Sandia National Laboratories

LAMMPS Users Meeting 2021: Visualization Tutorial

SAND2021-9634 C

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Why Bother With Viz?

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?

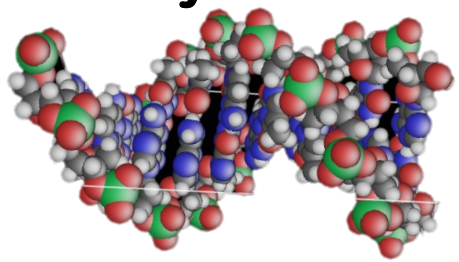
Wish List

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"

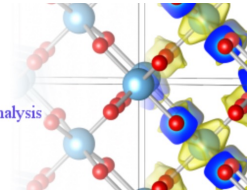
OVITO
Open Visualization Tool

AtomEye

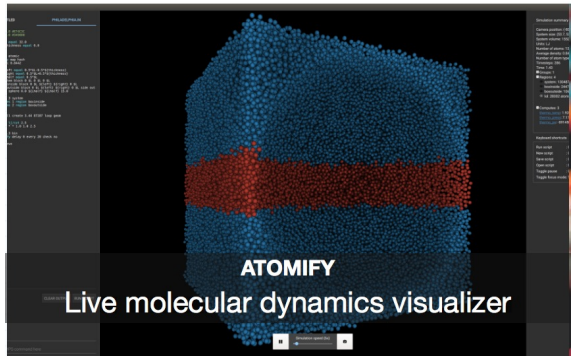


VMD
Visual Molecular Dynamics

VESTA
Visualization for Electronic and STructural Analysis



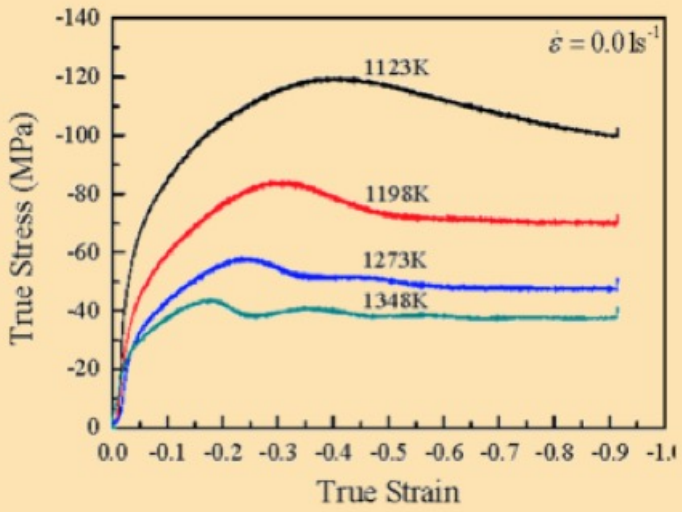
ParaView



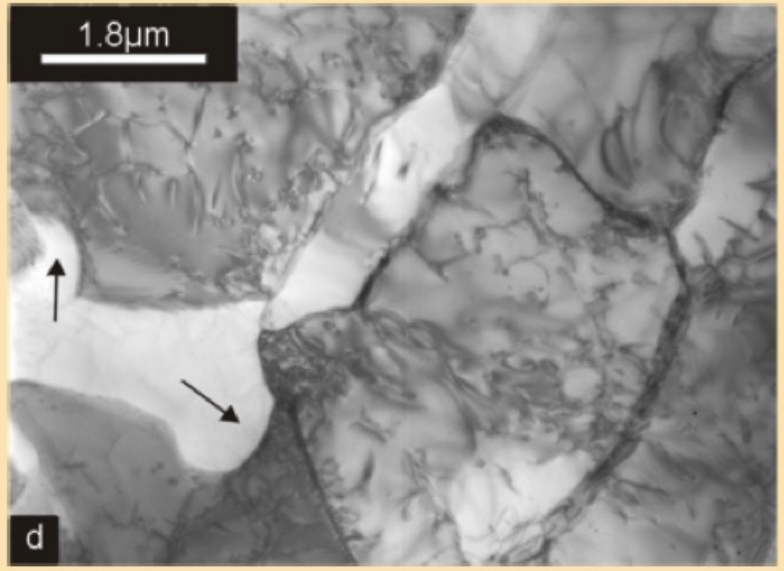
And many more…

Value by Analogy

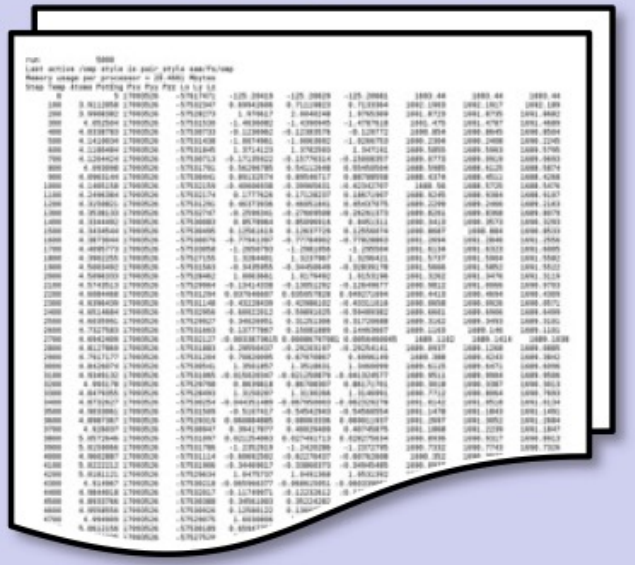
To only look at the raw output of an experiment / simulation is limiting your insight into 'what happened'



Microscopy & Imaging

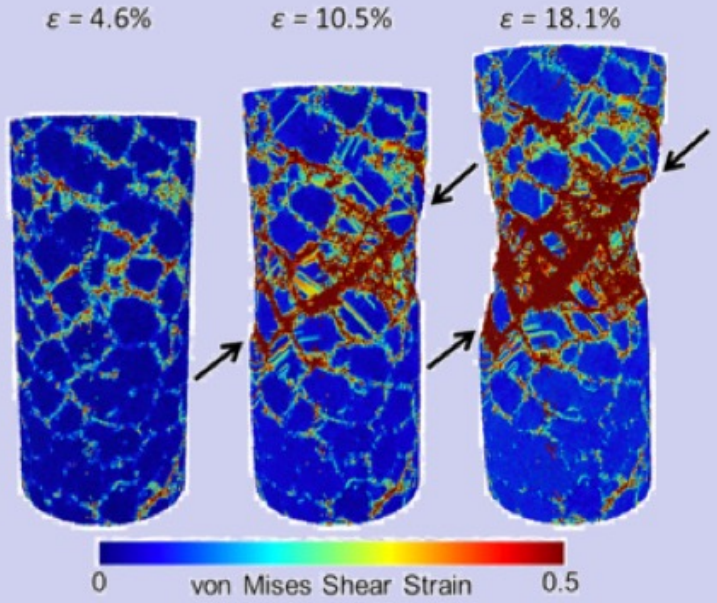


Raw output data

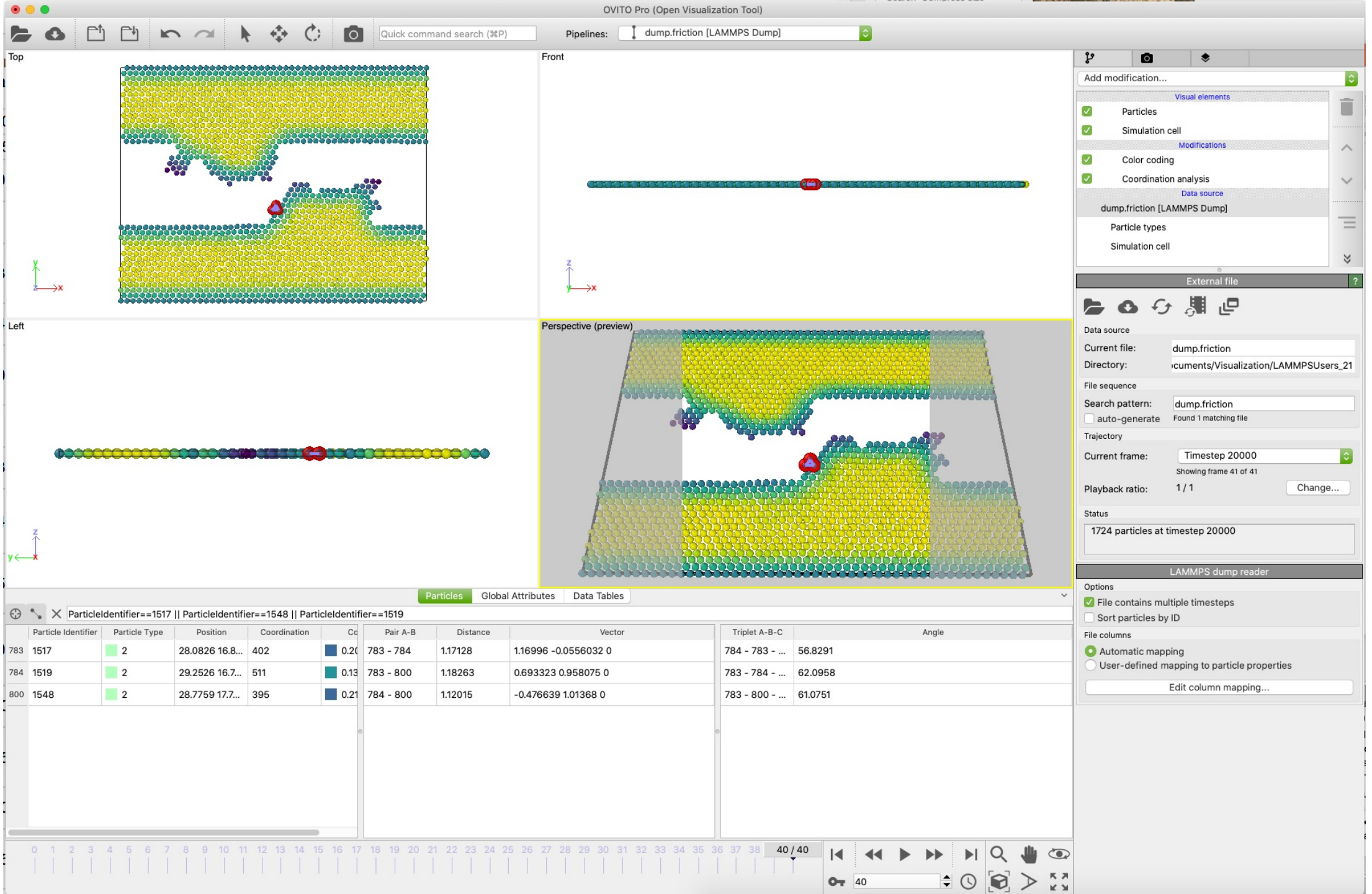


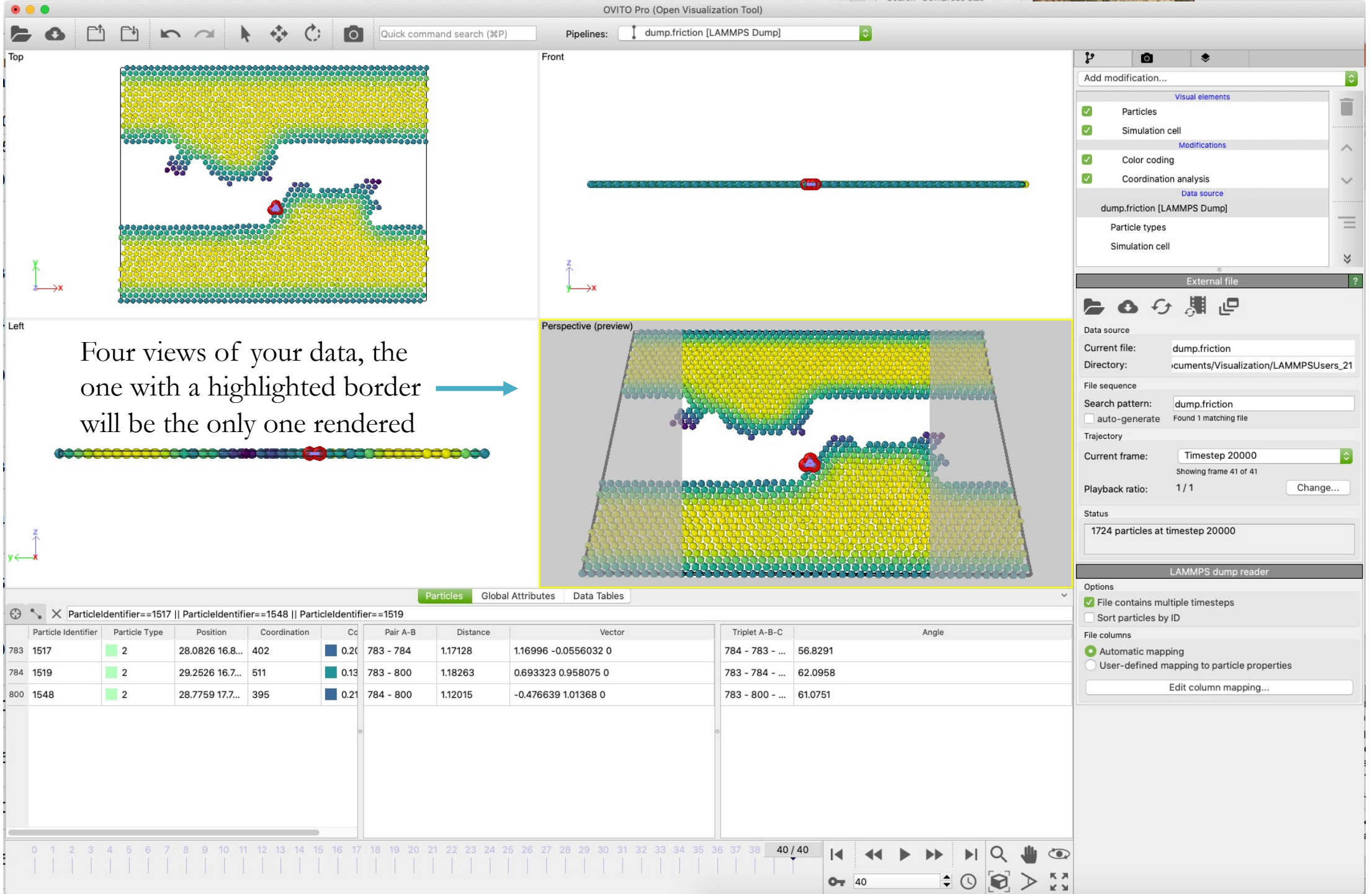
Data analysis & Visualization

"in-silico microscopy"



(Credit A. Stukowski LAMMPS Users Meeting 2019)


OVITO Pro (Open Visualization Tool)
Quick command search (⌘P)
Pipelines:
dump.friction [LAMMPS Dump]
Top
Front
Left
Perspective (preview)
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: ɔcuments/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...
Particles
Global Attributes
Data Tables
ParticleIdentifier==1517 || ParticleIdentifier==1548 || ParticleIdentifier==1519
Particle Identifier
Particle Type
Position
Coordination
Pair A-B
Distance
Vector
Triplet A-B-C
Angle
783 1517 2 28.0826 16.8... 402 783 - 784 1.17128 1.16996 -0.0556032 0 784 - 783 - ... 56.8291
784 1519 2 29.2526 16.7... 511 783 - 800 1.18263 0.693323 0.958075 0 783 - 784 - ... 62.0958
800 1548 2 28.7759 17.7... 395 784 - 800 1.12015 -0.476639 1.01368 0 783 - 800 - ... 61.0751
40 / 40
40


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
Add modification...
Visual elements
Particles
Simulation cell
Modifications
Color coding
Coordination analysis
Data source
dump.friction [LAMMPS Dump]
Particle types
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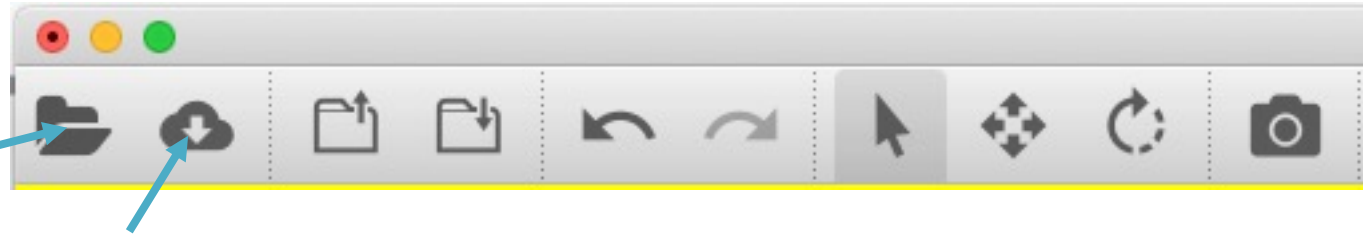
40 / 40
40

GUI Walkthrough

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.

GUI Walkthrough

Save/Load an OVITO session

(Covered in tutorial)

Load a local file on your machine

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

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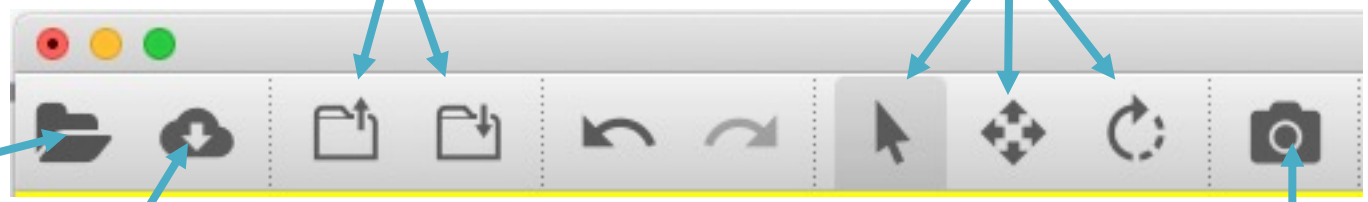

Save/Load an OVITO session

(Covered in tutorial)

Quick access to swap your left-click mouse function to Select/Move/Rotate

Load a local file on your machine

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

Render active viewport, this is one of four panels highlighted in yellow

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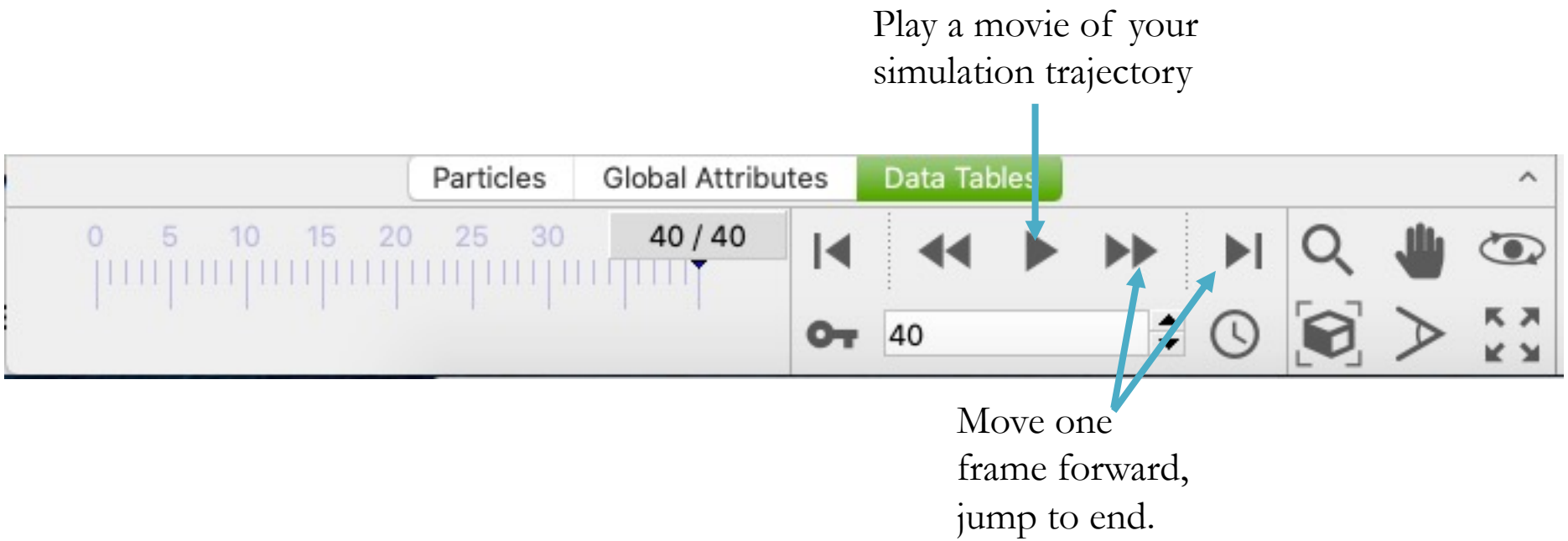
GUI Walkthrough



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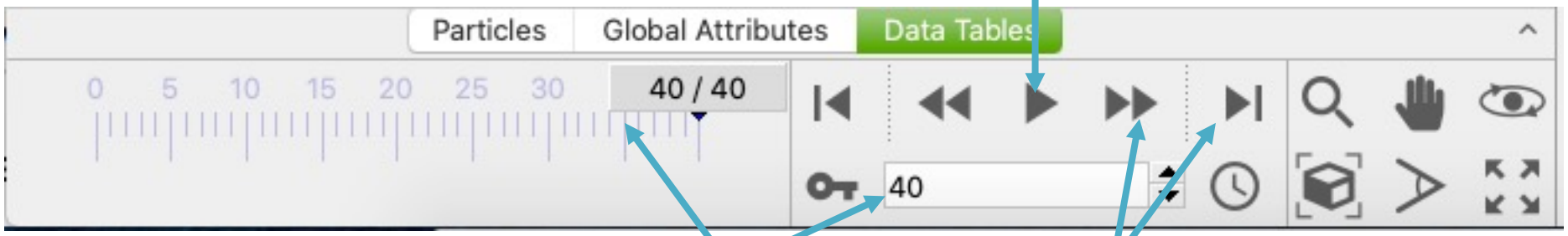
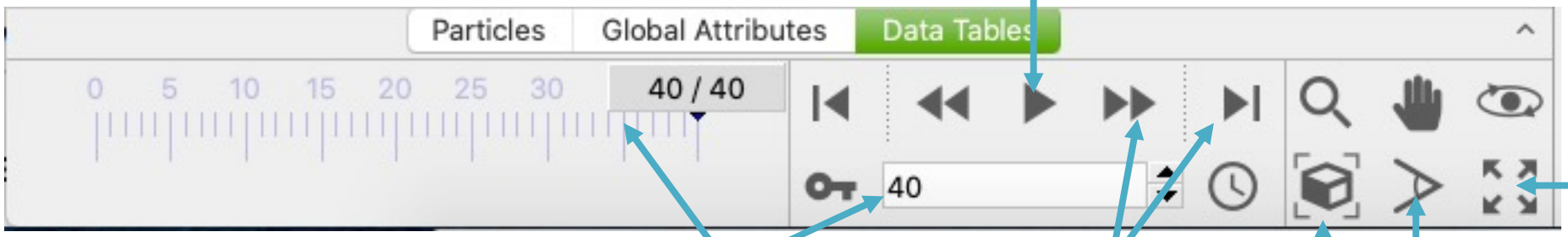


GUI Walkthrough



Play a movie of your simulation trajectory

Select a particular frame to view

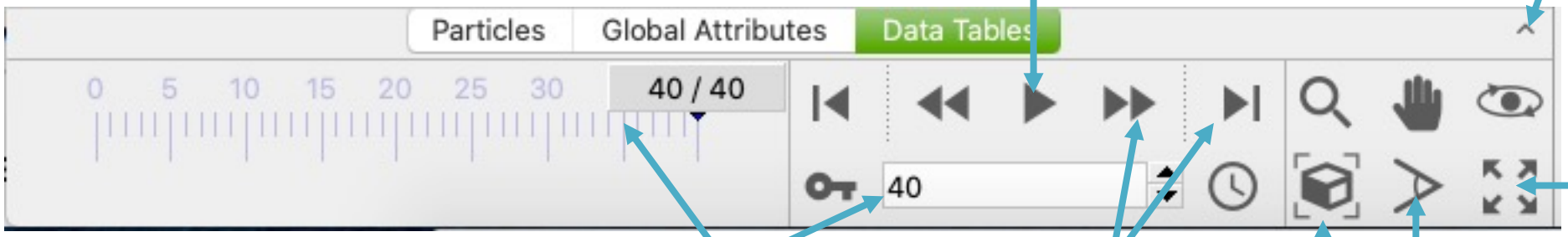
Move one frame forward, jump to end.

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

GUI Walkthrough



Play a movie of your simulation trajectory

Detailed information tables stored here

Focus on one viewing panel, click again to see all

Select a particular frame to view

Move one frame forward, jump to end.

Adjust Zoom, left-click and drag up/down

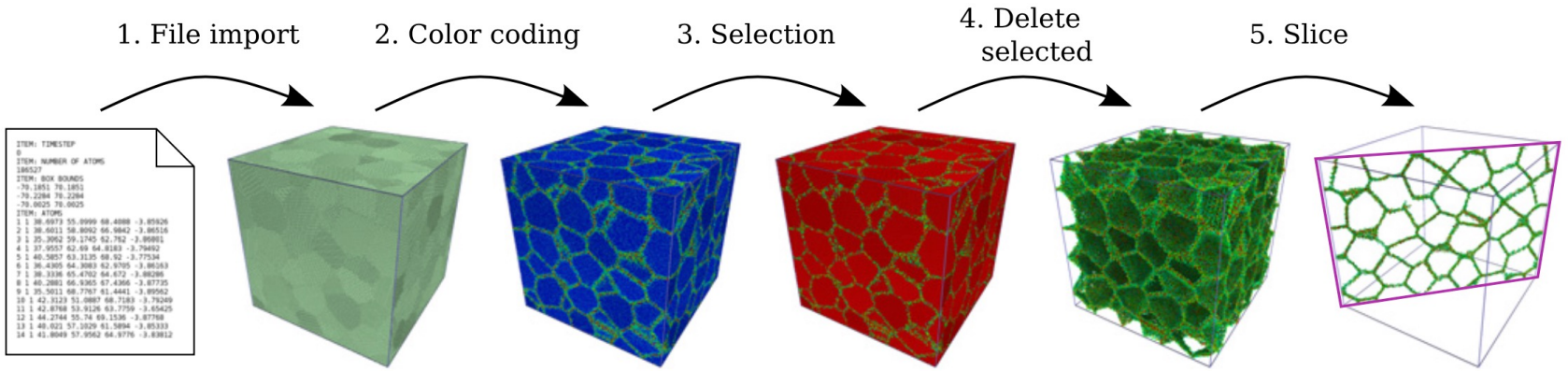
Auto-Zoom to fit all atoms into the view

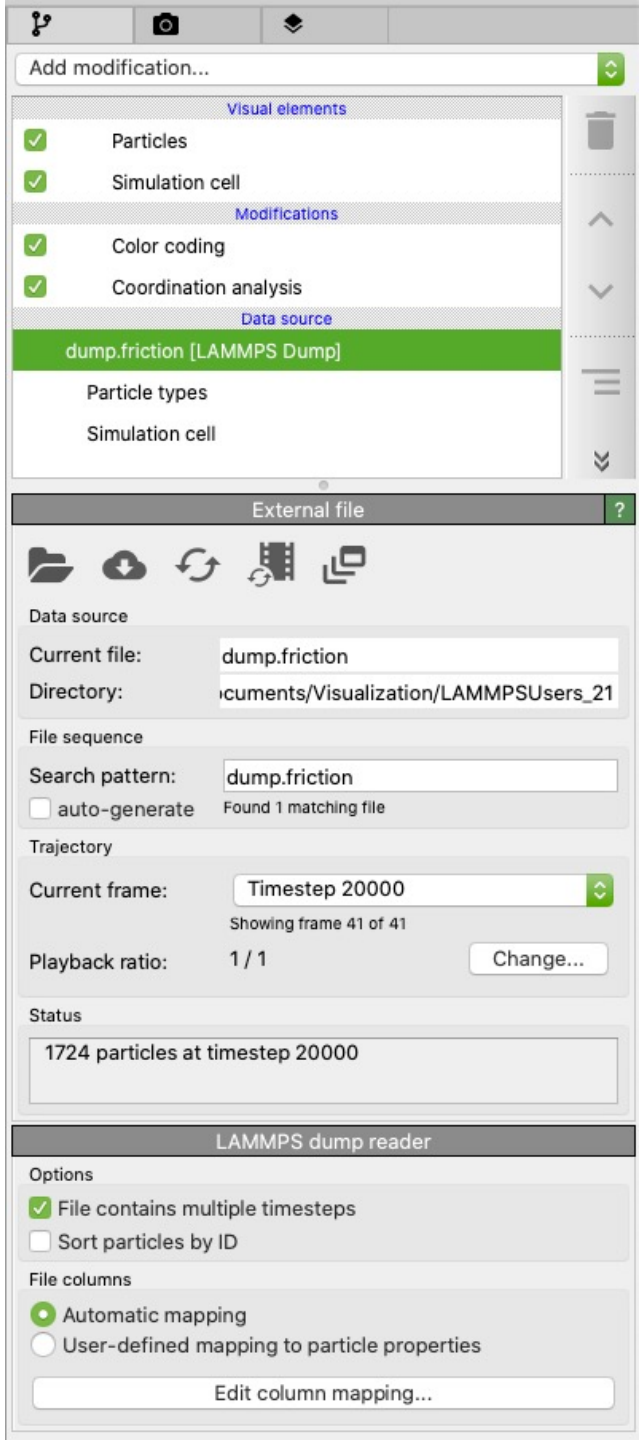
GUI Walkthrough

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.

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





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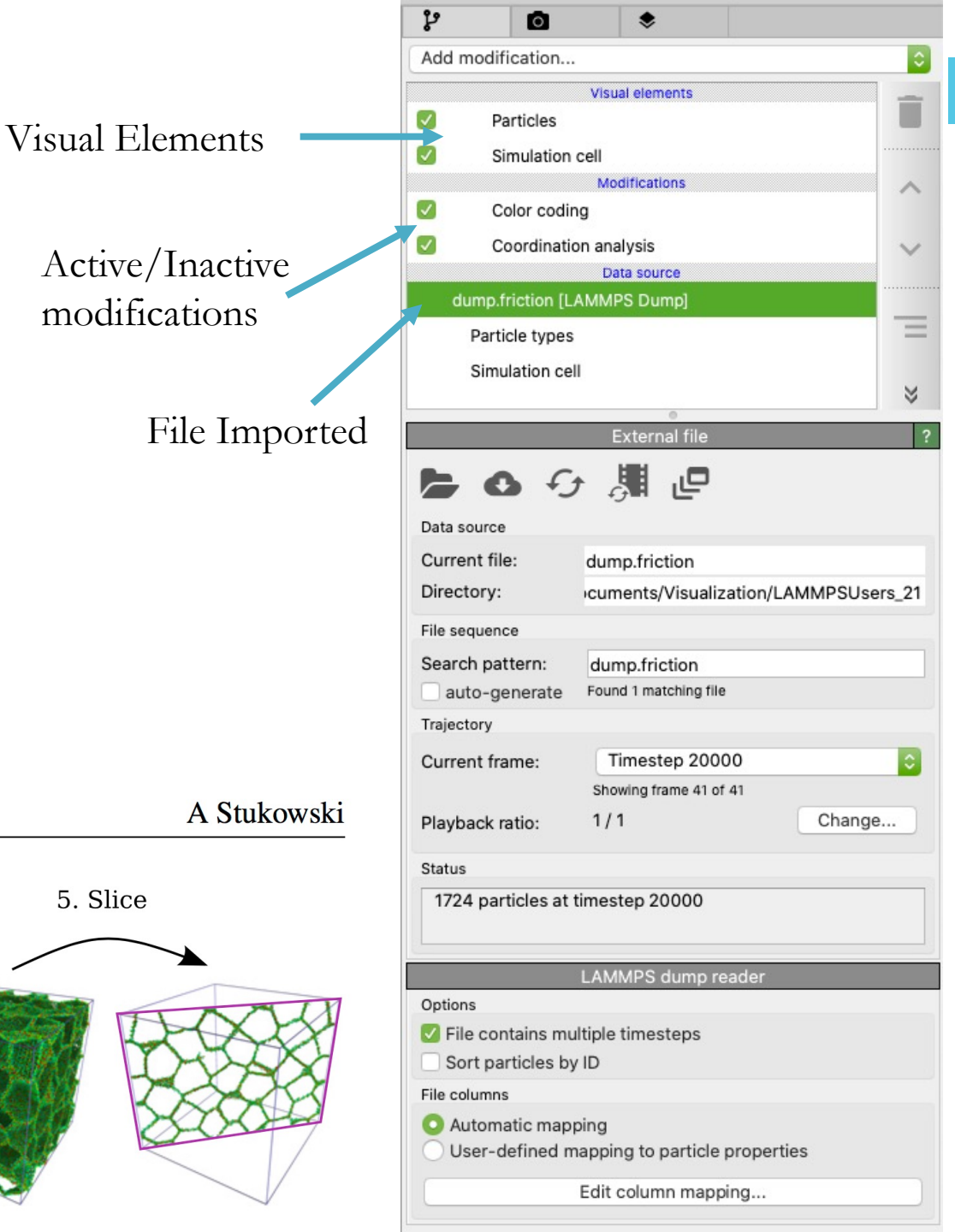

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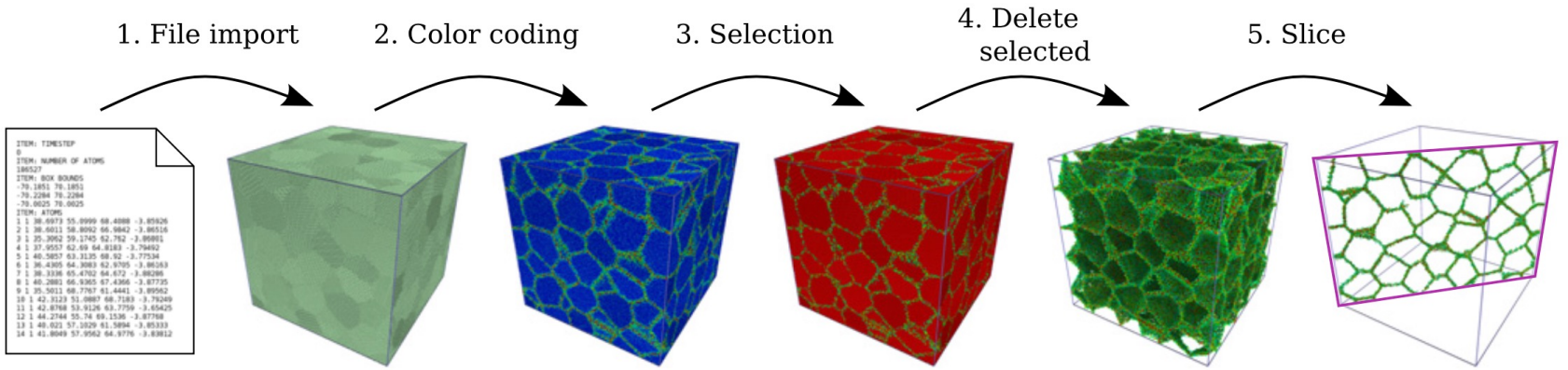
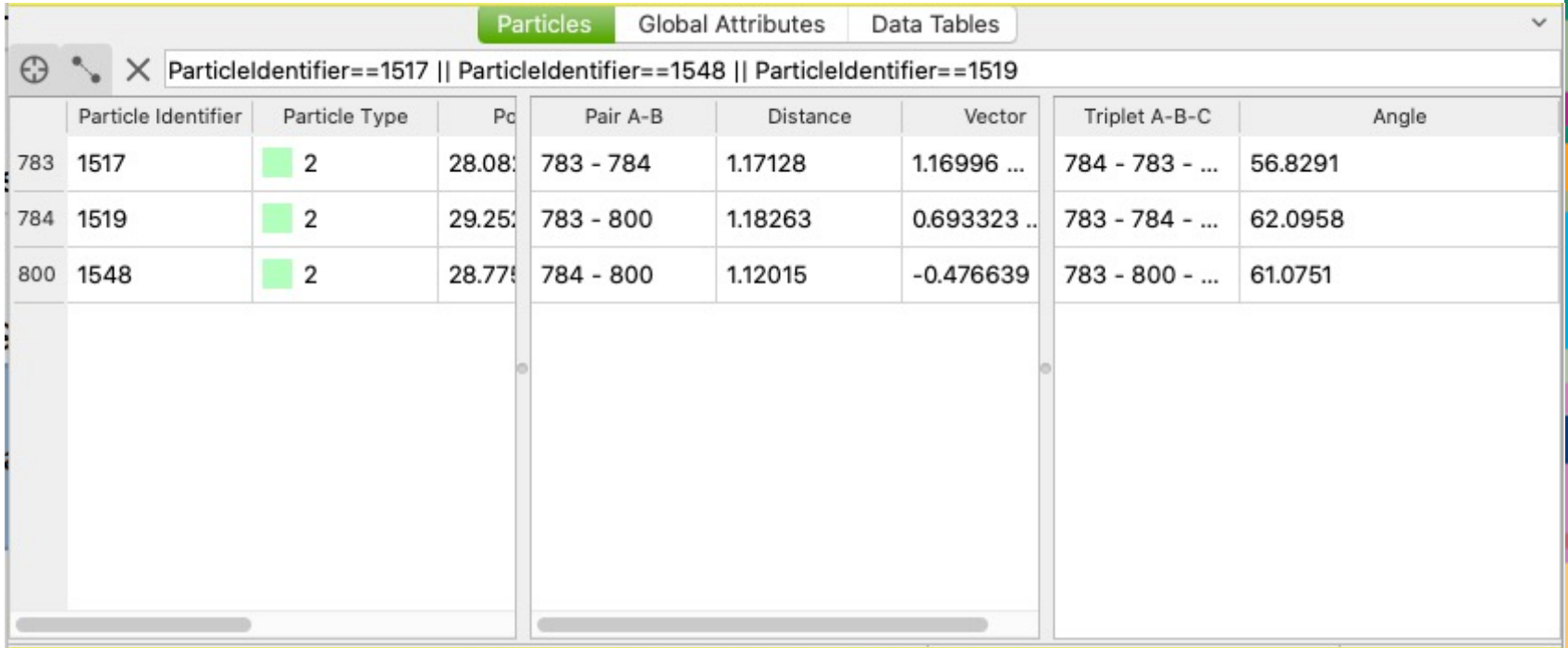
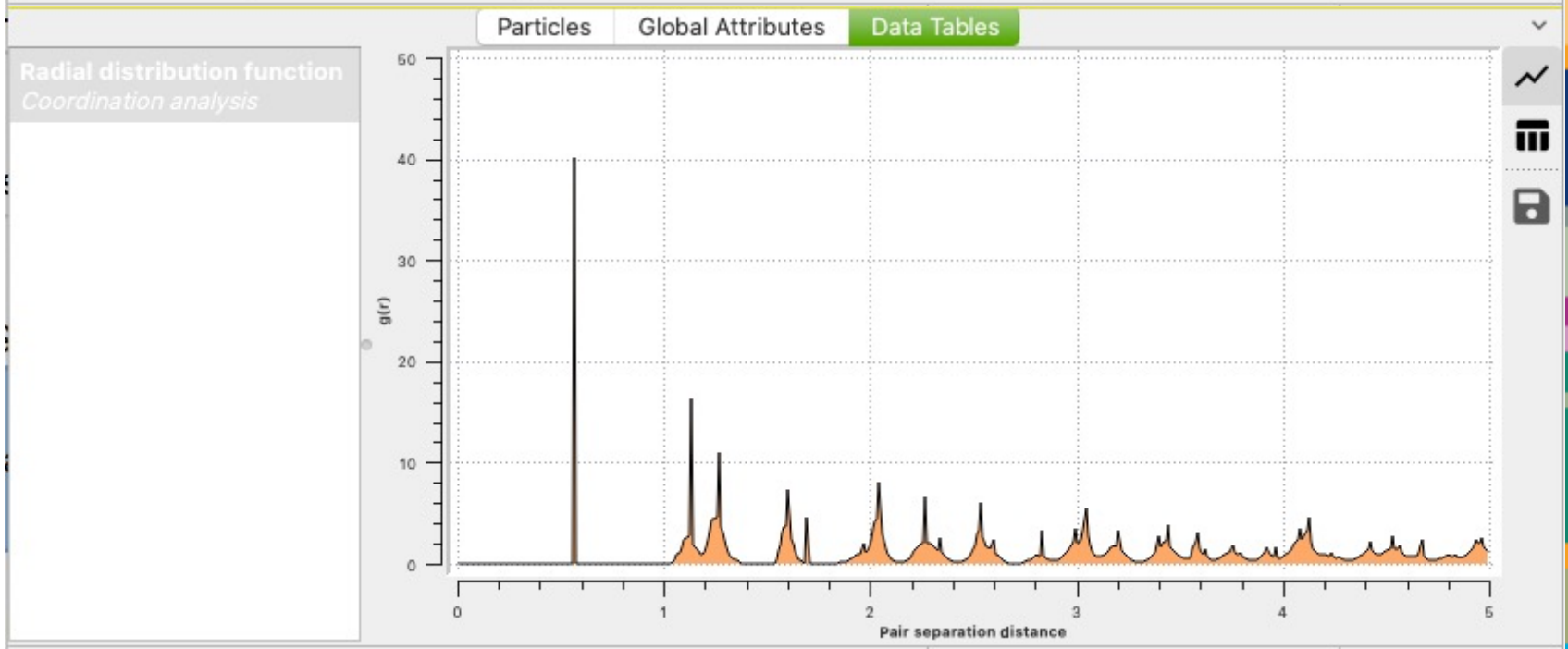
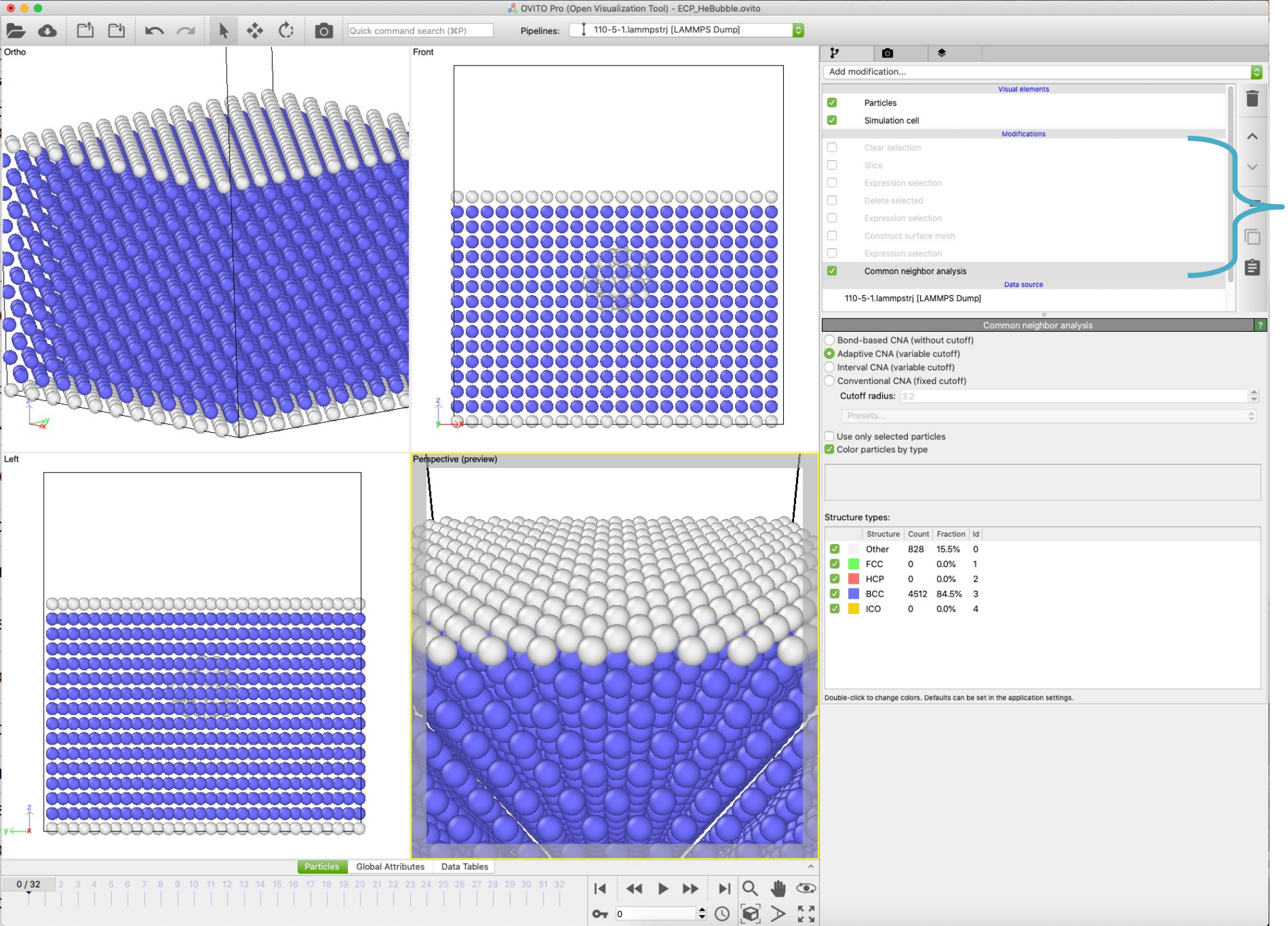


GUI Walkthrough

- 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



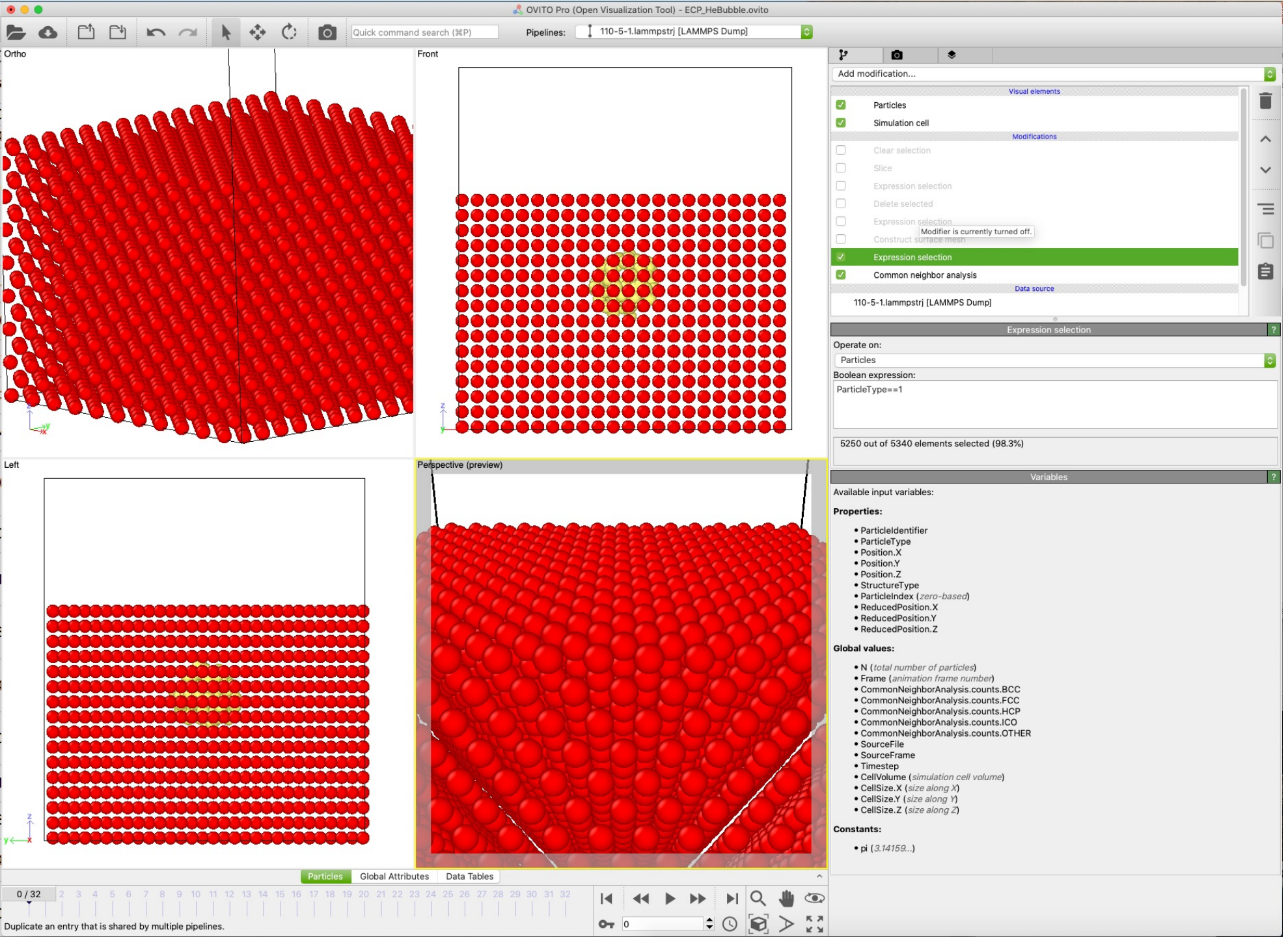




Modification stack read from bottom to top

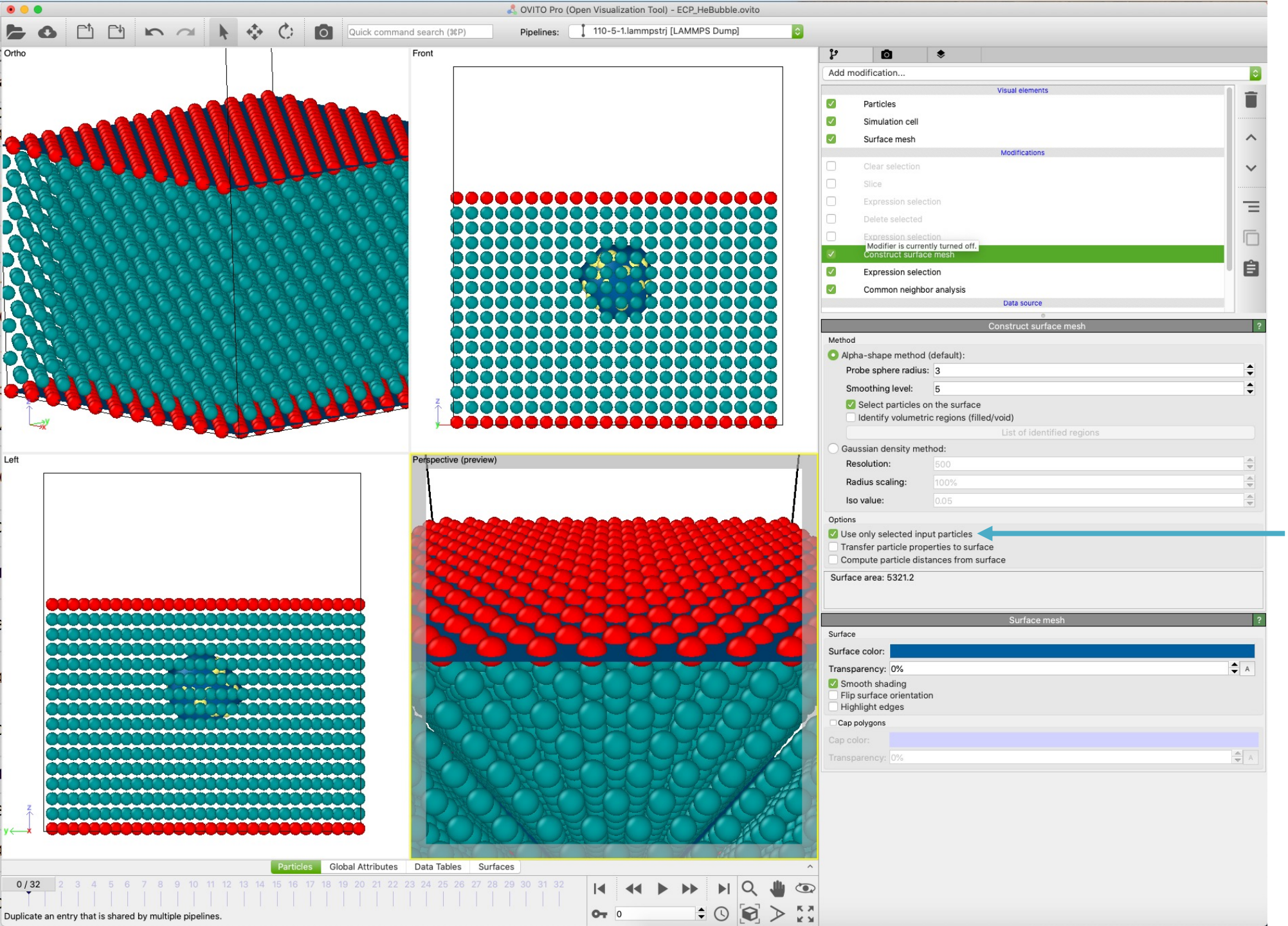
Common Neighbor Analysis is used to identify the surfaces, and internal cavity in the sample

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



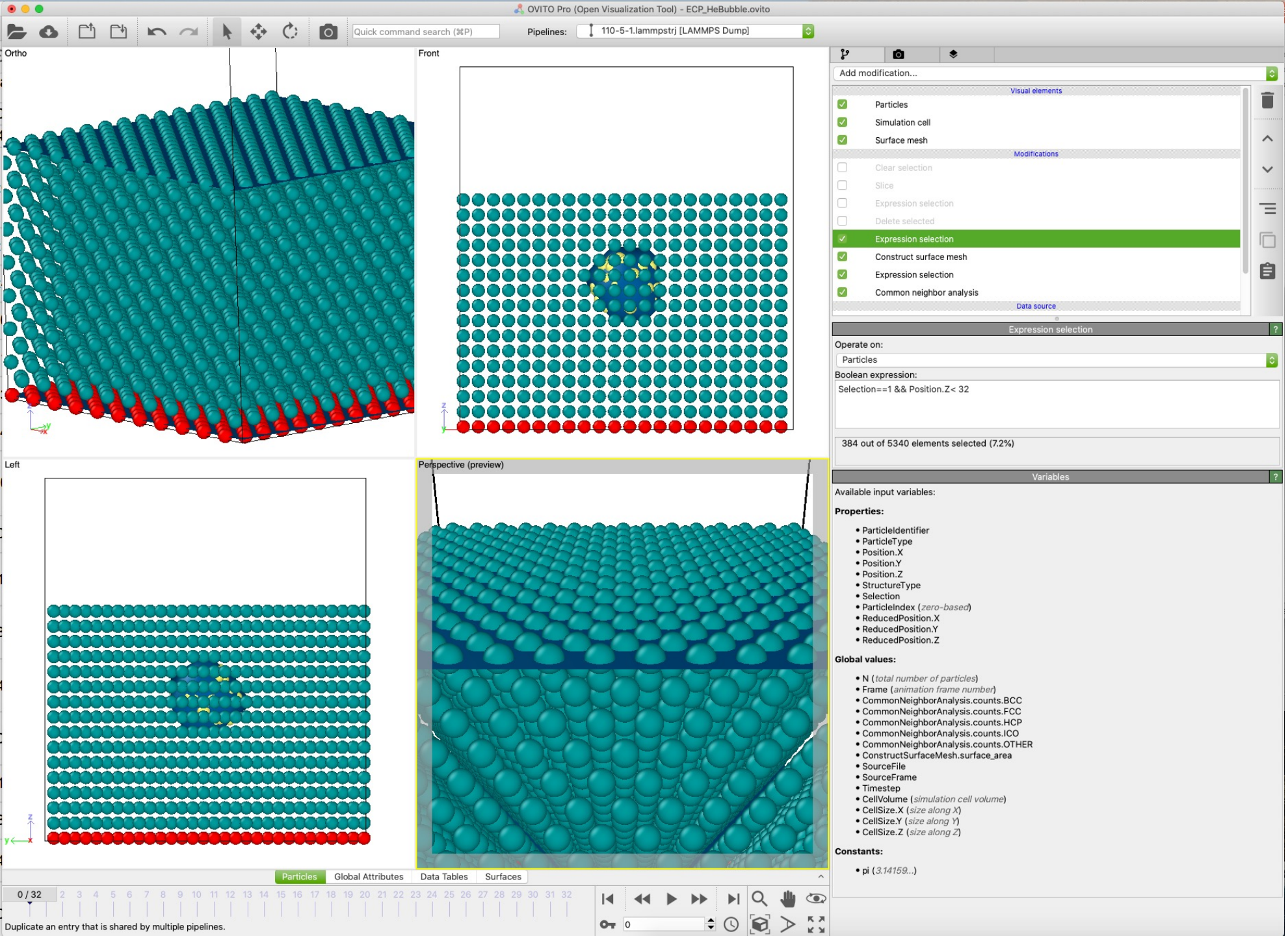
ParticleType is used to create a selection of particles (now colored in red).

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



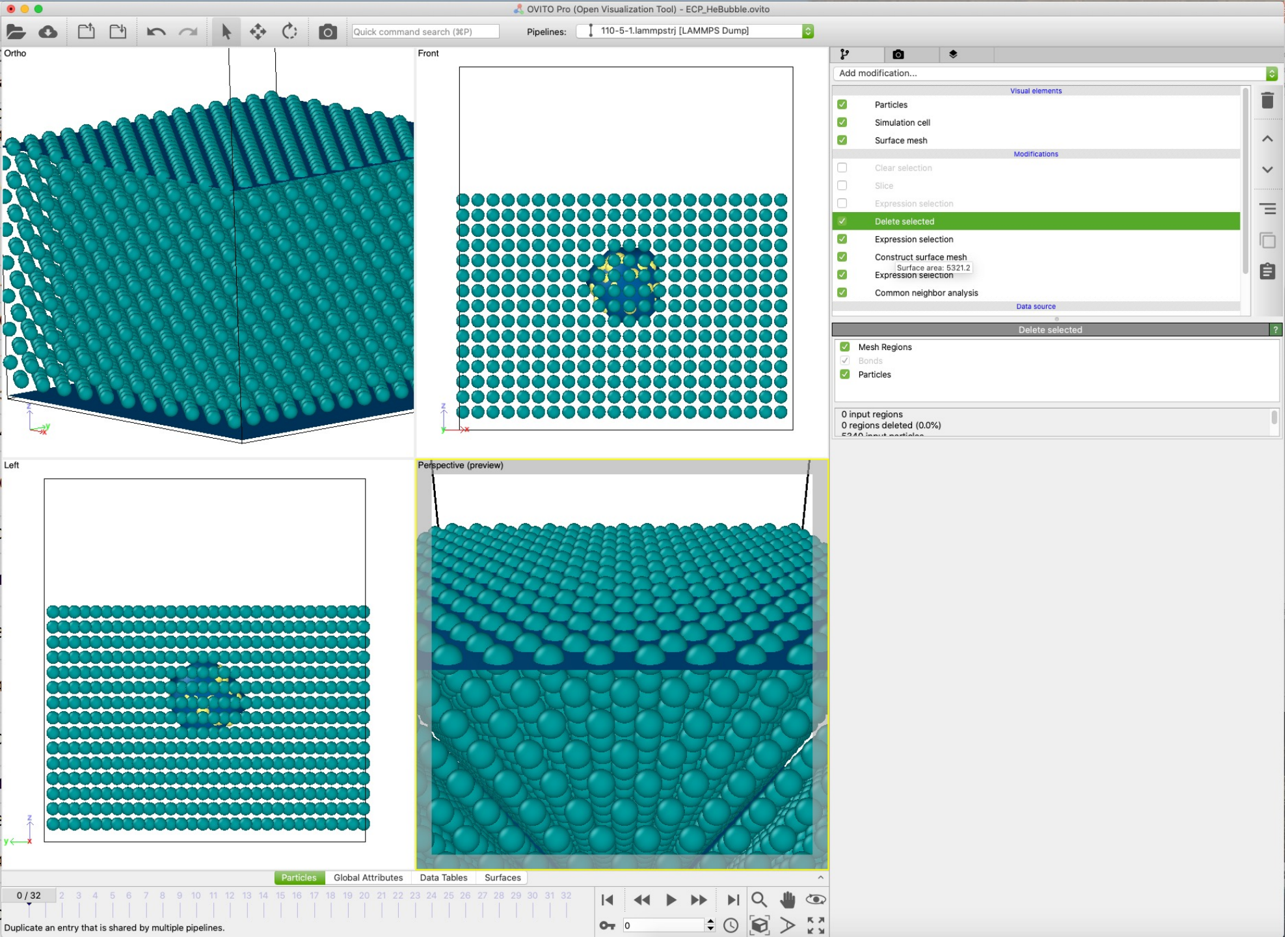
Construct Surface Mesh modifier is added

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

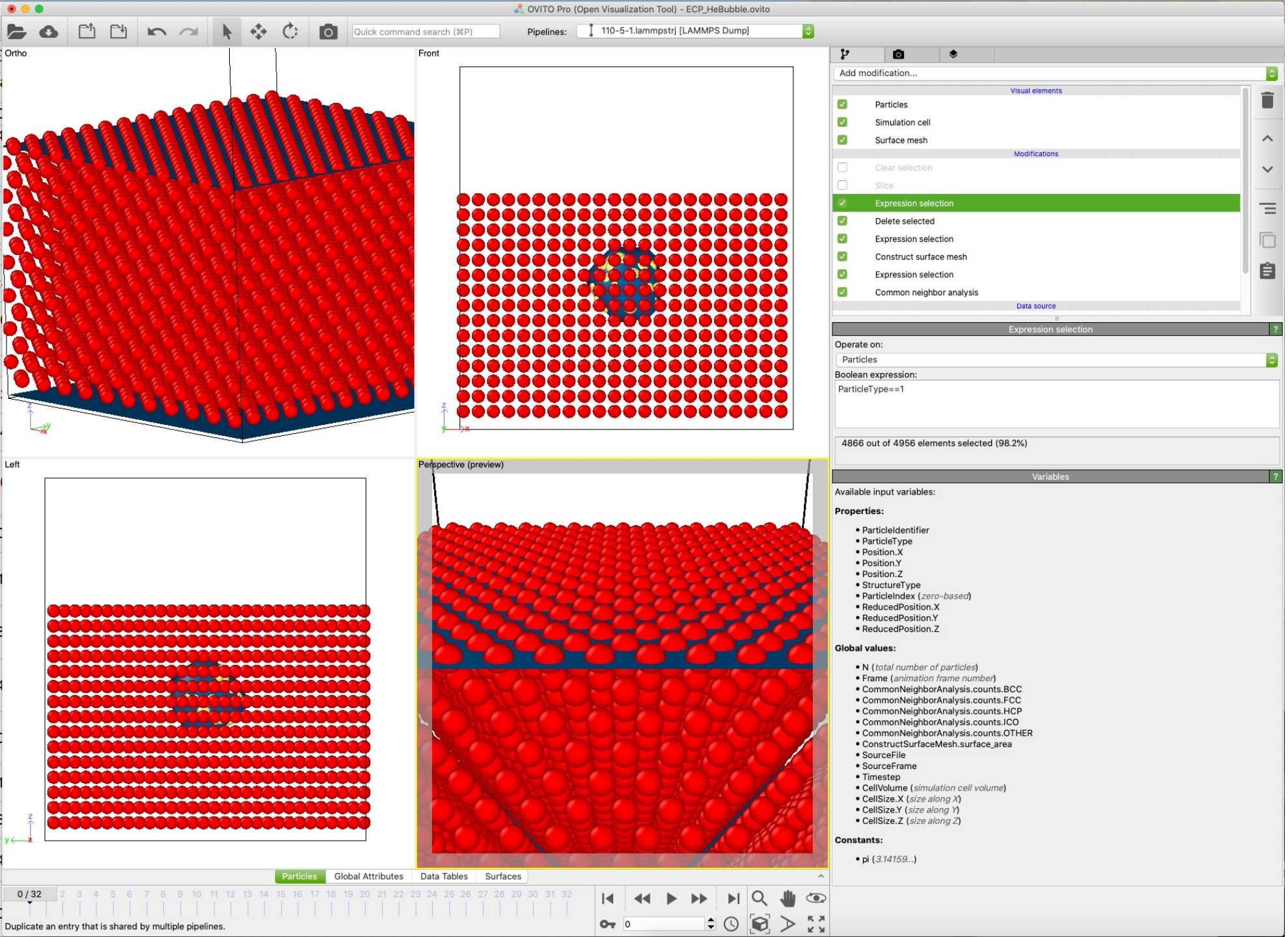


Atoms are given a value of 0/1 called **Selection**, can use this to make a compound expression

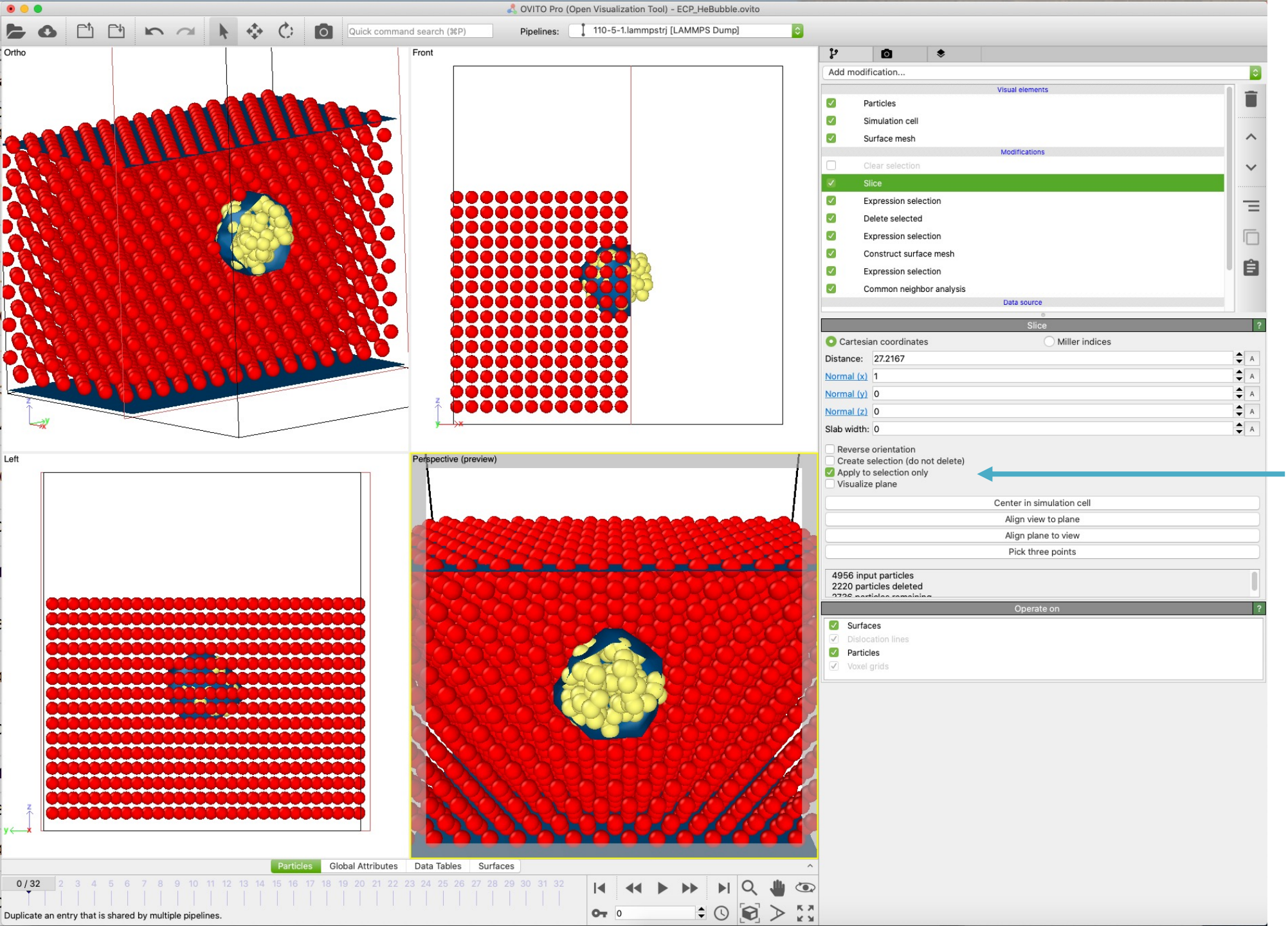
We want to select atoms on the surface (**Selection**==1) and below the cavity (**Position.Z**<32)



Delete Selected to make the bottom surface look pretty

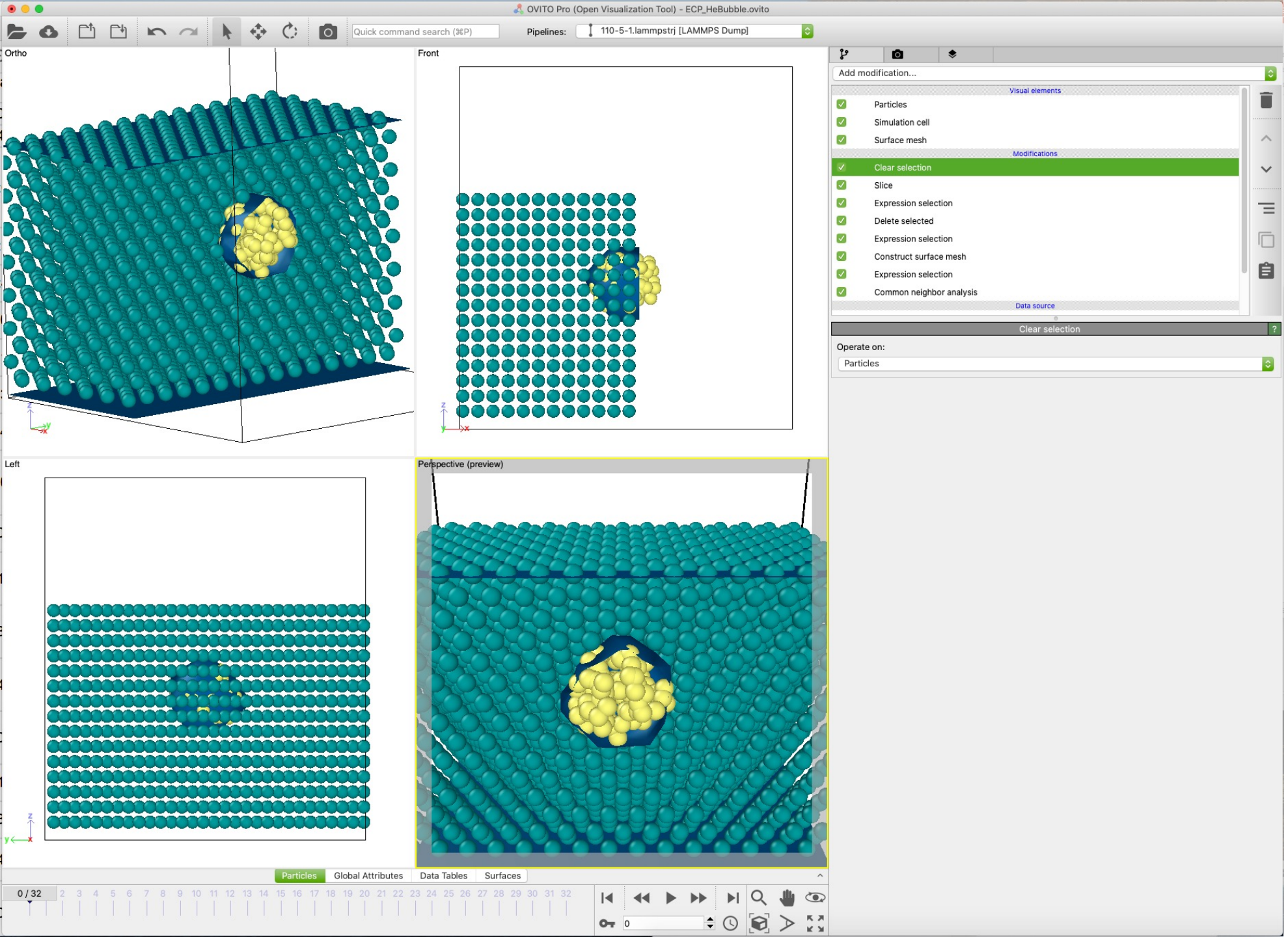


Create a new **Expression Selection** to grab the atoms in the solid again (**ParticleType**==1).

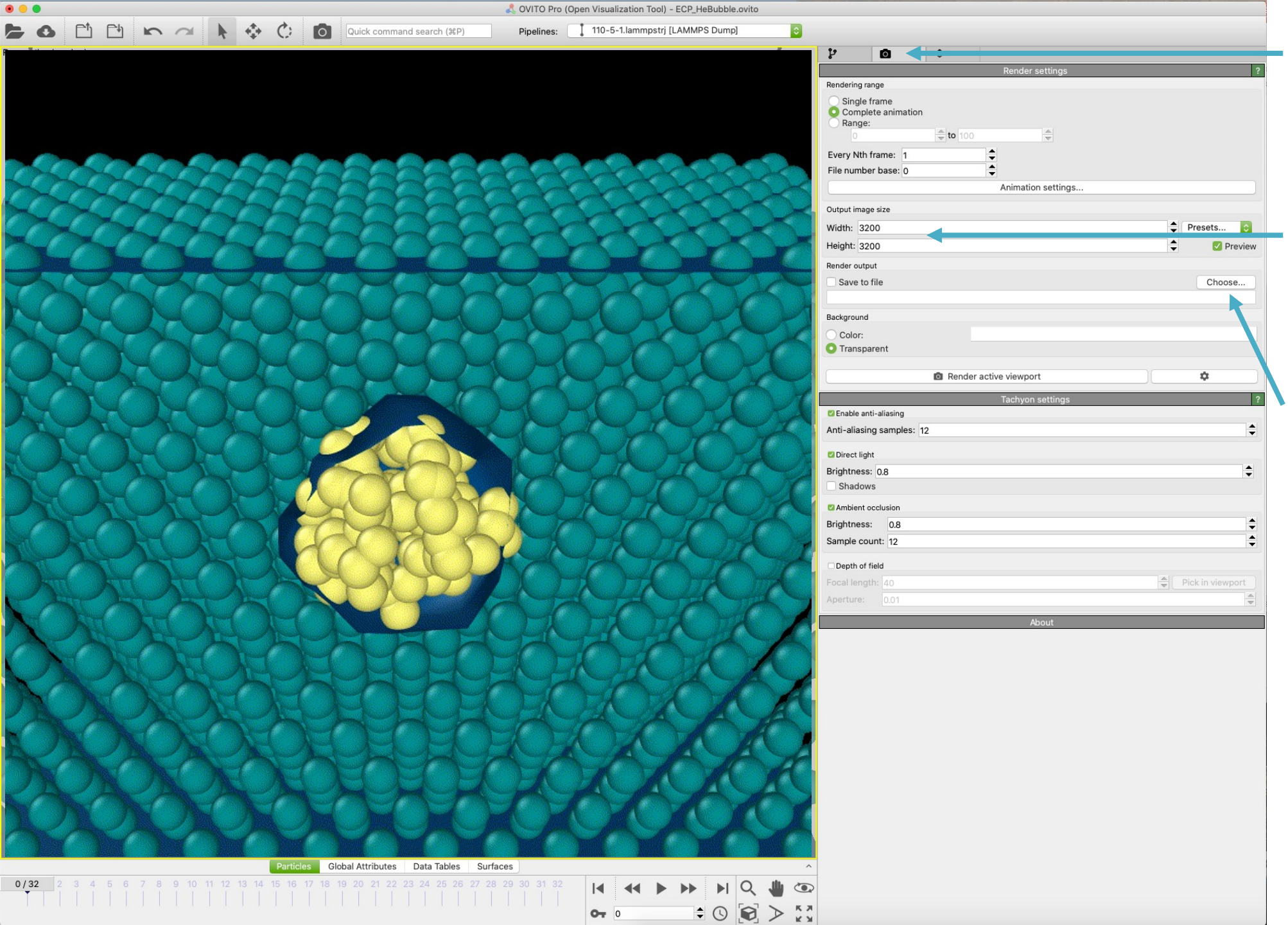


Slice modification allows us to look inside the sample

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.

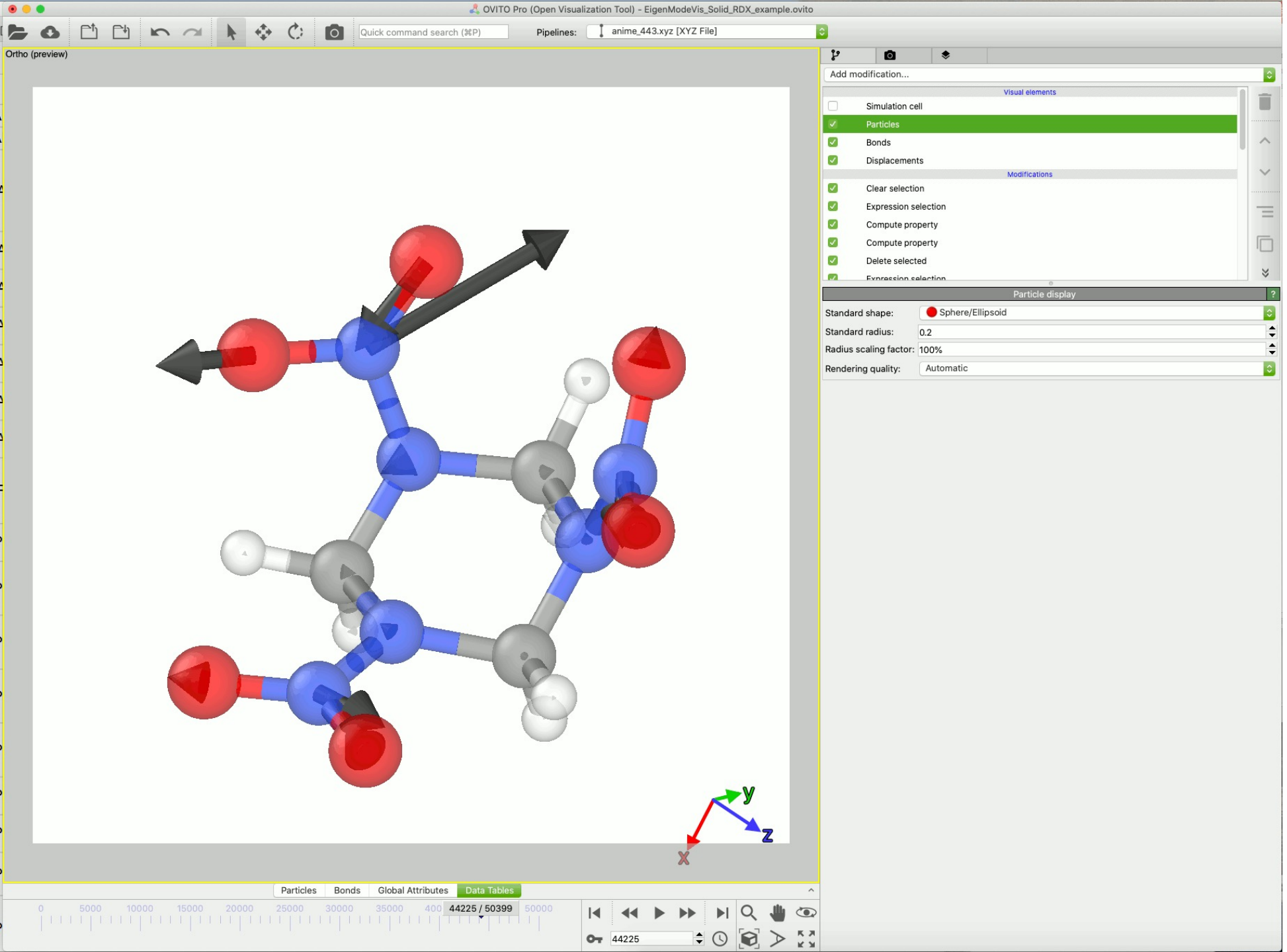


Now over on the rendering tab

Adjust size of image here

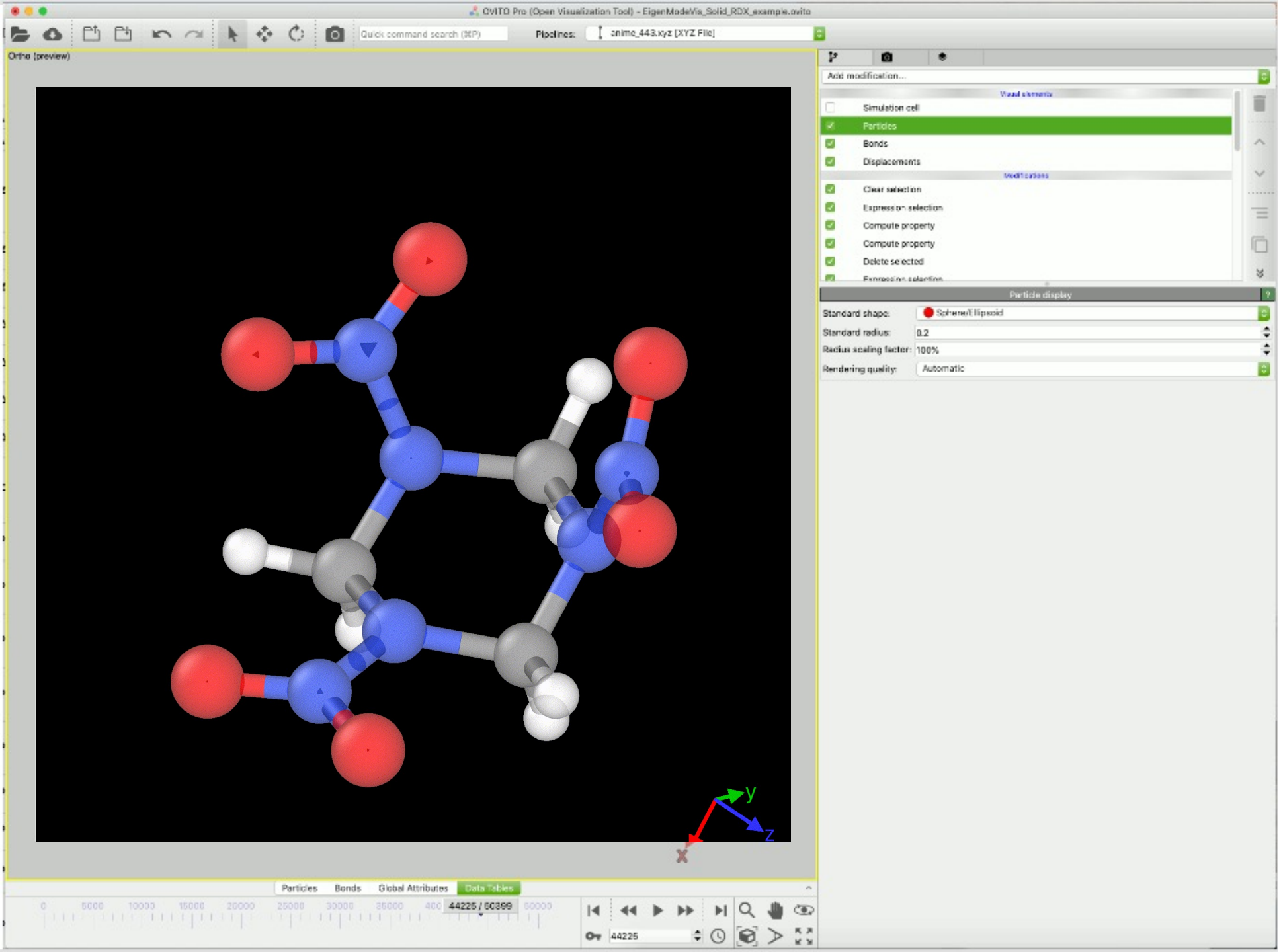
Can save as single images, gif, or other movie formats

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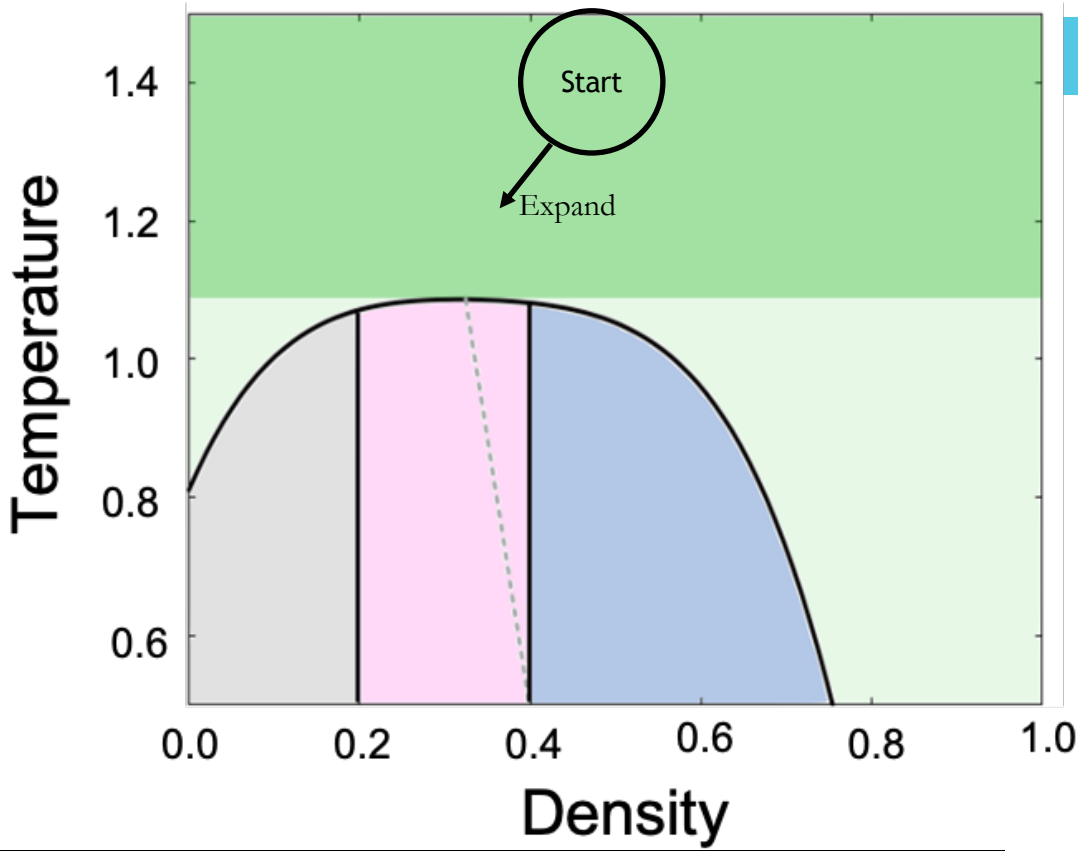
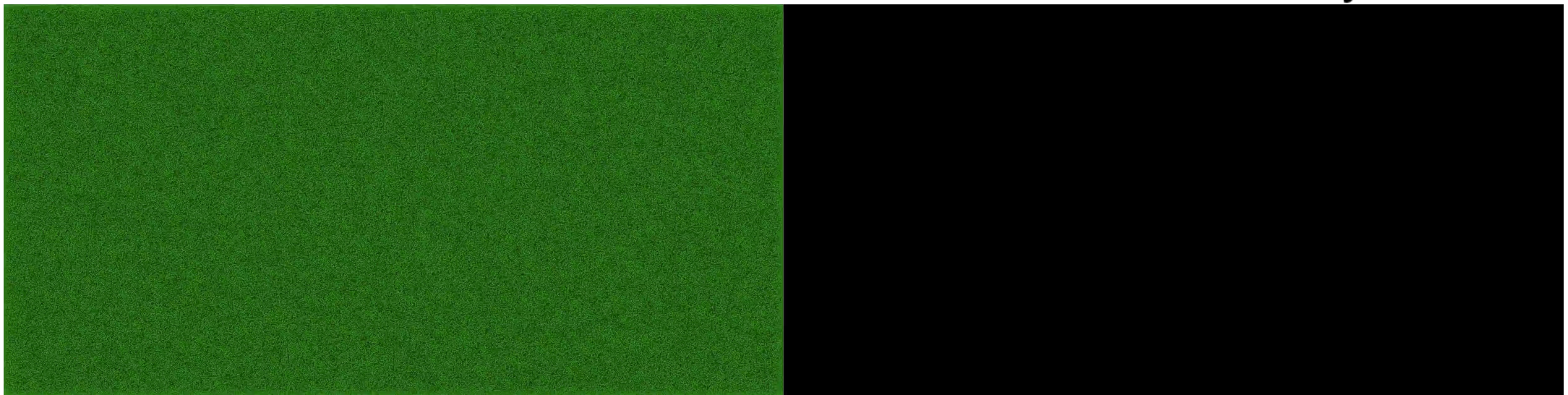
Identify molecules with **Cluster Analysis** > Select one molecule with **ClusterID** > Generate displacement vectors, scale by mass of atoms > Adjust the **Transparency** of atoms and bonds with **Compute Property**

Advanced Features

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

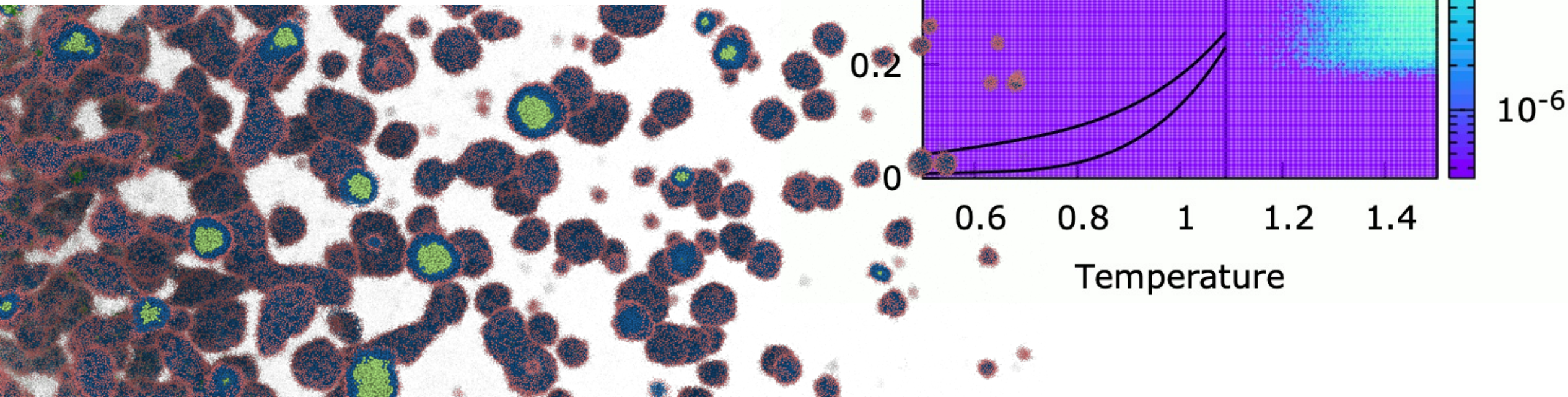




Advanced Features

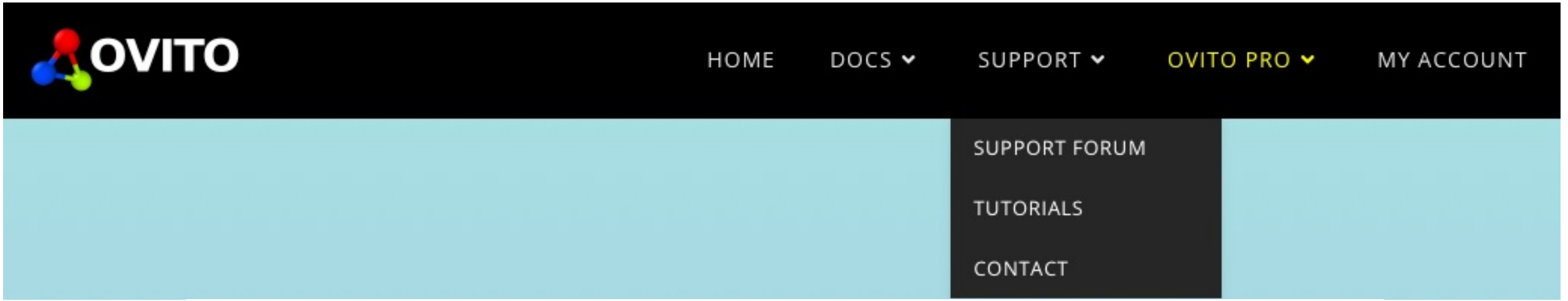
Analyzing Large Simulations

- 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



Support Forum

https://www.ovito.org/forum/



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

Potpourri

mitwood@sandia.gov