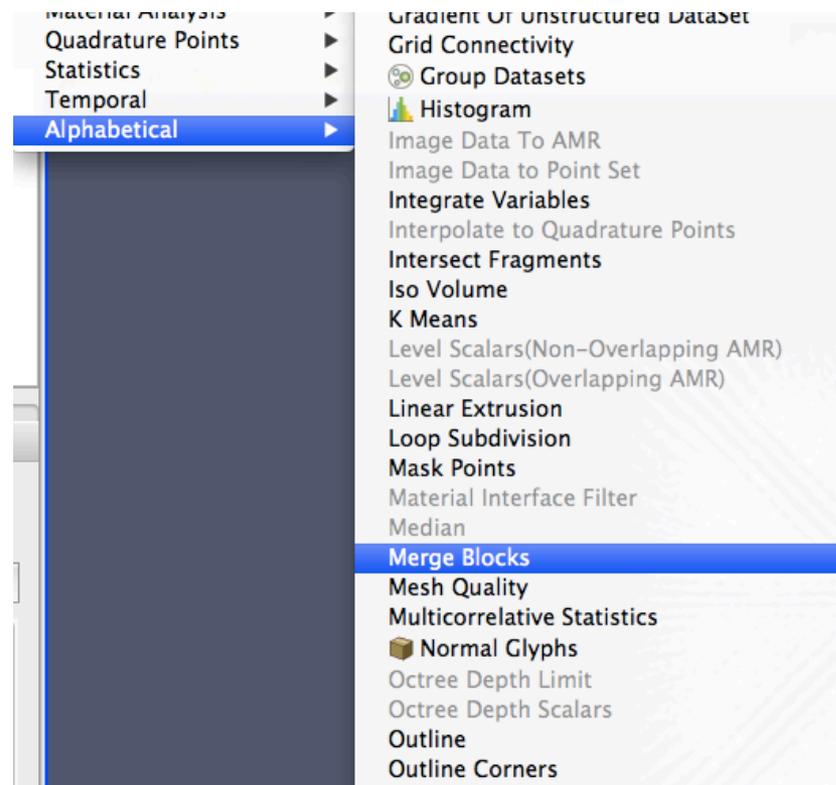
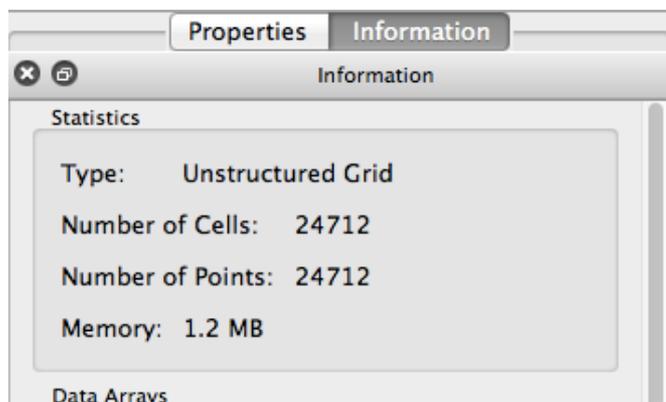
# Baseline View





# Visualization Pipeline

- Merge multi-block data
  - Only one block anyway
  - Easier to work with later
- Filter menu
  - Merge Blocks
- VTK Unstructured Grid

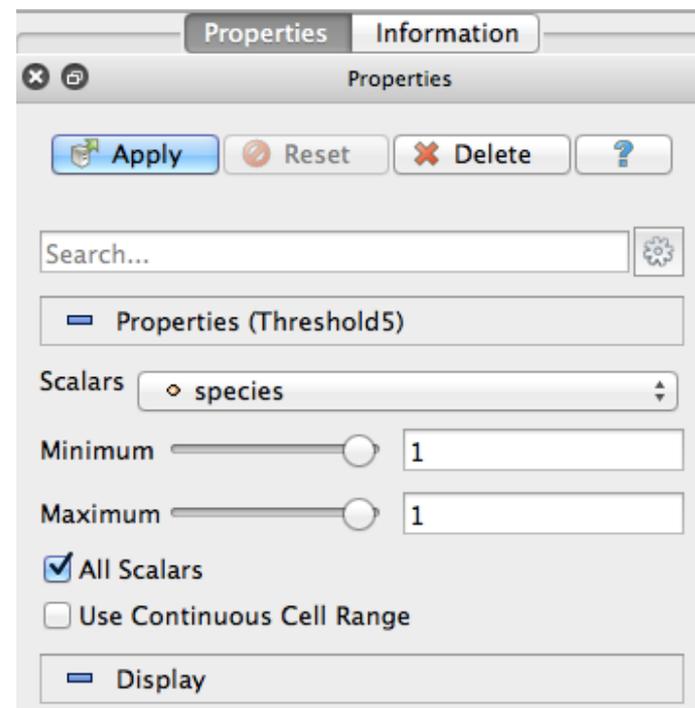




# Separate Helium from Tungsten



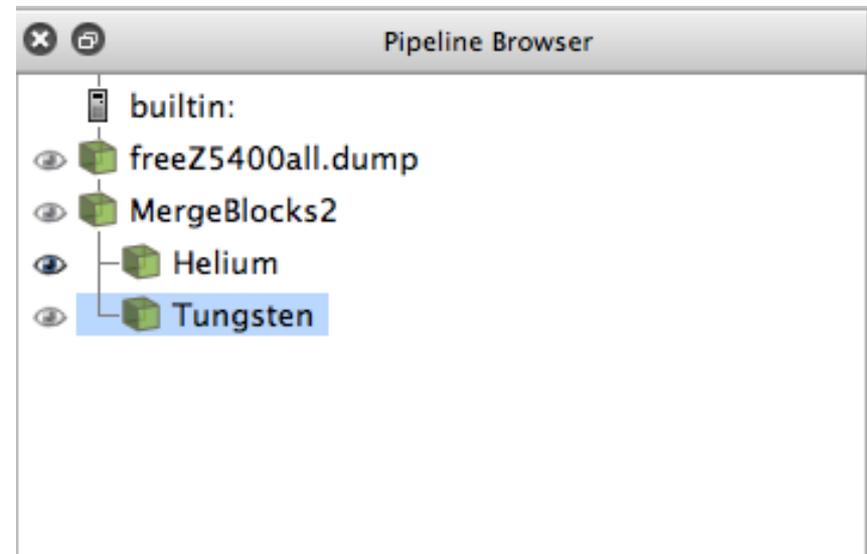
- He atoms
  - Click *Threshold* icon on toolbar
  - Change Scalars to “species”
  - Change Min/Max to 1
- W atoms
  - Same as He **but**
  - Select MergeBlocks
  - Set Min/Max to 0
- Change pipeline name





# Select Data to View

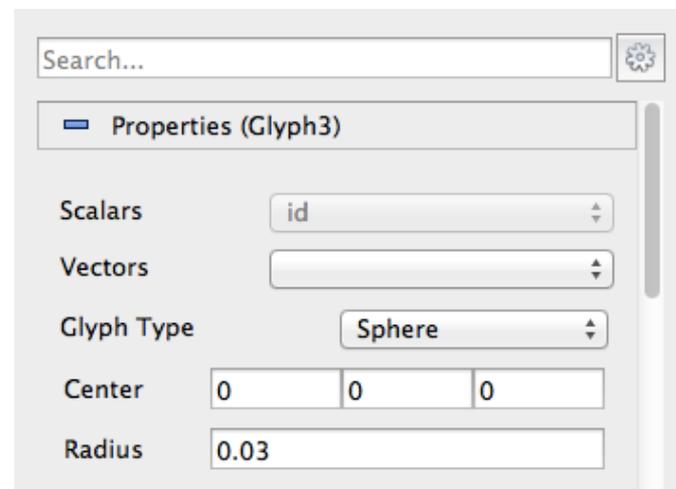
- Show/Hide data set with Eyeball icon
  - **Black** mean visible
  - Gray means hidden





# Helium Atoms as Spheres

- Select Helium
- Click *Glyph* icon 
- Glyph Type: Sphere
- Radius: 0.03
- Mask Points: Unchecked
- Random Mode: Unchecked



Search...

Properties (Glyph3)

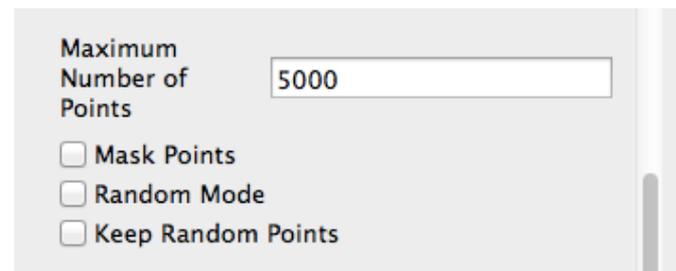
Scalars

Vectors

Glyph Type

Center

Radius



Maximum Number of Points

Mask Points

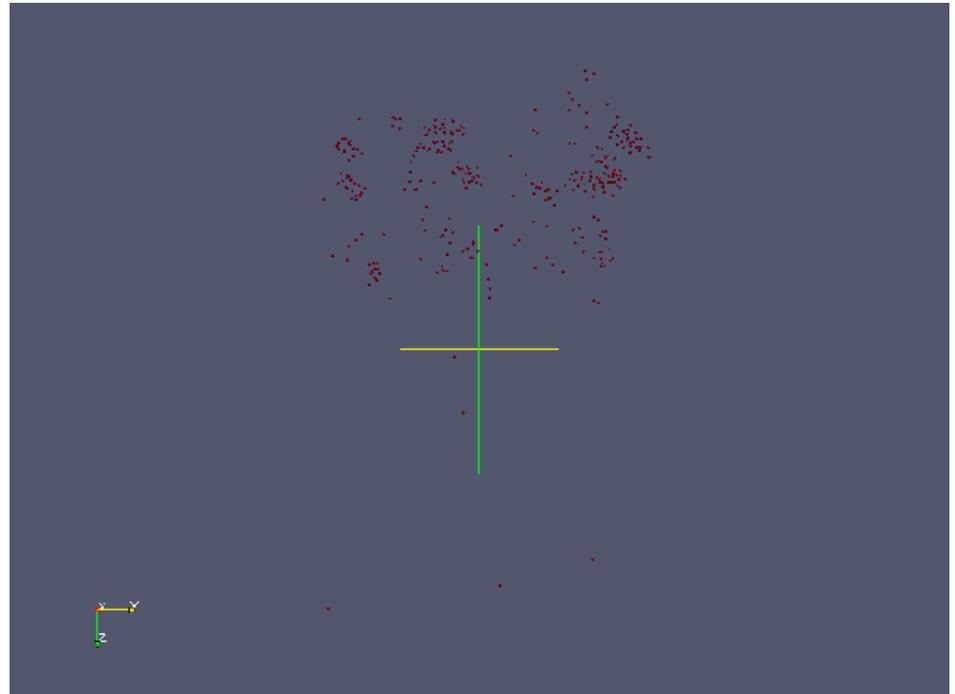
Random Mode

Keep Random Points



# Helium Atoms as Spheres

- Use small radius
  - Serve as visual aid
  - Interested in bubble
  - More on this later
- Large number of atoms
  - Show subset
  - Max Number of Points
  - Mask Points
  - Random Mode





# Problems of Unstructured Points

- Visualizing points as spheres
  - Very difficult to discern spatial distributions
  - Most visualization operations don't work
- Convert unstructured points to structured grids



# Reconstruct Helium Bubble

- Estimate Helium density
  - Convert discrete distribution to continuous
  - Replace each particle with a Gaussian
  - Resample density on a structured grid
- Approximate bubble surface
  - Draw a line in the sand
  - Call it the bubble surface



# Gaussian Resampling

- Select Helium
- Filter Menu
  - Gaussian Resampling
- Resampling Grid: 100, 100, 100
- Radius: 0.02
- Elliptical Splat: Unchecked
- Accumulation Mode: Sum

Resample Field

Resampling Grid

Extent to Resample

<input type="text" value="0"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="0"/>

Gaussian Splat Radius

Gaussian Exponent Factor

Scale Splats

Scale Factor

Elliptical Splats

Elliptical Eccentricity

Fill Volume Boundary

Fill Value

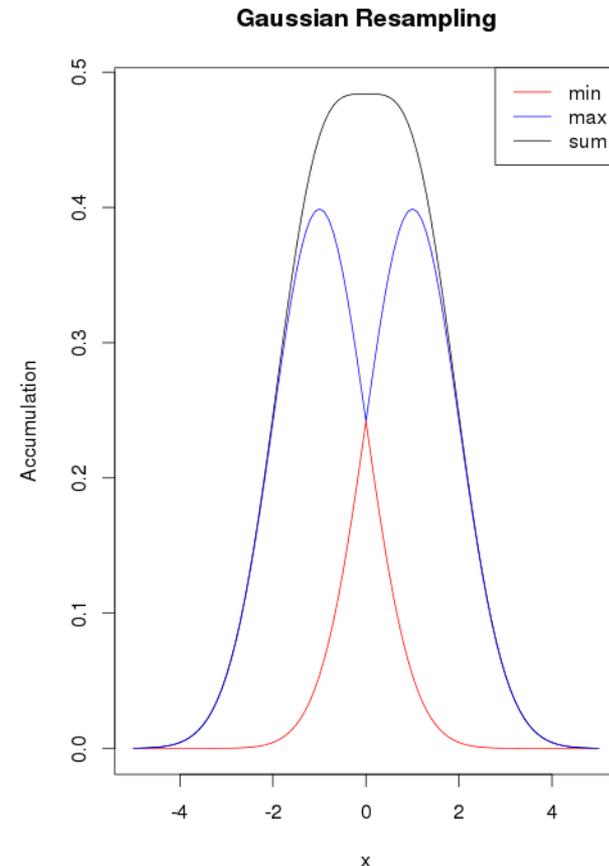
Splat Accumulation Mode

Empty Cell Value



# Issues with Gaussian Resampling

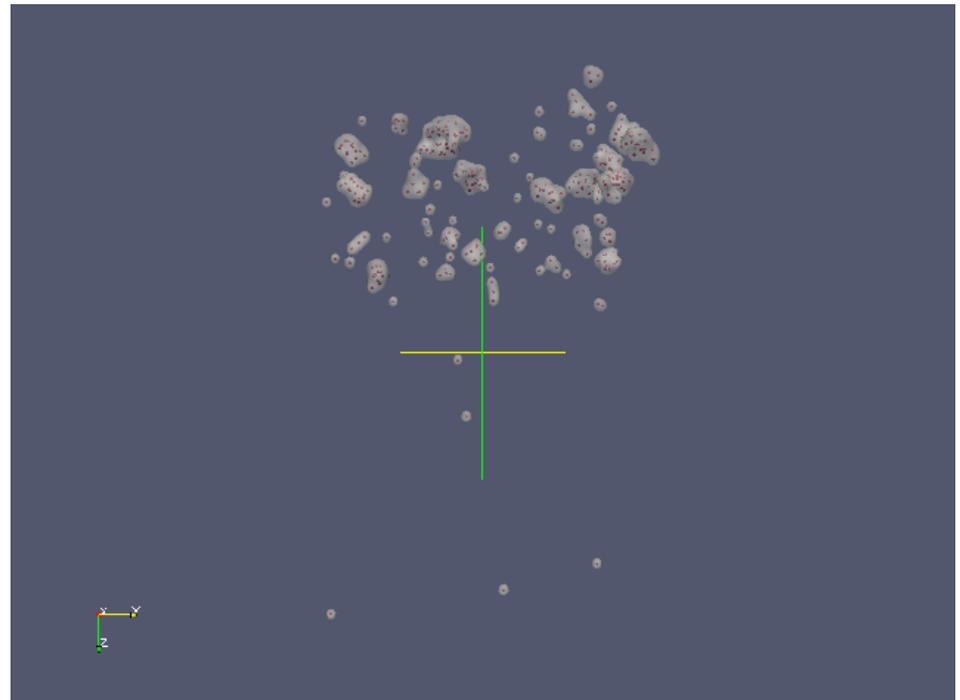
- Grid size
  - Smoothness of surface
  - Computational efficiency
- Radius
  - Classical clustering problem
  - Computational efficiency
- Accumulation mode
  - Min: Intersection
  - Max: Union
  - Sum: Like Max but “smoother”





# Isosurface

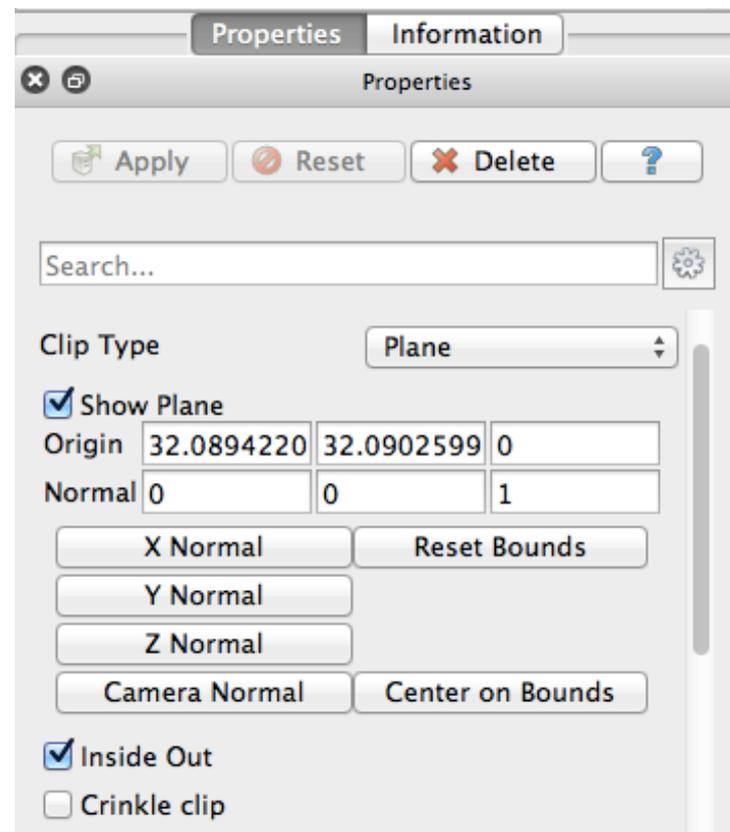
- Select Helium density
- Click *Contour* icon
- Isovalue: 0.5
- Opacity: 0.5





# Tungsten Surface

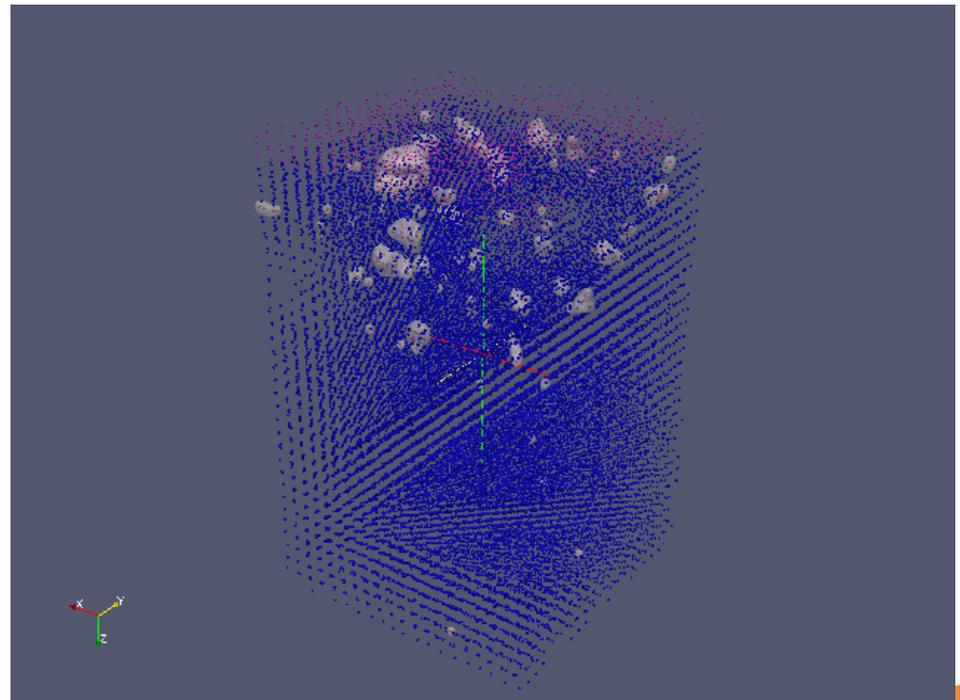
- Separate Tungsten atoms
- $Z > 0$ 
  - Select Tungsten
  - Click *Clip* icon 
  - Click Z Normal
  - Origin.Z: 0
  - Inside Out: Checked
- $Z < 0$ 
  - Same as above
  - Inside Out: Unchecked





# Tungsten Surface

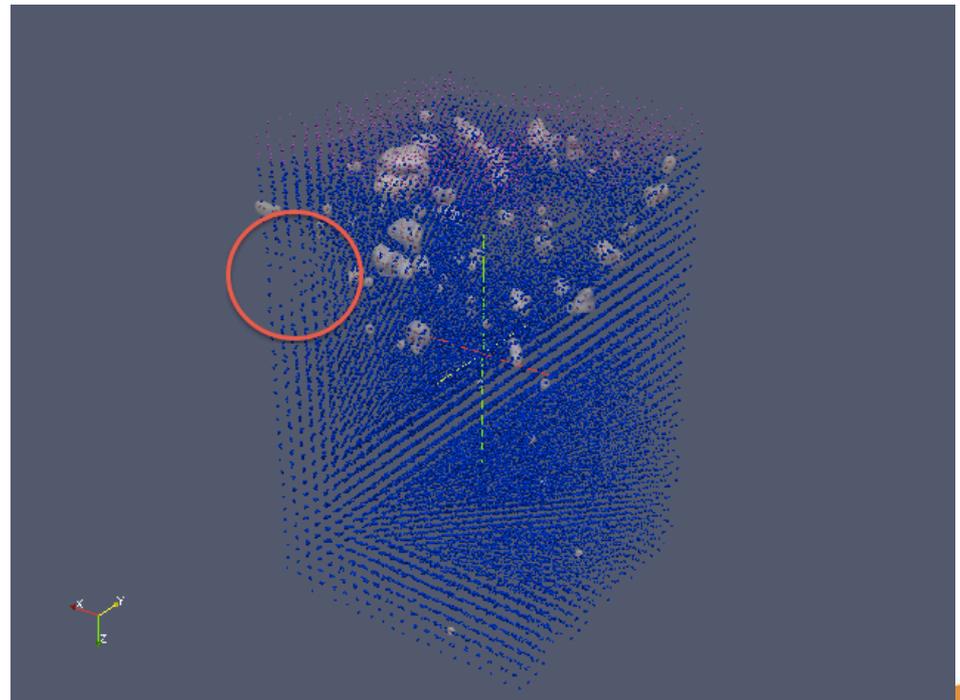
- Sphere glyph to represent Tungsten atoms
- Different colors for  $Z > 0$  and  $Z < 0$
- Keep the radius small





# Cavity

- Something “missing” in the picture
  - Reality or illusion?
- Same problem as He bubble
- Use the same trick!!!





# Cavity

- Select all Tungsten atoms
- Filter menu
  - Gaussian Resampling
- Resampling Grid: 128, 128, 128
- Radius: 0.06
- Elliptical Splat: Uncheck
- Accumulation Mode: Sum
- Contour
  - Isovalue: 0.5



# OOPS!!!

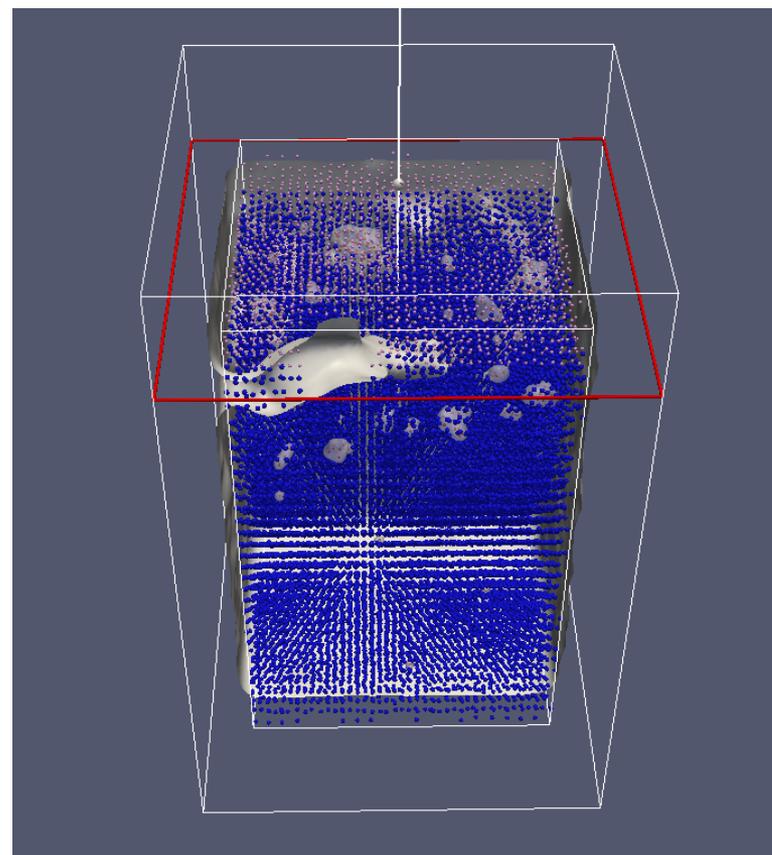
- Gaussian Splatter spills
- Fixed B.C. with density = 0
- Artifacts: “Shell” around the atoms





# What's Inside the Blob?

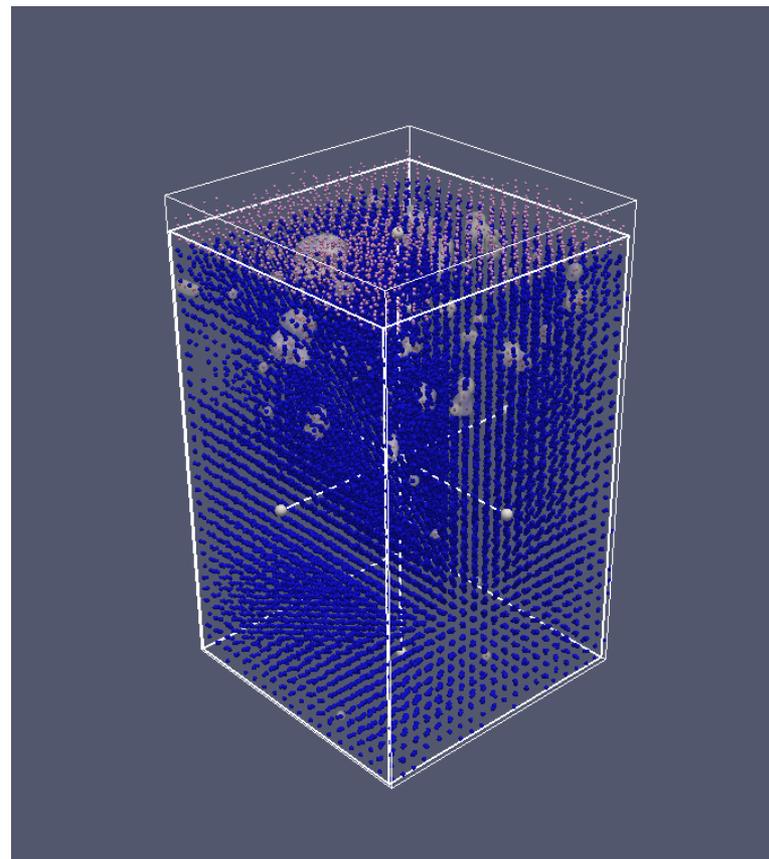
- Cut it out with *Clip*
- Plane with X Normal
- Plane with Z Normal





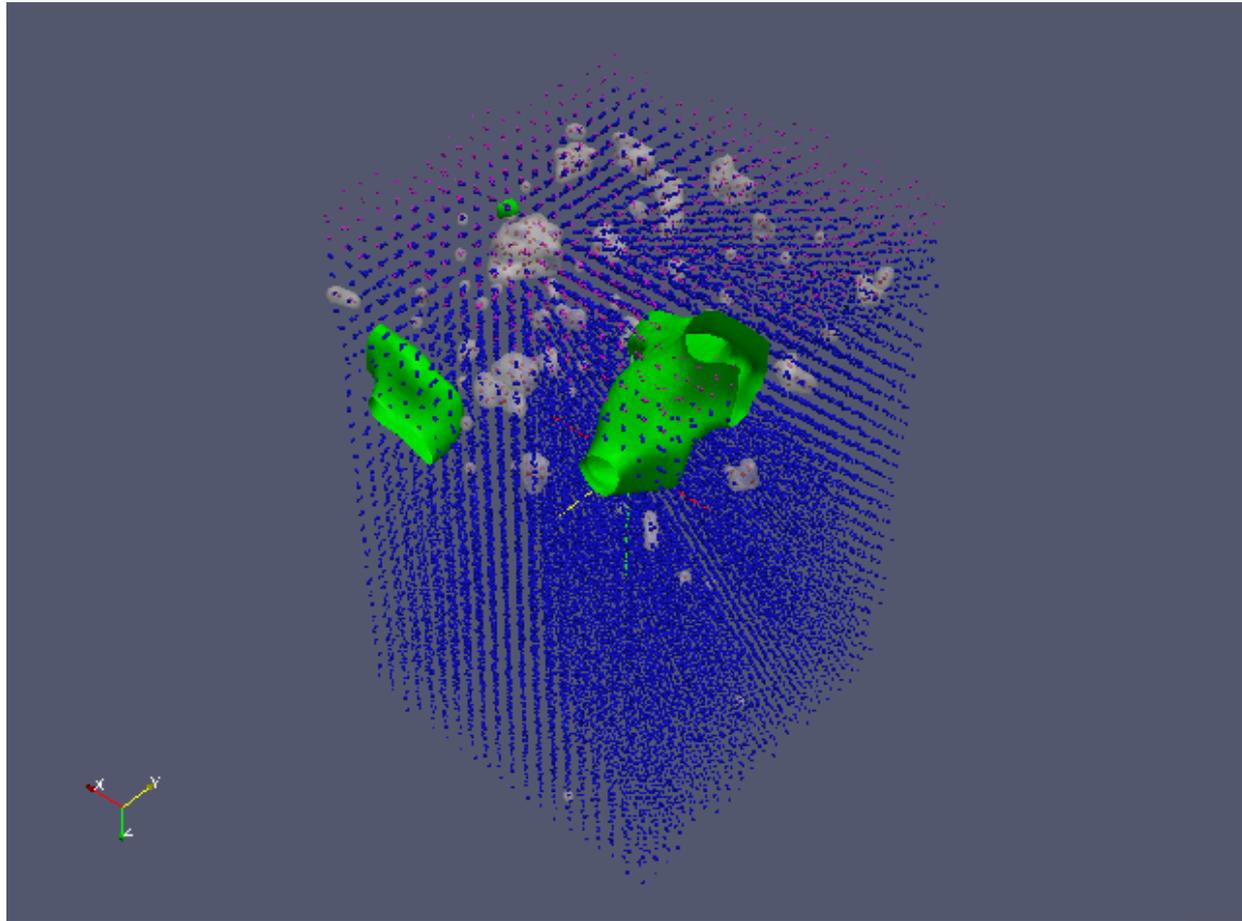
# Box Cut

- Remove the “shell” with a Box clip
- Match the box with the bounding box of atoms
- Isosurface





# Viola





# Summary

- ParaView as your interactive visualization tool
- Apply and combine simple visualization operations in a pipeline
- Avoid visual clutter and artifacts
- Practice makes perfect