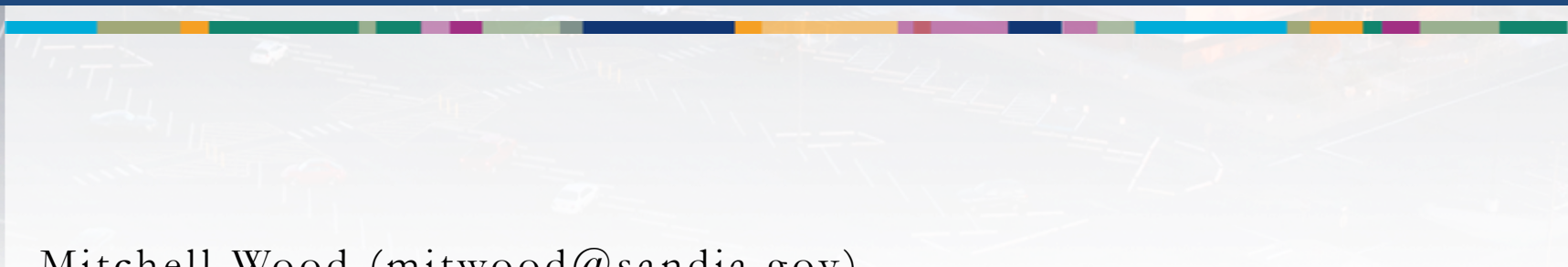




Sandia
National
Laboratories

LAMMPS Users Meeting 2021: Visualization Tutorial

SAND2021-9634 C



Mitchell Wood (mitwood@sandia.gov)

Center for Computing Research, Sandia National Labs

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It Looks Cool

- Communicating scientific results is not a trivial task, even between experts
- Debugging simulation crashes, planning new ones
- Mechanistic understanding a.k.a. the ‘unplotable’ data. Describe a splash or failure in words...
- Art?



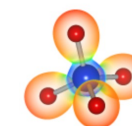
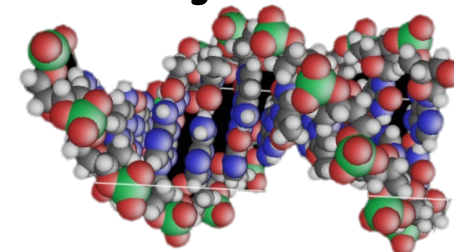


Another Zoo of Acronyms

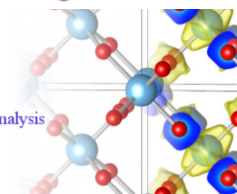
- Exploration
 - Fast manipulation of structures
 - Multiple supported file formats
- Science illustration
 - Built-in analysis tools (rdf, FFT, etc.)
 - High quality renderings
 - Scene manipulation
- Artistic or features (covers, websites, etc.)
 - Unusual styles, property mappings, “photoshopping”



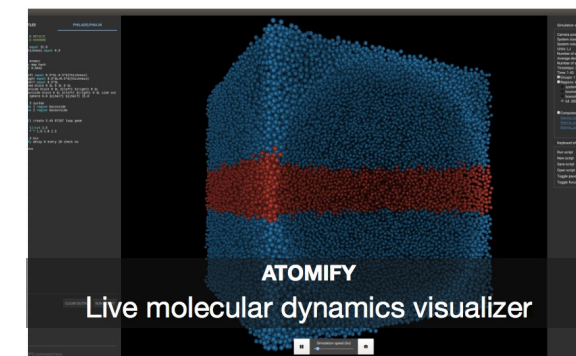
AtomEye

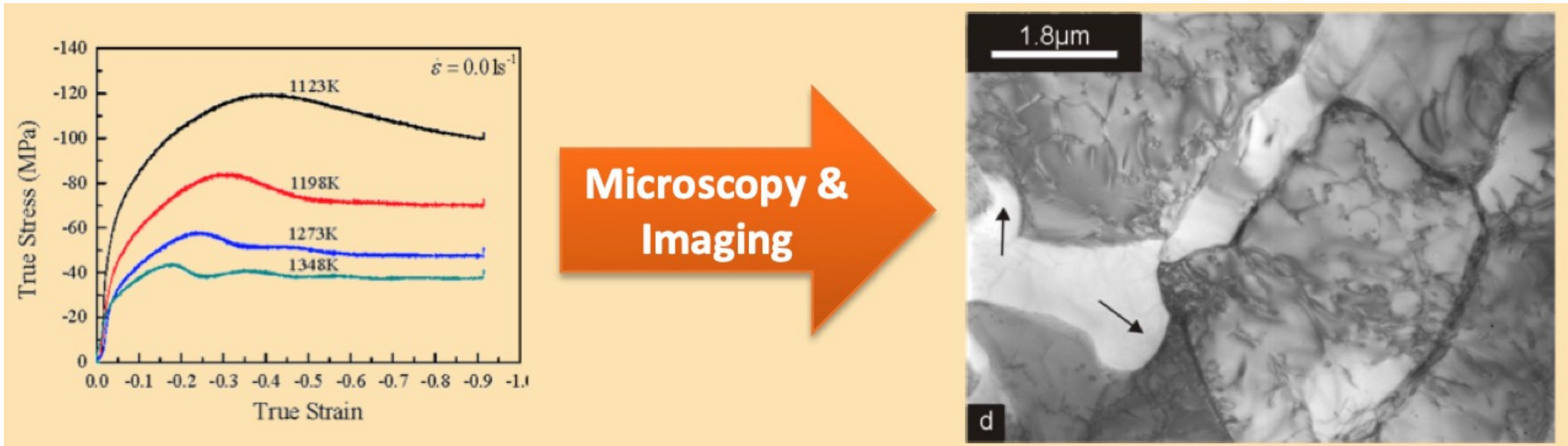


VESTA
Visualization for Electronic and STructural Analysis

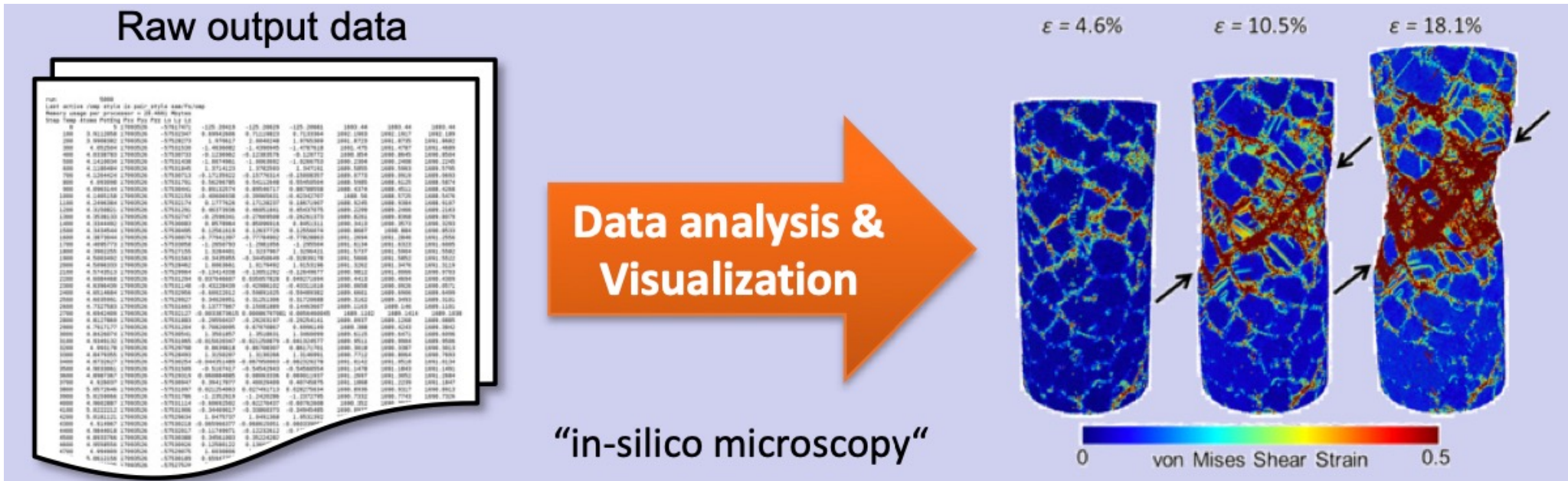


And many more...





To only look at the raw output of an experiment / simulation is limiting your insight into ‘what happened’



OVITO Pro (Open Visualization Tool)

Pipelines: dump.friction [LAMMPS Dump]

Top

Front

Left

Perspective (preview)

Particles Global Attributes Data Tables

ParticleIdentifier==1517 || ParticleIdentifier==1548 || ParticleIdentifier==1519

	Particle Identifier	Particle Type	Position	Coordination	Cc	Pair A-B	Distance	Vector	Triplet A-B-C	Angle
783	1517	2	28.0826 16.8...	402	0.20	783 - 784	1.17128	1.16996 -0.0556032 0	784 - 783 - ...	56.8291
784	1519	2	29.2526 16.7...	511	0.13	783 - 800	1.18263	0.693323 0.958075 0	783 - 784 - ...	62.0958
800	1548	2	28.7759 17.7...	395	0.21	784 - 800	1.12015	-0.476639 1.01368 0	783 - 800 - ...	61.0751

40 / 40

40

Add modification...

Visual elements

- Particles
- Simulation cell

Modifications

- Color coding
- Coordination analysis

Data source

dump.friction [LAMMPS Dump]

Particle types

Simulation cell

External file

Data source

Current file: dump.friction

Directory: cuments/Visualization/LAMMPSUsers_21

File sequence

Search pattern: dump.friction

auto-generate Found 1 matching file

Trajectory

Current frame: Timestep 20000

Showing frame 41 of 41

Playback ratio: 1 / 1

Change...

Status

1724 particles at timestep 20000

LAMMPS dump reader

Options

- File contains multiple timesteps
- Sort particles by ID

File columns

- Automatic mapping
- User-defined mapping to particle properties

Edit column mapping...

OVITO Pro (Open Visualization Tool)

Pipelines: dump.friction [LAMMPS Dump]

Top

Front

Left

Perspective (preview)

Four views of your data, the one with a highlighted border will be the only one rendered

Particles Global Attributes Data Tables

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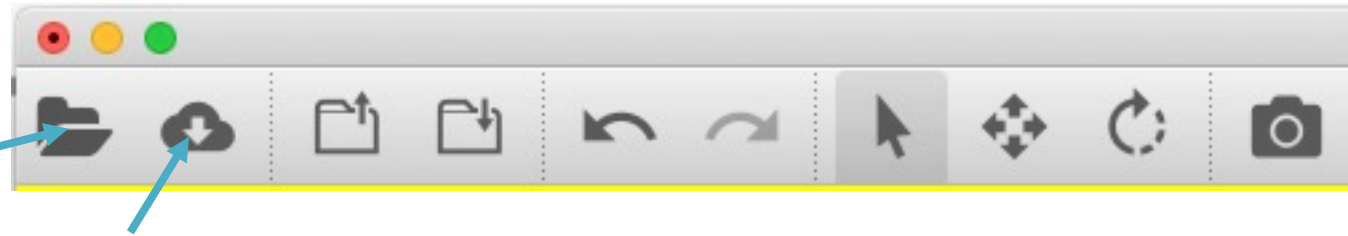
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File columns

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- User-defined mapping to particle properties

Edit column mapping...

Load a local file on
your machine



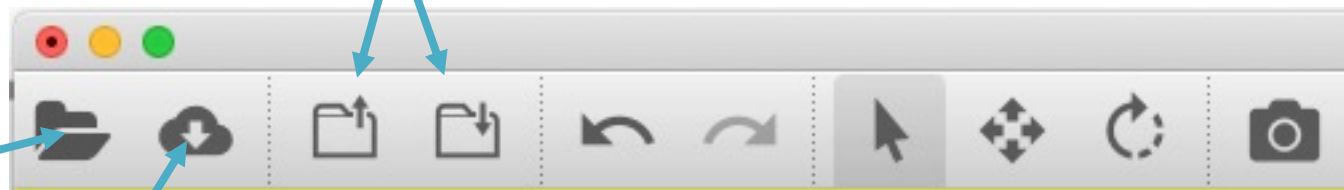
Load a remote file with
`sftp://user@machine//Path/To/The/LAMMPS.data`

Very useful because OVITO deletes the temporary file
when the app is closed, saving you a ton of disk space.

Save/Load an OVITO session

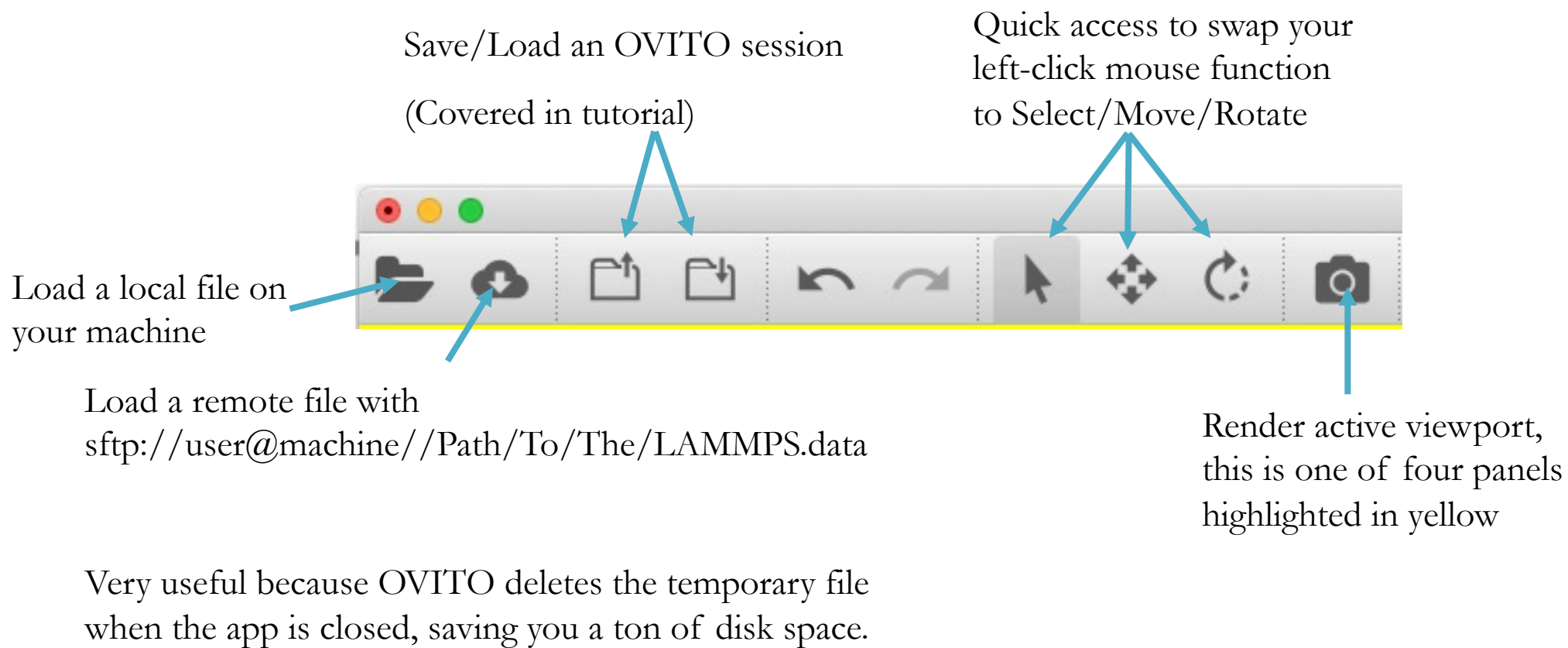
(Covered in tutorial)

Load a local file on
your machine



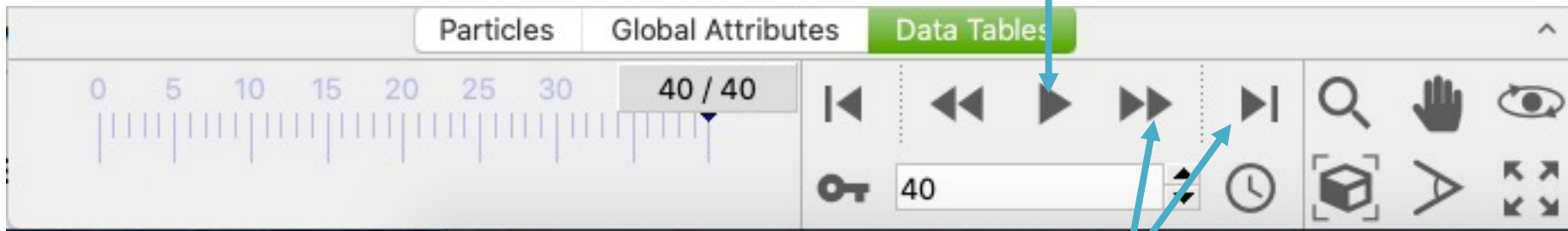
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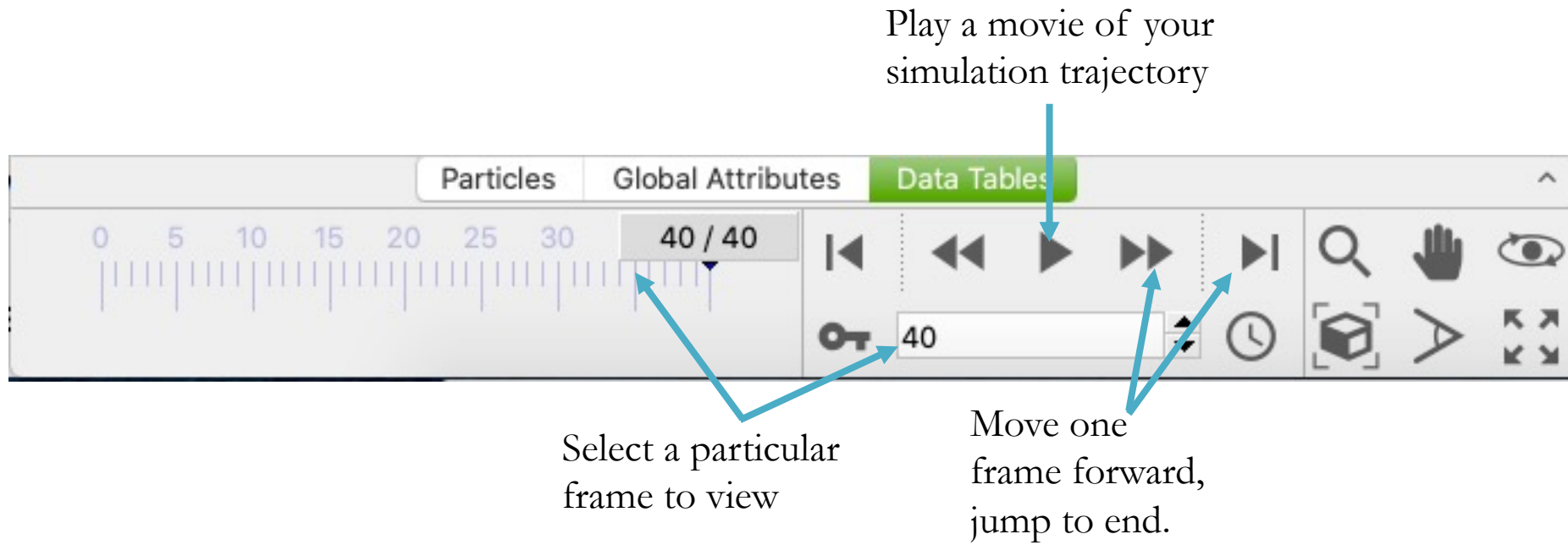




Play a movie of your
simulation trajectory



Move one
frame forward,
jump to end.





The screenshot shows a software interface with three tabs: 'Particles', 'Global Attributes', and 'Data Tables' (which is highlighted in green). Below the tabs is a timeline with a scale from 0 to 30 and a current frame indicator at 40 / 40. To the right of the timeline is a set of playback controls including buttons for previous frame, previous 10 frames, play/pause, next 10 frames, and next frame. Below these is a key icon and a text input field containing the number 40. Further right is a set of viewing controls including a magnifying glass, a hand icon, an eye icon, a 3D box icon, a zoom-in arrow, and a full-screen icon. Annotations with arrows point to various elements: 'Play a movie of your simulation trajectory' points to the play/pause button; 'Select a particular frame to view' points to the 40 / 40 frame indicator; 'Move one frame forward, jump to end.' points to the next frame and next 10 frames buttons; 'Auto-Zoom to fit all atoms into the view' points to the 3D box icon; 'Adjust Zoom, left-click and drag up/down' points to the zoom-in arrow; and 'Focus on one viewing panel, click again to see all' points to the full-screen icon.

Play a movie of your simulation trajectory

Select a particular frame to view

Move one frame forward, jump to end.

Auto-Zoom to fit all atoms into the view

Adjust Zoom, left-click and drag up/down

Focus on one viewing panel, click again to see all



The image shows a screenshot of a simulation GUI with several tabs: 'Particles', 'Global Attributes', and 'Data Tables' (which is highlighted in green). Below the tabs is a timeline with a scale from 0 to 30, and a current frame indicator showing '40 / 40'. To the right of the timeline are playback controls: a single frame back button, a double frame back button, a single frame forward button, a double frame forward button, and a play button. Below these is a text input field containing the number '40' and a key icon. Further right are icons for search, hand (pan), eye (visibility), a 3D box (auto-zoom), a magnifying glass with a hand (adjust zoom), and a focus icon. Annotations with arrows point to various elements: 'Play a movie of your simulation trajectory' points to the play button; 'Detailed information tables stored here' points to the top right corner; 'Select a particular frame to view' points to the '40 / 40' frame indicator; 'Move one frame forward, jump to end.' points to the single frame forward button; 'Auto-Zoom to fit all atoms into the view' points to the 3D box icon; 'Adjust Zoom, left-click and drag up/down' points to the magnifying glass with a hand icon; and 'Focus on one viewing panel, click again to see all' points to the focus icon.

Play a movie of your simulation trajectory

Detailed information tables stored here

Select a particular frame to view

Move one frame forward, jump to end.

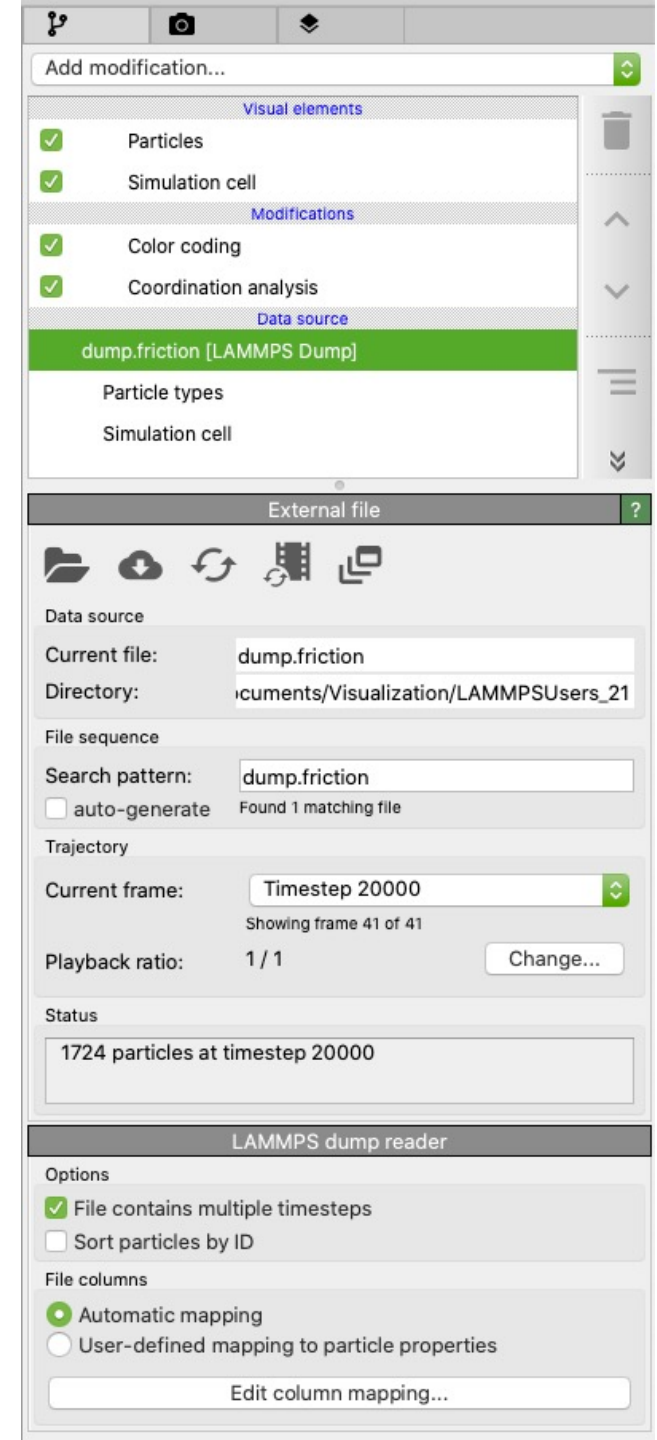
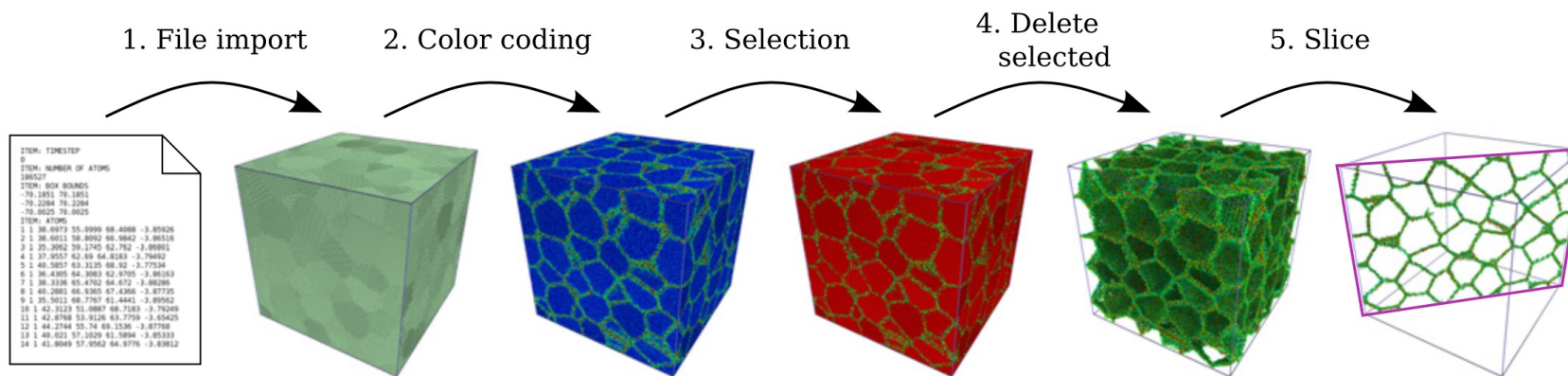
Auto-Zoom to fit all atoms into the view

Adjust Zoom, left-click and drag up/down

Focus on one viewing panel, click again to see all

Building a Viz Workflow

- The flexibility of OVITO comes in its library of modifications that can be made
- Bottom-up evaluation: Data is loaded, modifications added, visual elements are generated for rendering
- Multiple files can be loaded if **Search Pattern** is given a filename with '*' or '?' in it.

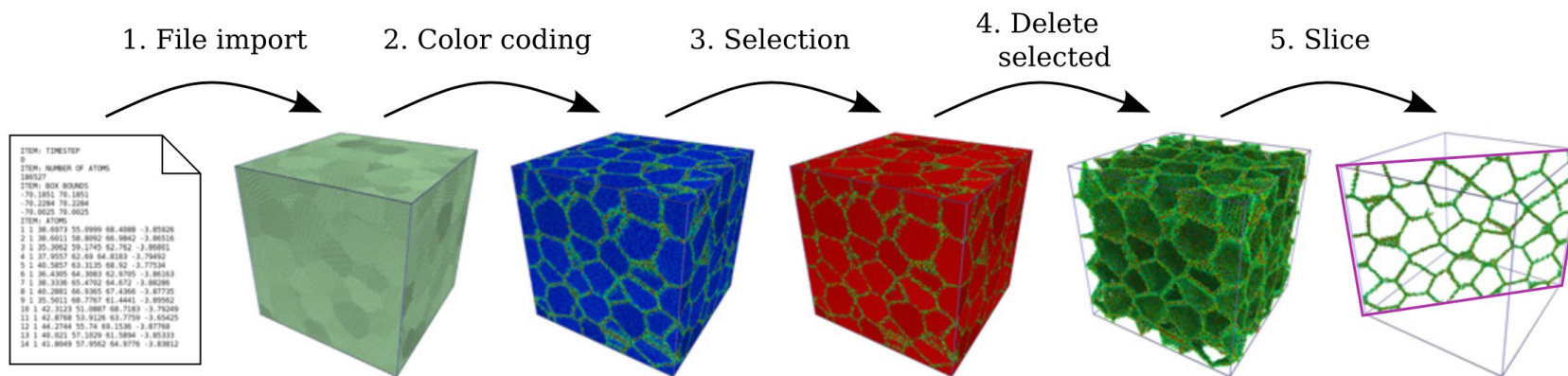


Building a Viz Workflow

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Modelling Simul. Mater. Sci. Eng. **18** (2010) 015012

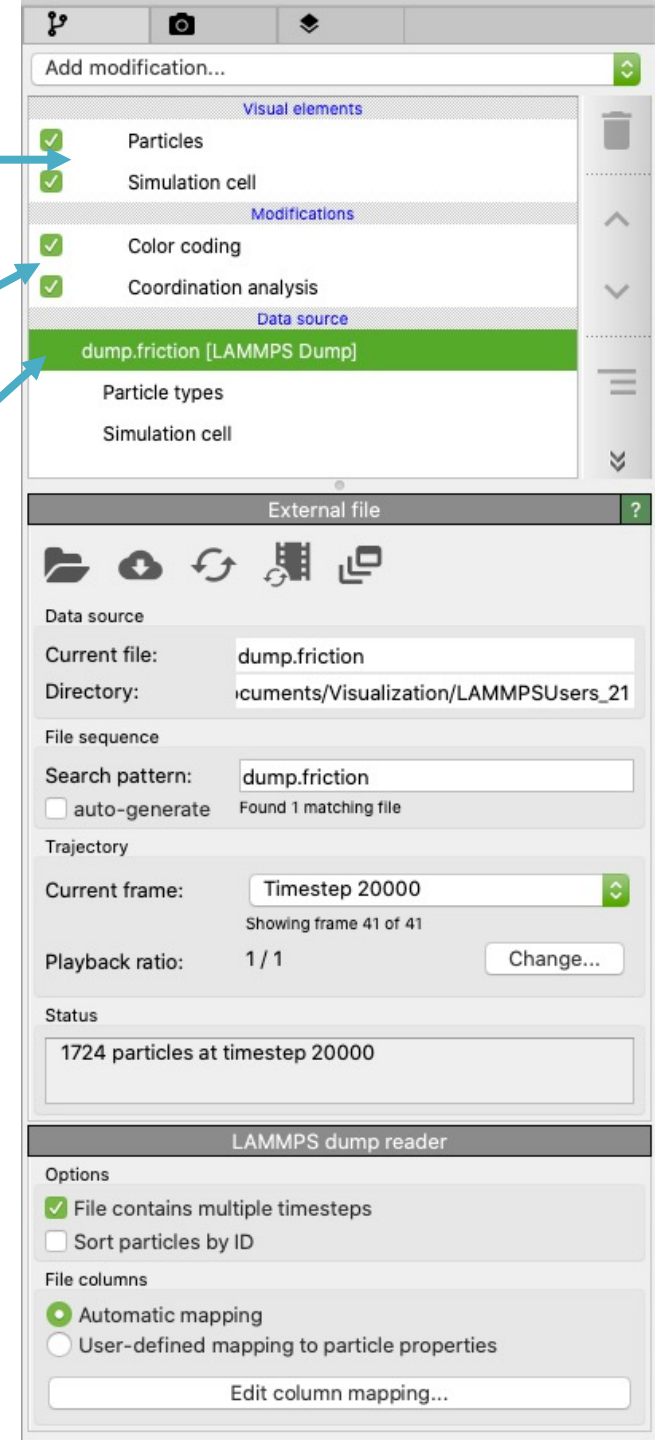
A Stukowski



Visual Elements

Active/Inactive
modifications

File Imported



GUI Walkthrough



Change left-click to inspect particles



Inspect properties of multiple particles (bond length, angles)



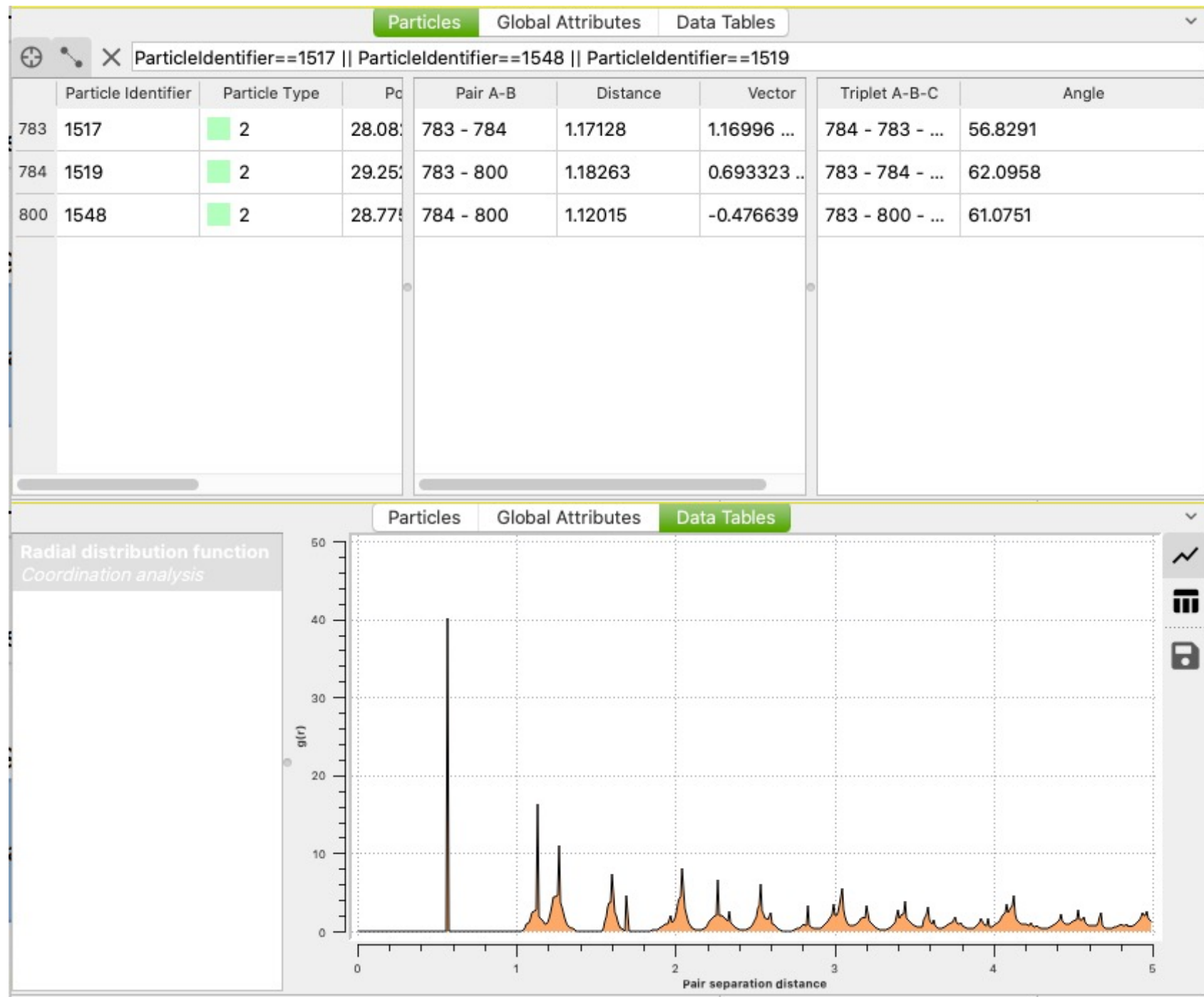
View plots generated by modifications

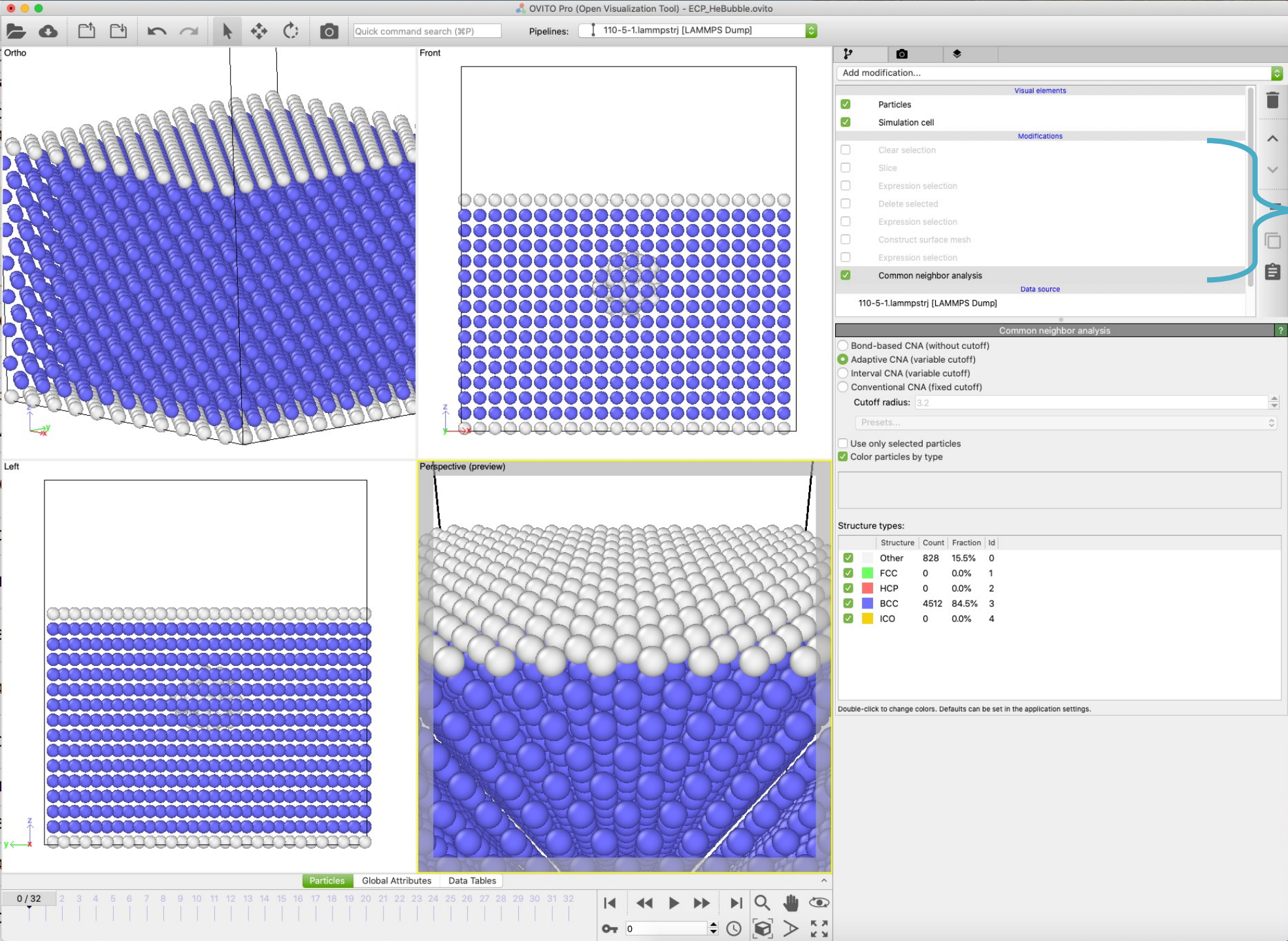


View data tables generated by modifications



Export data tables or plots generated by modifications

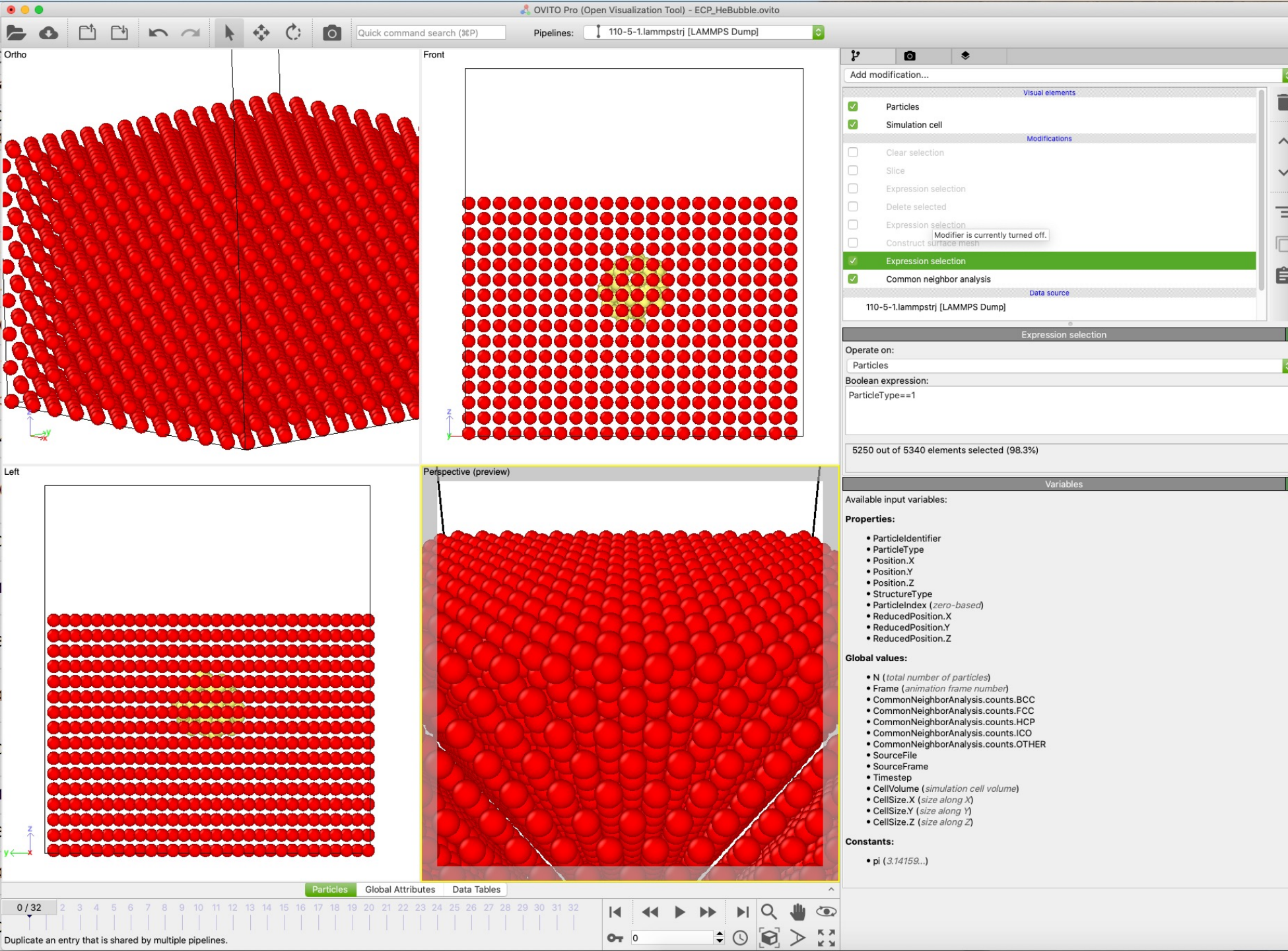




Modification stack read from bottom to top

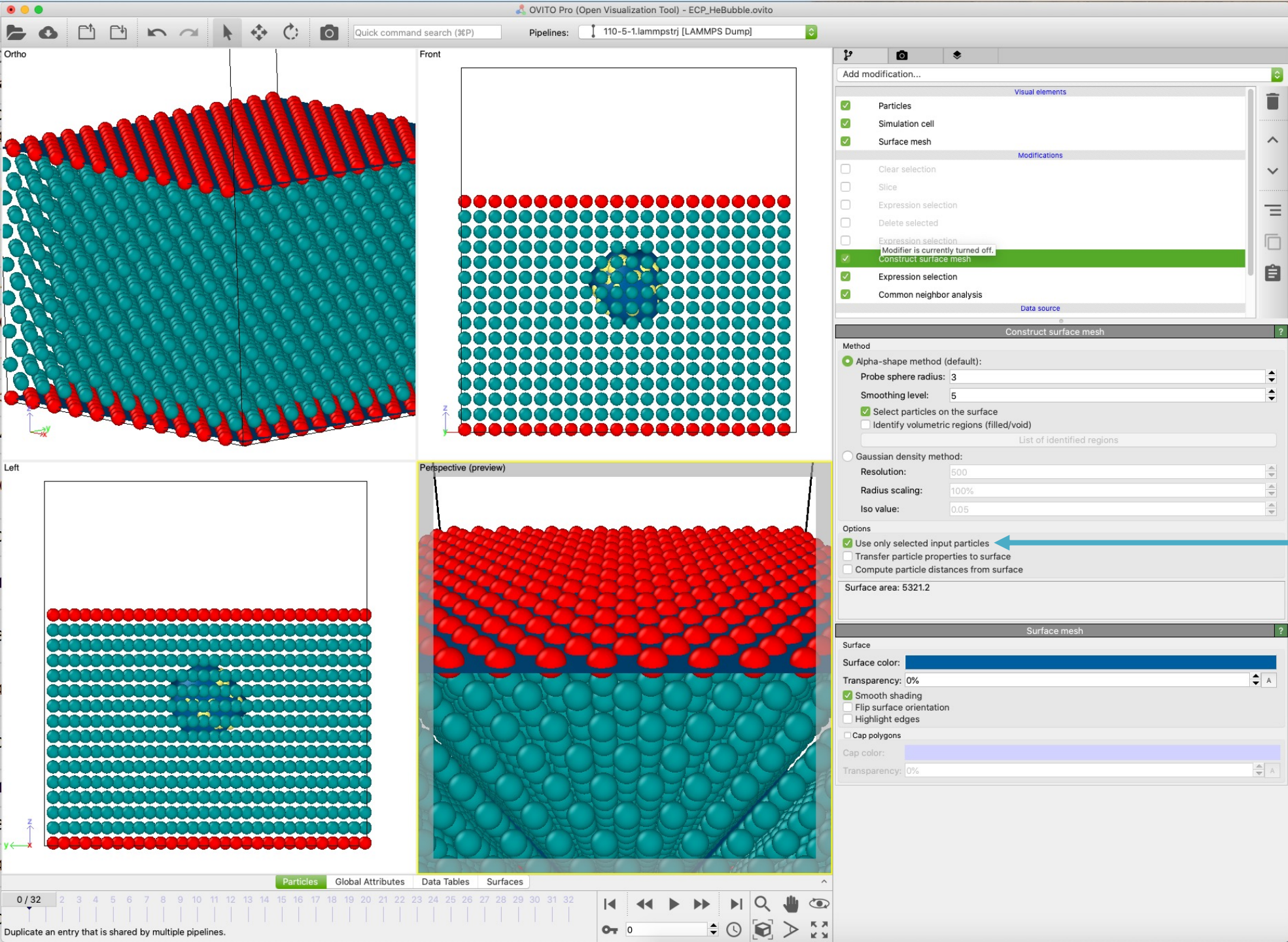
Common Neighbor Analysis is used to identify the surfaces, and internal cavity in the sample

Atoms will now have a property called **StructureType**



ParticleType is used to create a selection of particles (now colored in red).

Setting up for the next step where we want to identify the surfaces that surround only the solid material.



Construct Surface Mesh
modifier is added

Important box to check,
will create surfaces based
on the selection

OVITO Pro (Open Visualization Tool) - ECP_HeBubble.ovito

Pipelines: 110-5-1.lammpstrj [LAMMPS Dump]

Ortho

Front

Left

Perspective (preview)

Particles

Global Attributes

Data Tables

Surfaces

0 / 32

Duplicate an entry that is shared by multiple pipelines.

Add modification...

Visual elements

- ✓ Particles
- ✓ Simulation cell
- ✓ Surface mesh

Modifications

- ☐ Clear selection
- ☐ Slice
- ☐ Expression selection
- ☐ Delete selected
- ✓ Expression selection
- ✓ Construct surface mesh
- ✓ Expression selection
- ✓ Common neighbor analysis

Data source

Expression selection

Operate on:

Particles

Boolean expression:

Selection==1 && Position.Z < 32

384 out of 5340 elements selected (7.2%)

Variables

Available input variables:

Properties:

- ParticleIdentifier
- ParticleType
- Position.X
- Position.Y
- Position.Z
- StructureType
- Selection
- ParticleIndex (zero-based)
- ReducedPosition.X
- ReducedPosition.Y
- ReducedPosition.Z

Global values:

- N (total number of particles)
- Frame (animation frame number)
- CommonNeighborAnalysis.counts.BCC
- CommonNeighborAnalysis.counts.FCC
- CommonNeighborAnalysis.counts.HCP
- CommonNeighborAnalysis.counts.ICO
- CommonNeighborAnalysis.counts.OTHER
- ConstructSurfaceMesh.surface_area
- SourceFile
- SourceFrame
- Timestep
- CellVolume (simulation cell volume)
- CellSize.X (size along X)
- CellSize.Y (size along Y)
- CellSize.Z (size along Z)

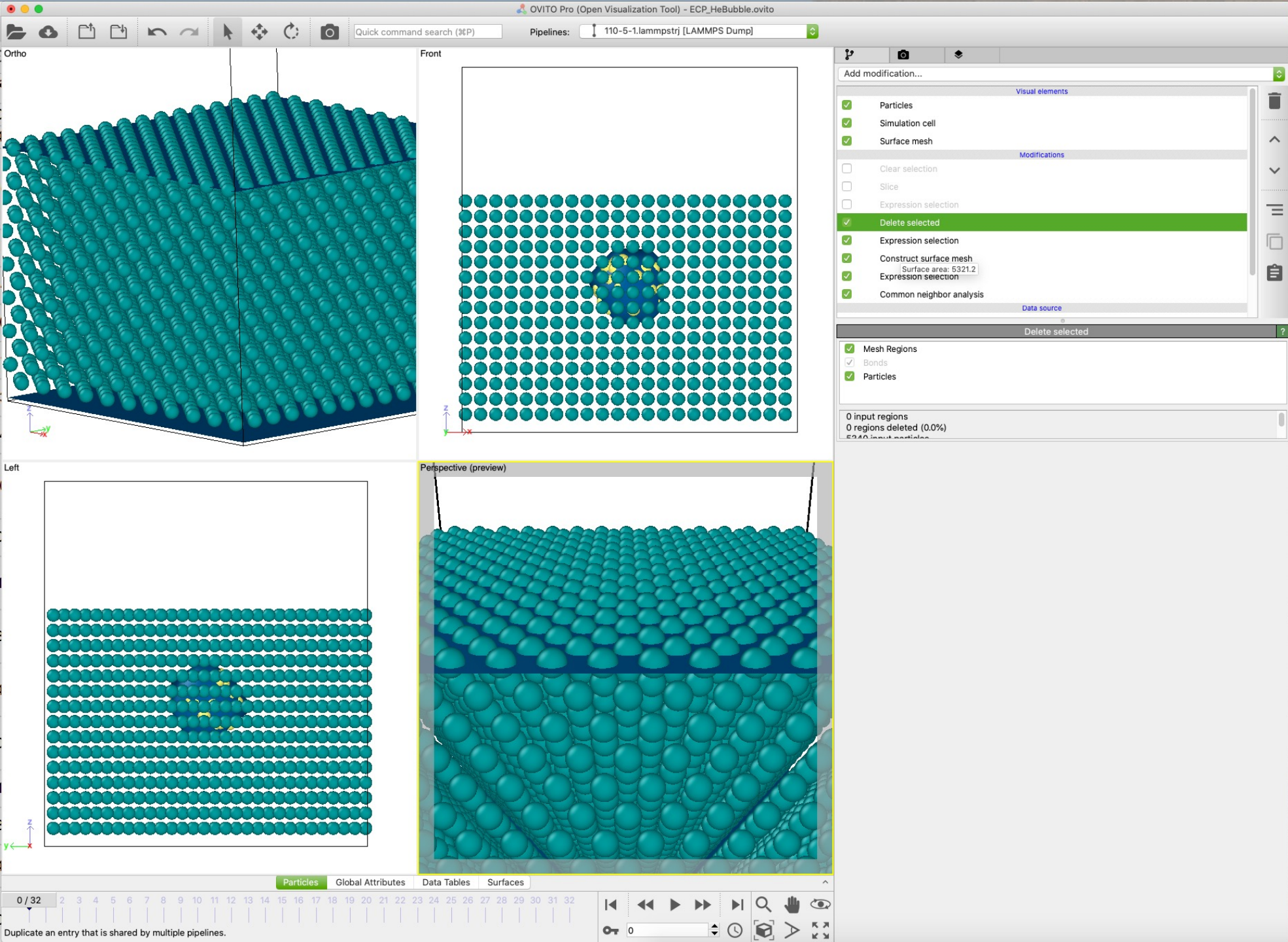
Constants:

- pi (3.14159...)



Atoms are given a value of 0/1 called **Selection**, can use this to make a compound expression

We want to select atoms on the surface (**Selection**==1) and below the cavity (**Position.Z**<32)



Delete Selected to make
the bottom surface look
pretty

OVITO Pro (Open Visualization Tool) - ECP_HeBubble.ovito

Pipelines: 110-5-1.lammpstrj [LAMMPS Dump]

Ortho

Front

Left

Perspective (preview)

Particles

Global Attributes

Data Tables

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0 / 32

Duplicate an entry that is shared by multiple pipelines.

Add modification...

Visual elements

- ☒ Particles
- ☒ Simulation cell
- ☒ Surface mesh

Modifications

- ☐ Clear selection
- ☐ Slice
- ☒ Expression selection
- ☒ Delete selected
- ☒ Expression selection
- ☒ Construct surface mesh
- ☒ Expression selection
- ☒ Common neighbor analysis

Data source

Expression selection

Operate on:

Particles

Boolean expression:

ParticleType==1

4866 out of 4956 elements selected (98.2%)

Variables

Available input variables:

Properties:

- ParticleIdentifier
- ParticleType
- Position.X
- Position.Y
- Position.Z
- StructureType
- ParticleIndex (zero-based)
- ReducedPosition.X
- ReducedPosition.Y
- ReducedPosition.Z

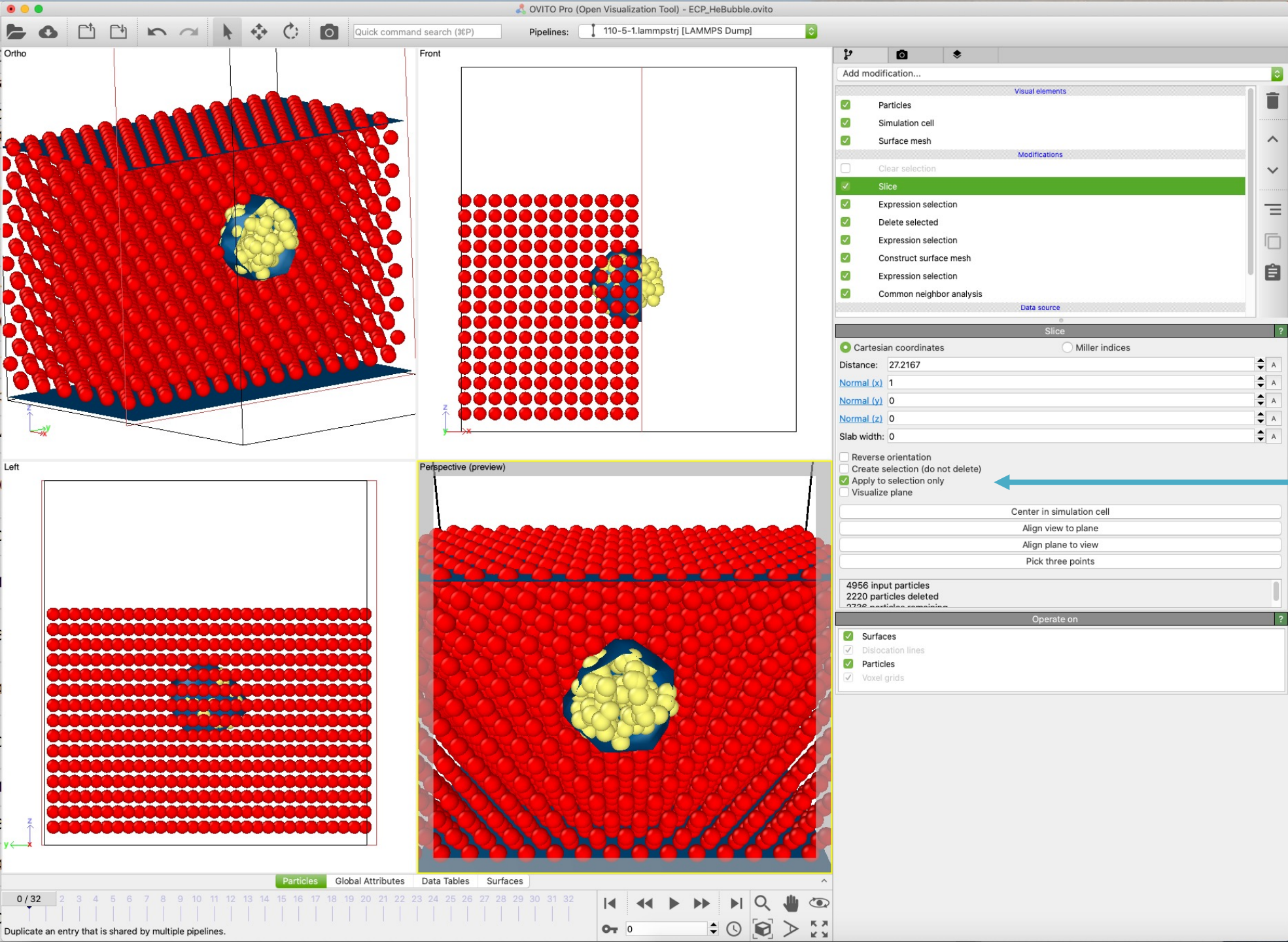
Global values:

- N (total number of particles)
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- CommonNeighborAnalysis.counts.BCC
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- CommonNeighborAnalysis.counts.HCP
- CommonNeighborAnalysis.counts.ICO
- CommonNeighborAnalysis.counts.OTHER
- ConstructSurfaceMesh.surface_area
- SourceFile
- SourceFrame
- Timestep
- CellVolume (simulation cell volume)
- CellSize.X (size along X)
- CellSize.Y (size along Y)
- CellSize.Z (size along Z)

Constants:

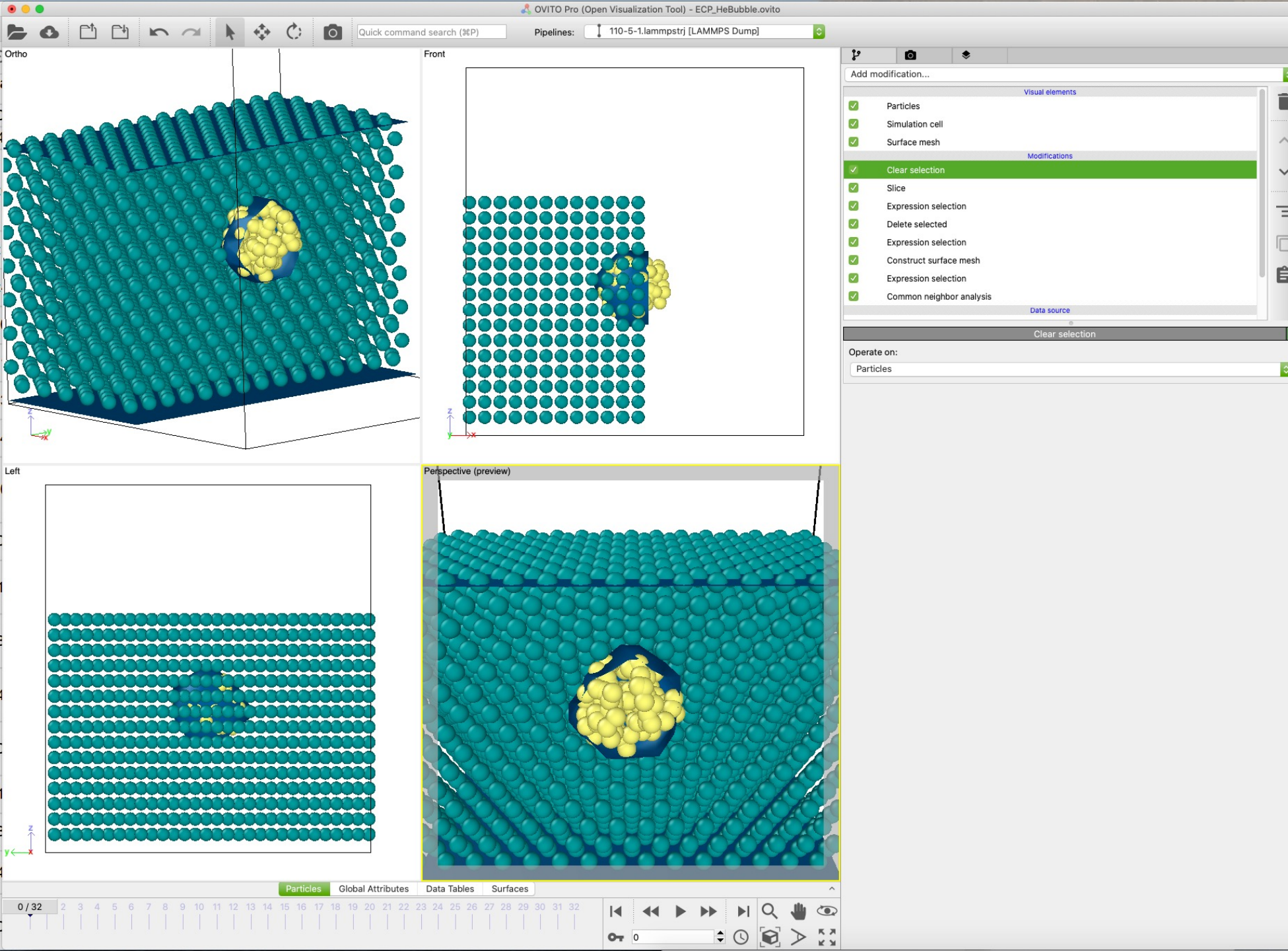
- pi (3.14159...)

Create a new **Expression Selection** to grab the atoms in the solid again (**ParticleType==1**).

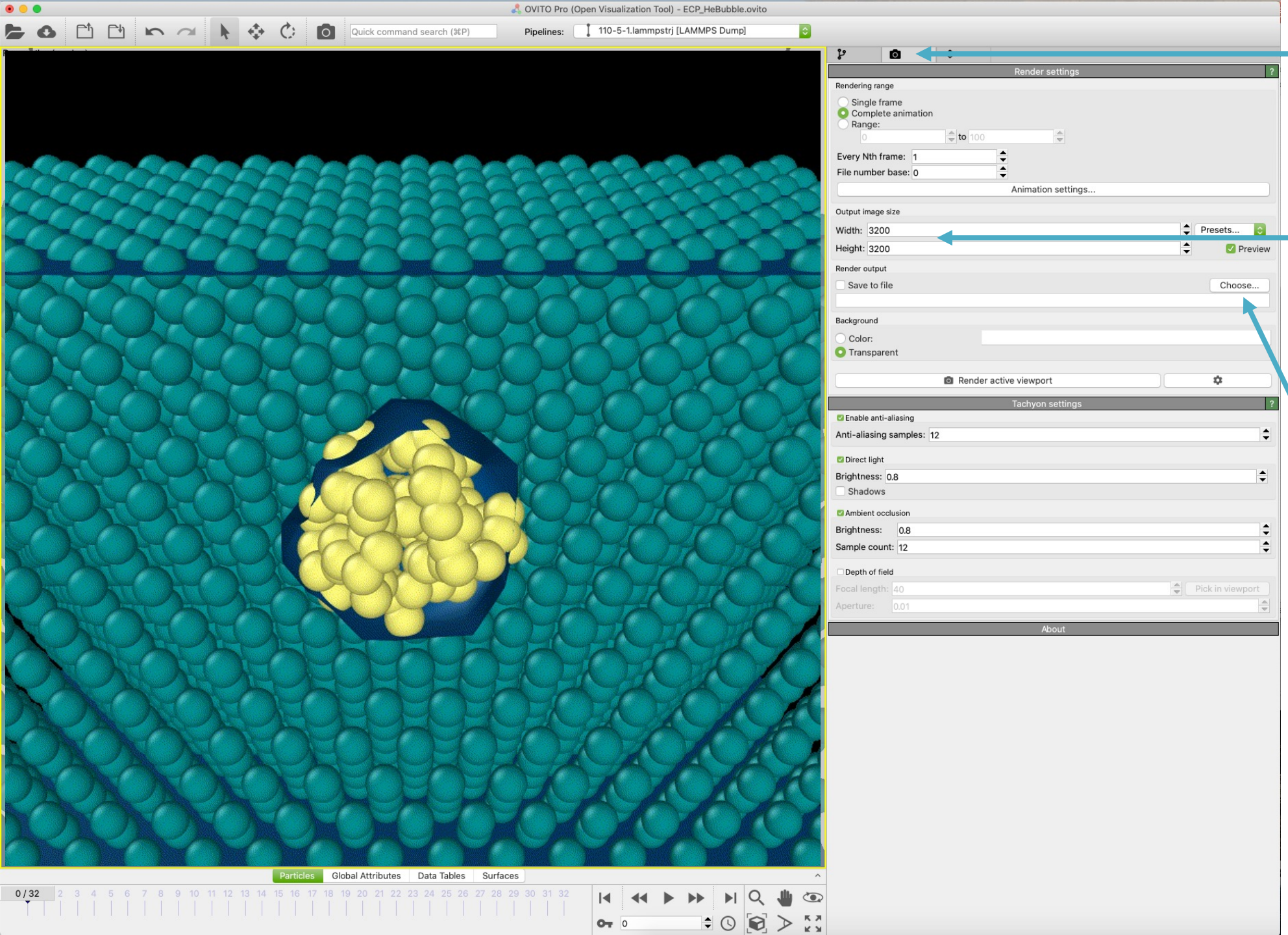


Slice modification allows us to look inside the sample

Important box to check, will only cut out atoms that are part of the previous **Expression Selection**



Clear Selection to get rid of that ugly red color and get back to our original atom coloring.



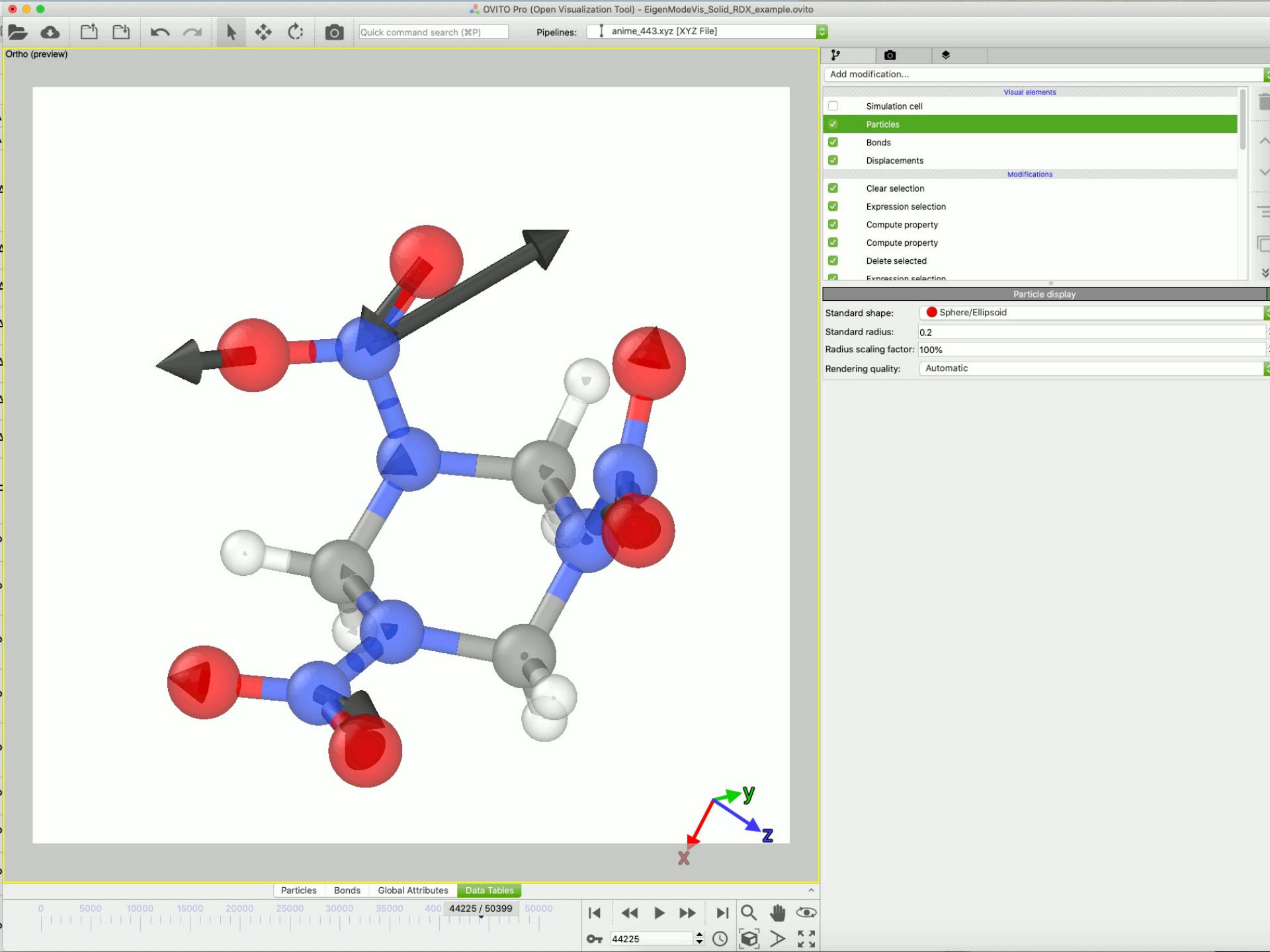
Now over on the rendering tab



Adjust size of image here

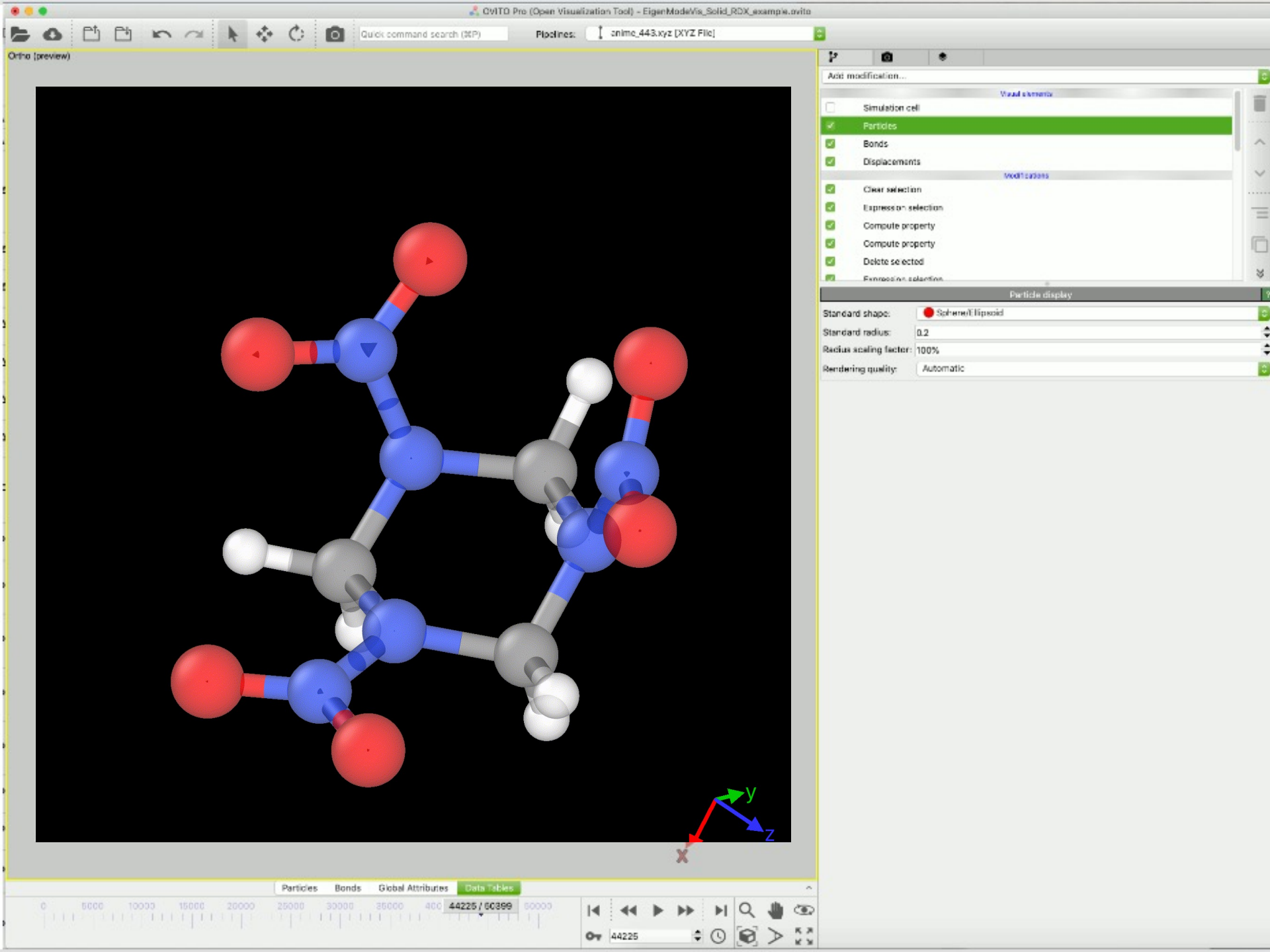
Can save as single images, gif, or other movie formats

I chose the bottom right panel to render as a gif



Quick run through the modifications needed to visualize a normal mode of vibration in a molecule

Identify molecules with **Cluster Analysis** > Select one molecule with **ClusterID** > Generate displacement vectors, scale by mass of atoms > Adjust the **Transparency** of atoms and bonds with **Compute Property**

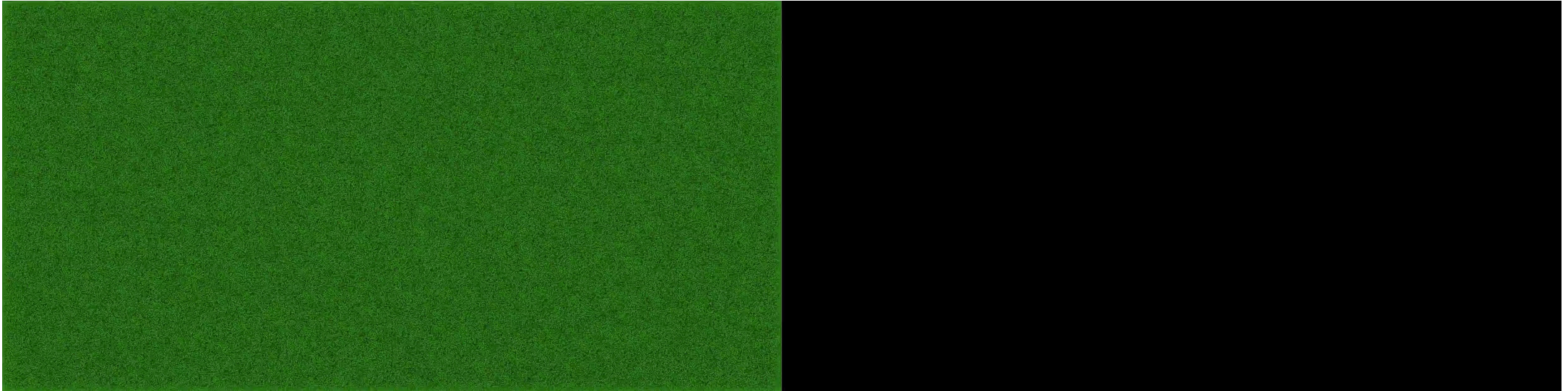
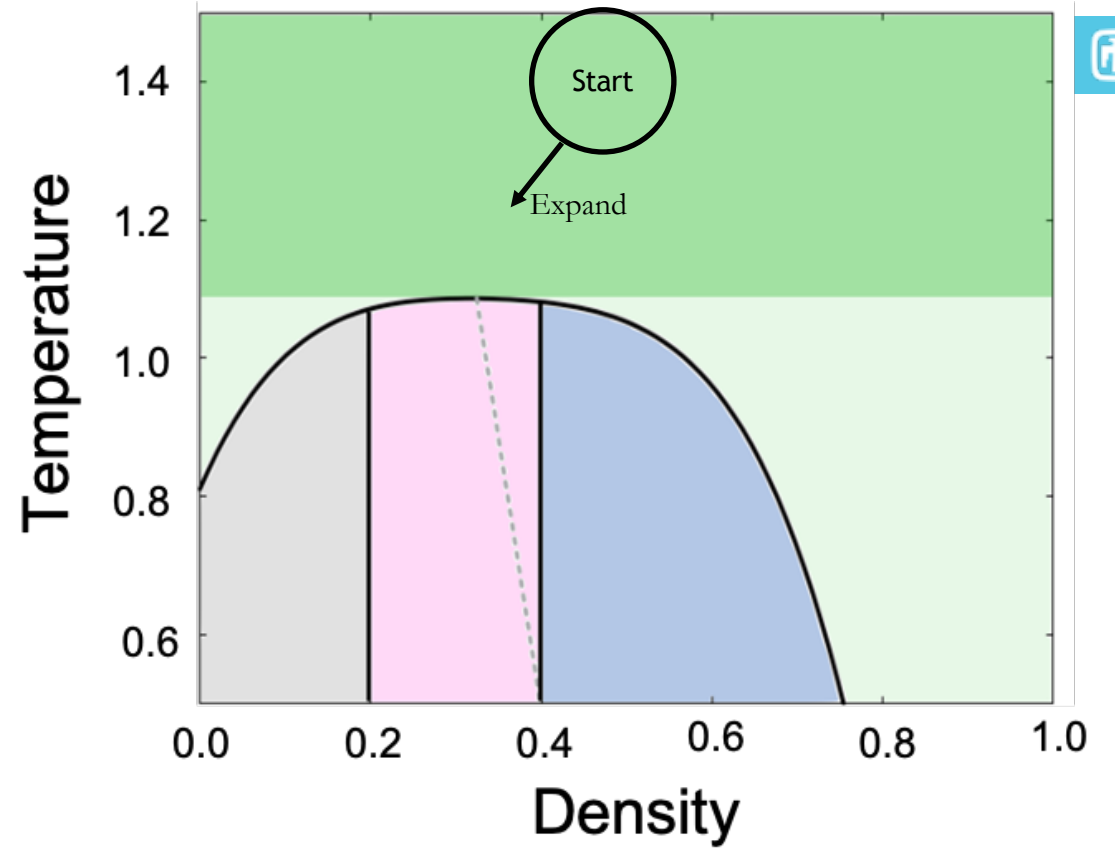


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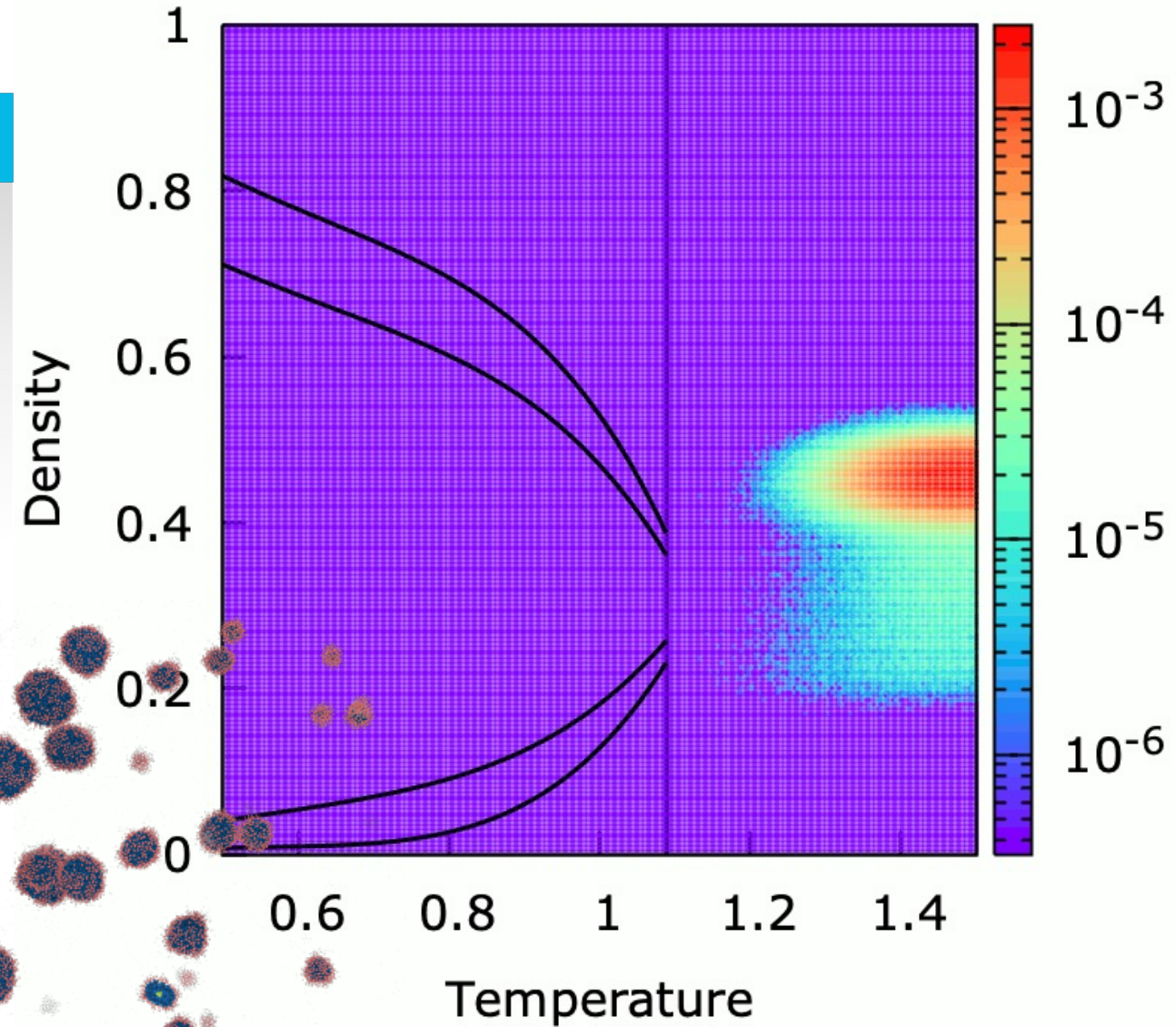
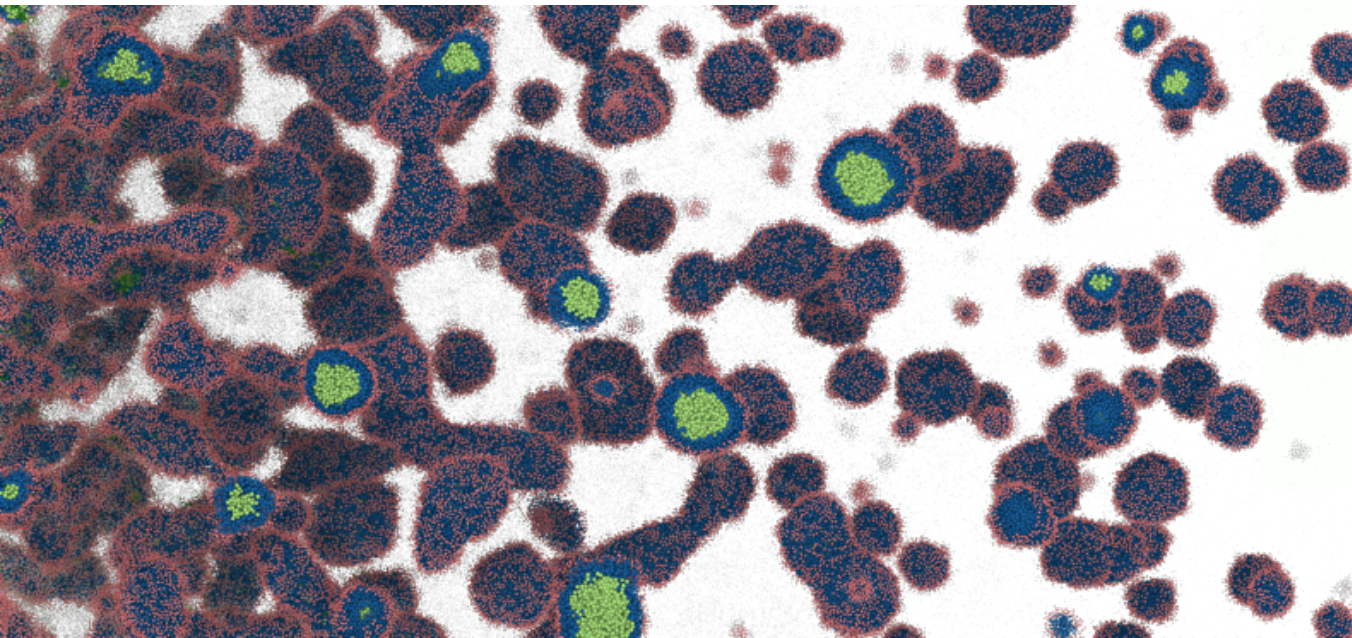
Analyzing Large Simulations

- If you really enjoy the features of OVITO, there is a paid version that will enable python scripting
- This also allows for batch processing on a cluster computing resource
- Example is a >1B atom simulation of a Liquid to Vapor phase transition



Analyzing Large Simulations

- Example is a >1B atom simulation of a Liquid to Vapor phase transition
- OVITO calculated properties can be outputted to make for unique analysis of your simulations




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General questions

Feel free to post any questions regarding the usage of OVITO here.

[1](#) [2](#) [3](#) [Last »](#)[+ New Topic](#)

Topics		Last post
	NearestNeighborFinder-periodic image By sepideh kavousi 4 Replies · 64 Views	 6 hours ago Alexander Stukowski
	LAMMPS trajectory files with bonds By Botond Tyukodi 11 Replies · 683 Views	 20 hours ago Cong Dai
	Creating bonds NOT based on distance. By Anna Lappala 1 Reply · 11 Views	 1 day ago Alexander Stukowski

PMMA Short Chains, $\lambda = 24\text{nm}$ $U_p = 2.25\text{ km/s}$, $SF_{ac} = 1.0$

Time 1ps

