



Exceptional service in the national interest

OVITO Visualization for LAMMPS Users

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LAMMPS Workshop, Albuquerque, 2025



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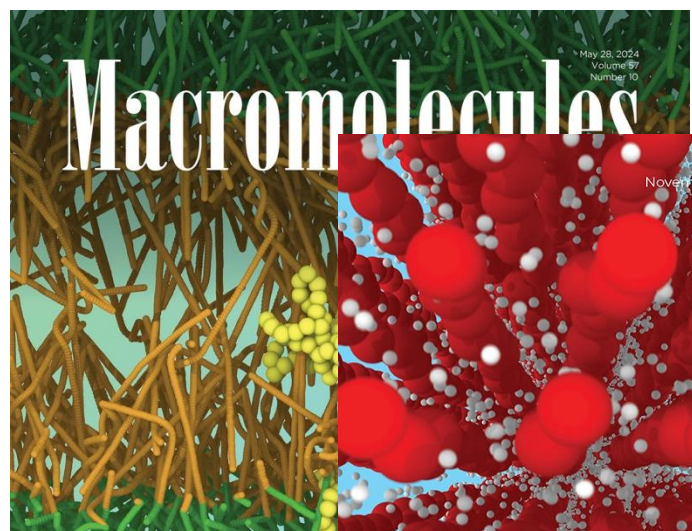
Follow along by downloading at ovito.org !

SAND2025-09998C



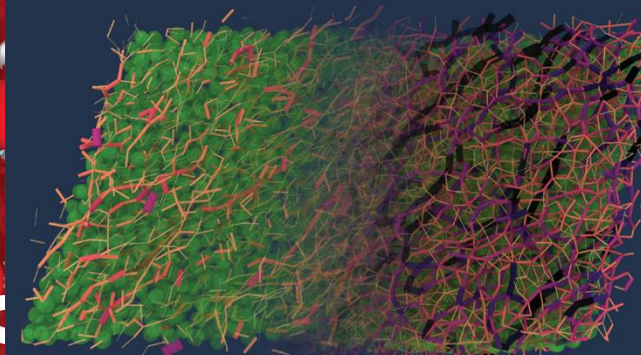
Why Bother with Visualization?

- 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 any of these journal covers in just words...
- Art?

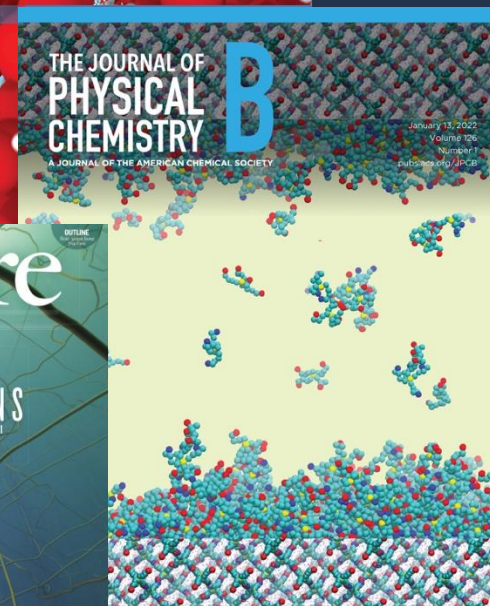
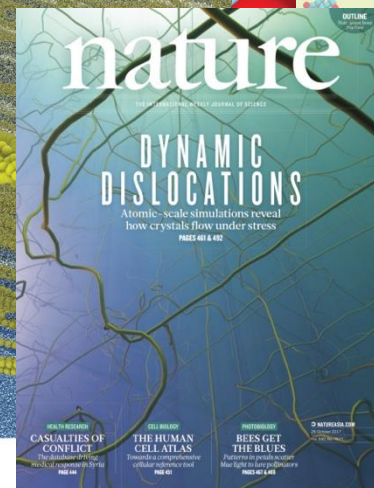
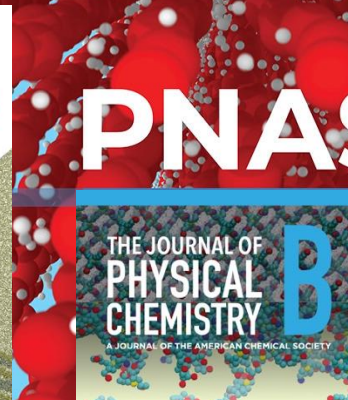


Soft Matter

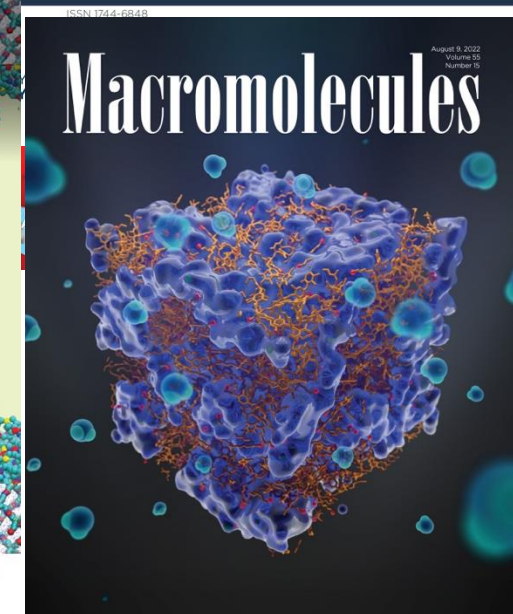
rsc.li/soft-matter-journal



ACS Publications
Most Trusted. Most Cited. Most Read.



Publications
Most Trusted. Most Cited. Most Read.



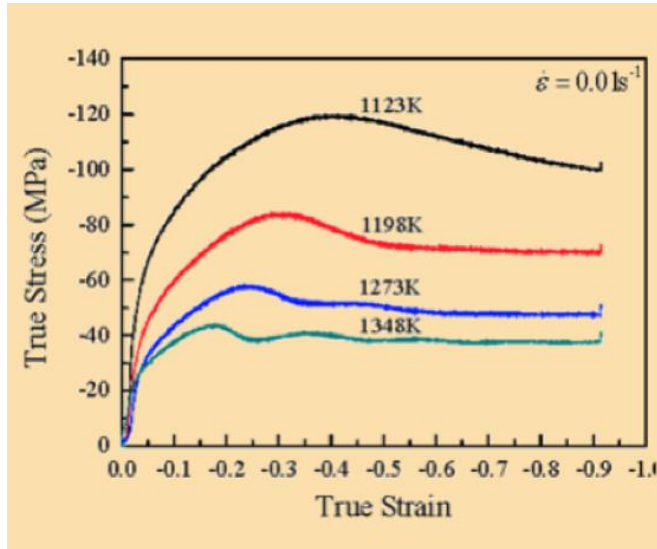
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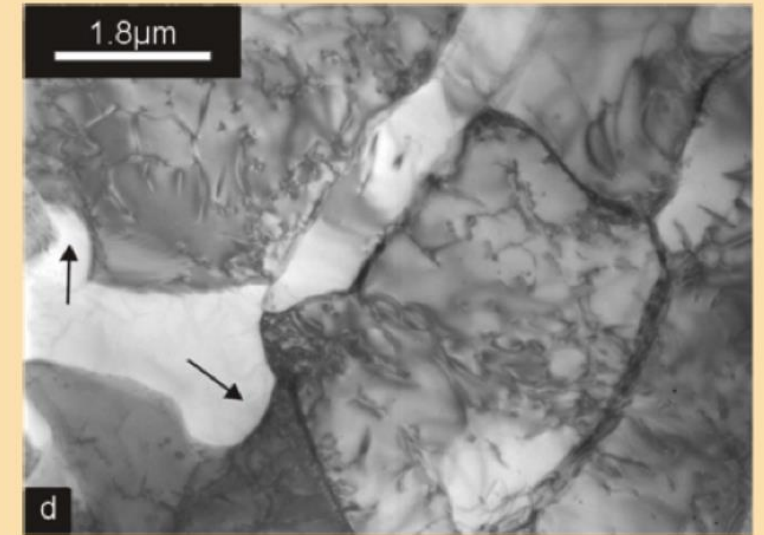


Value by Analogy

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



Microscopy & Imaging

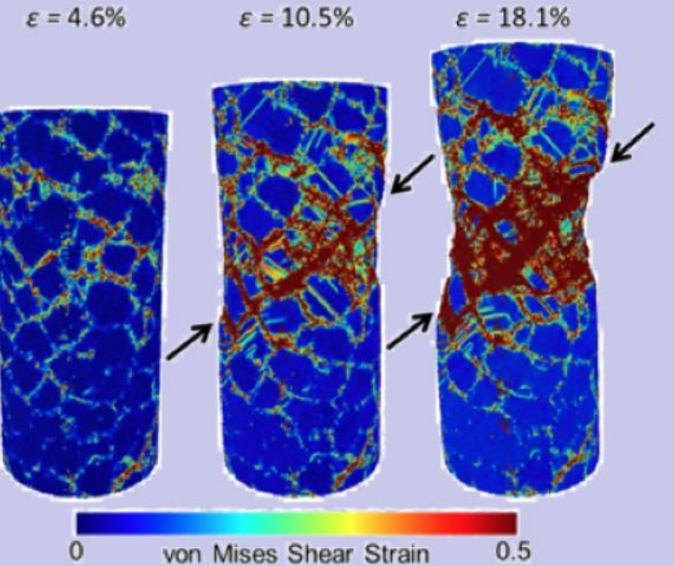


Raw output data



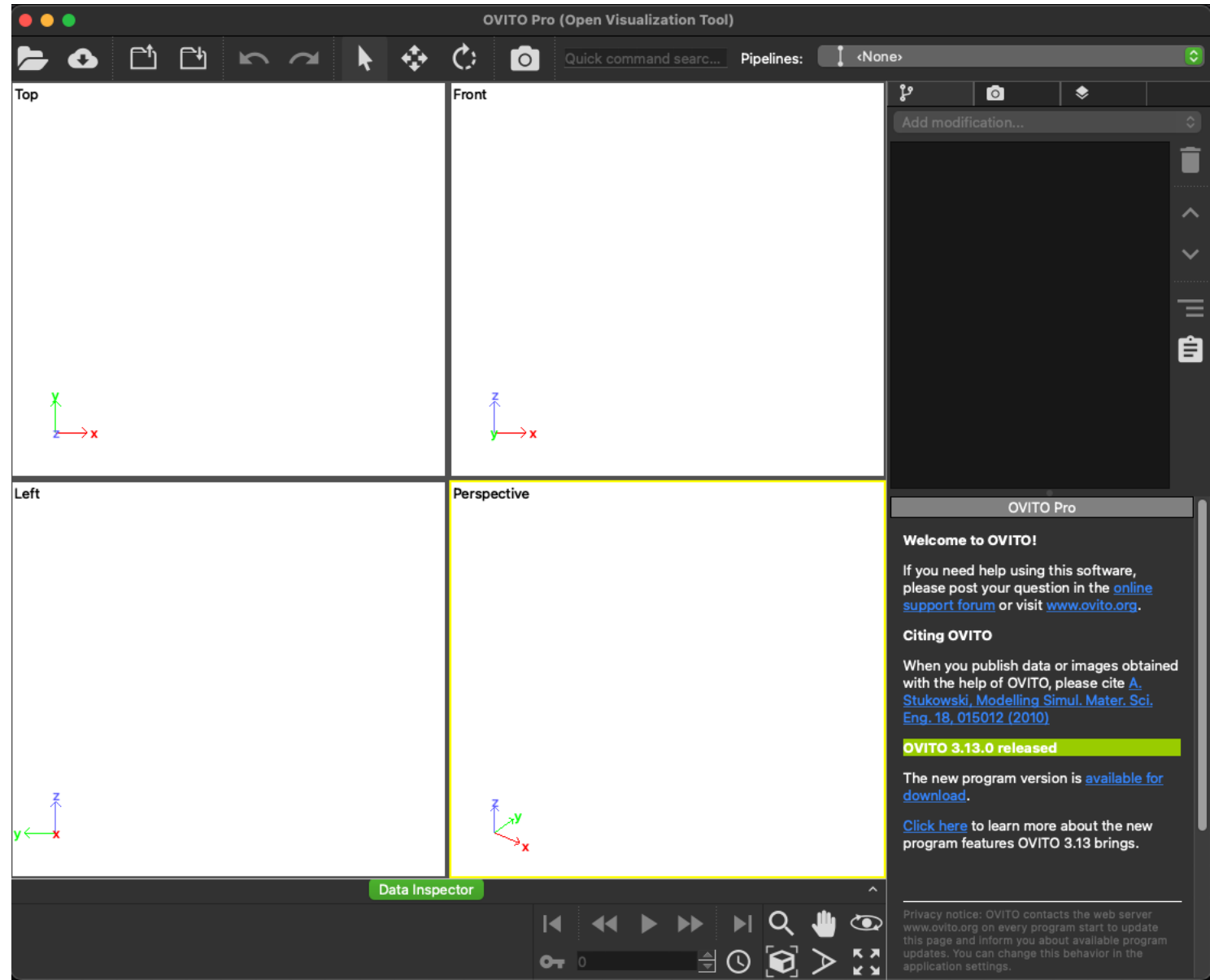
Data analysis & Visualization

"in-silico microscopy"



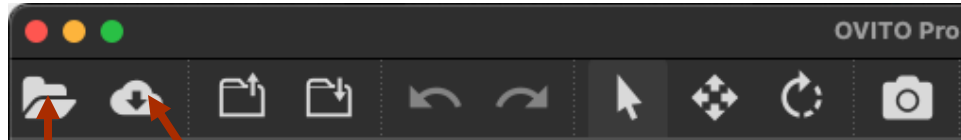


GUI Walkthrough



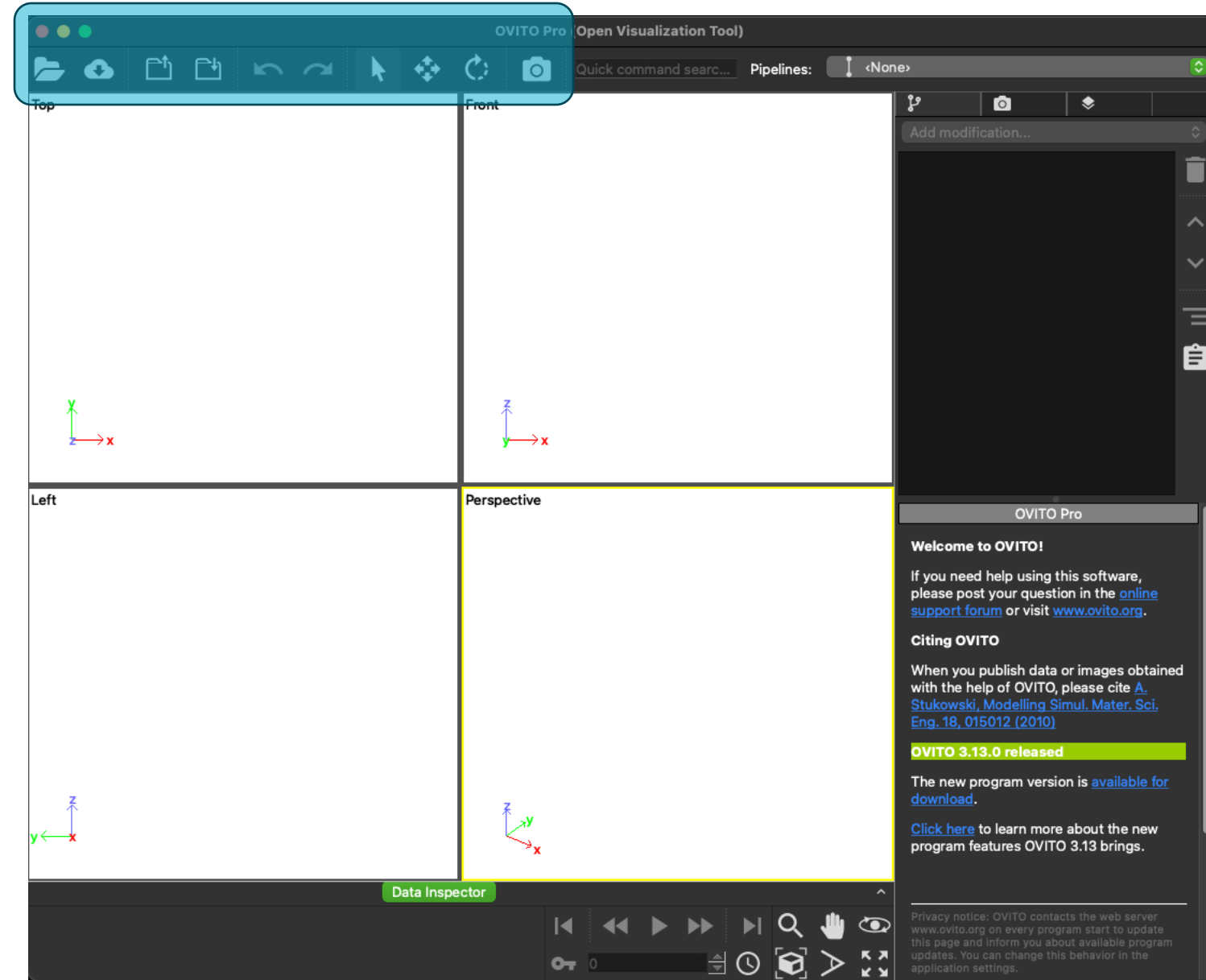


GUI Walkthrough



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

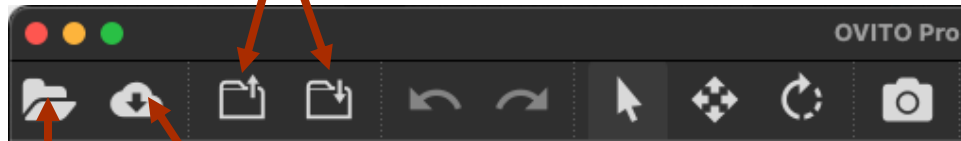
Load a local file on
your machine





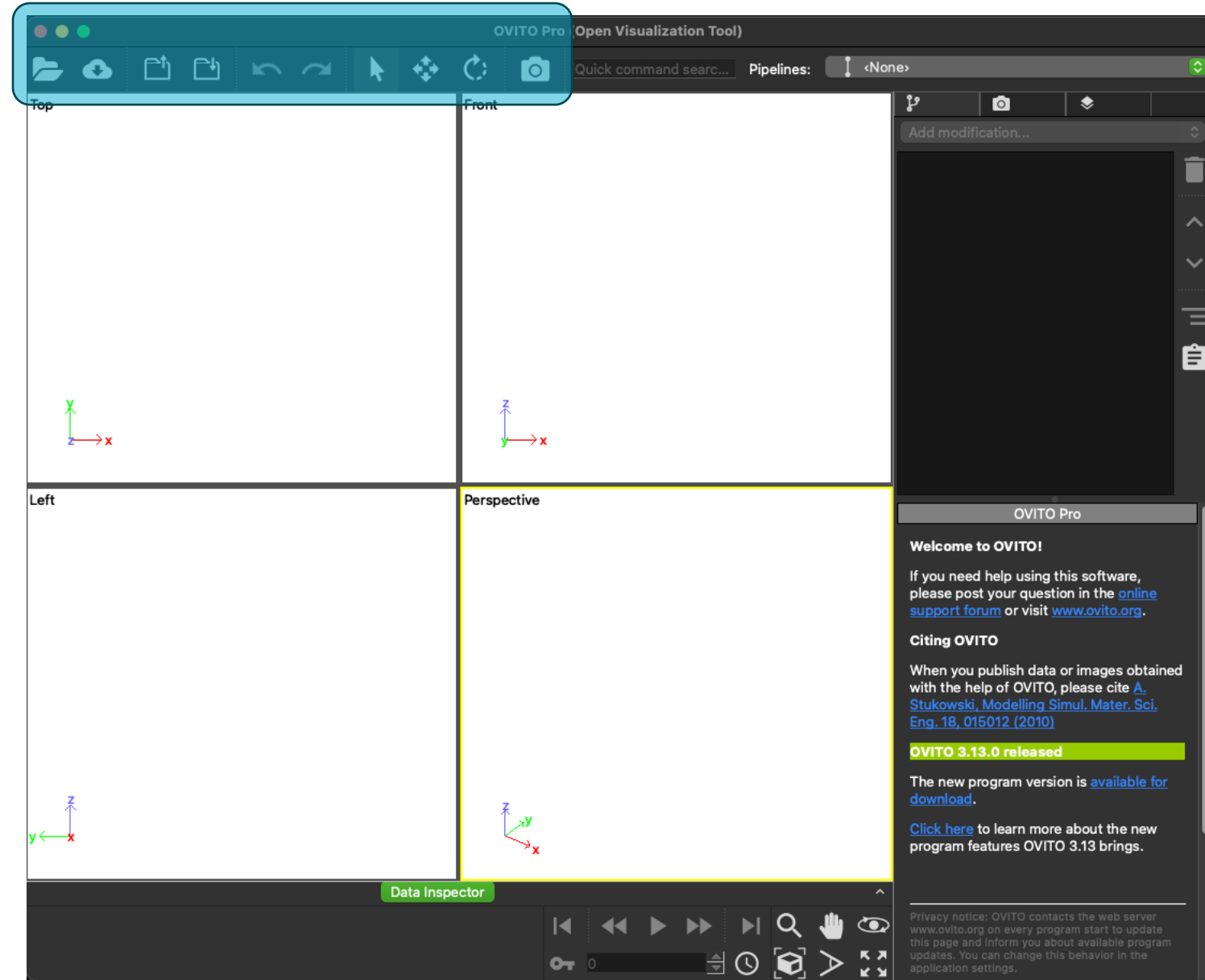
GUI Walkthrough

Save/Load an OVITO session



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

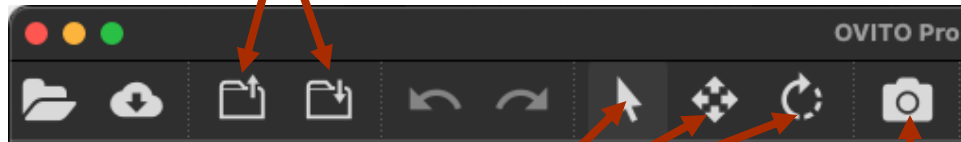
Load a local file on
your machine





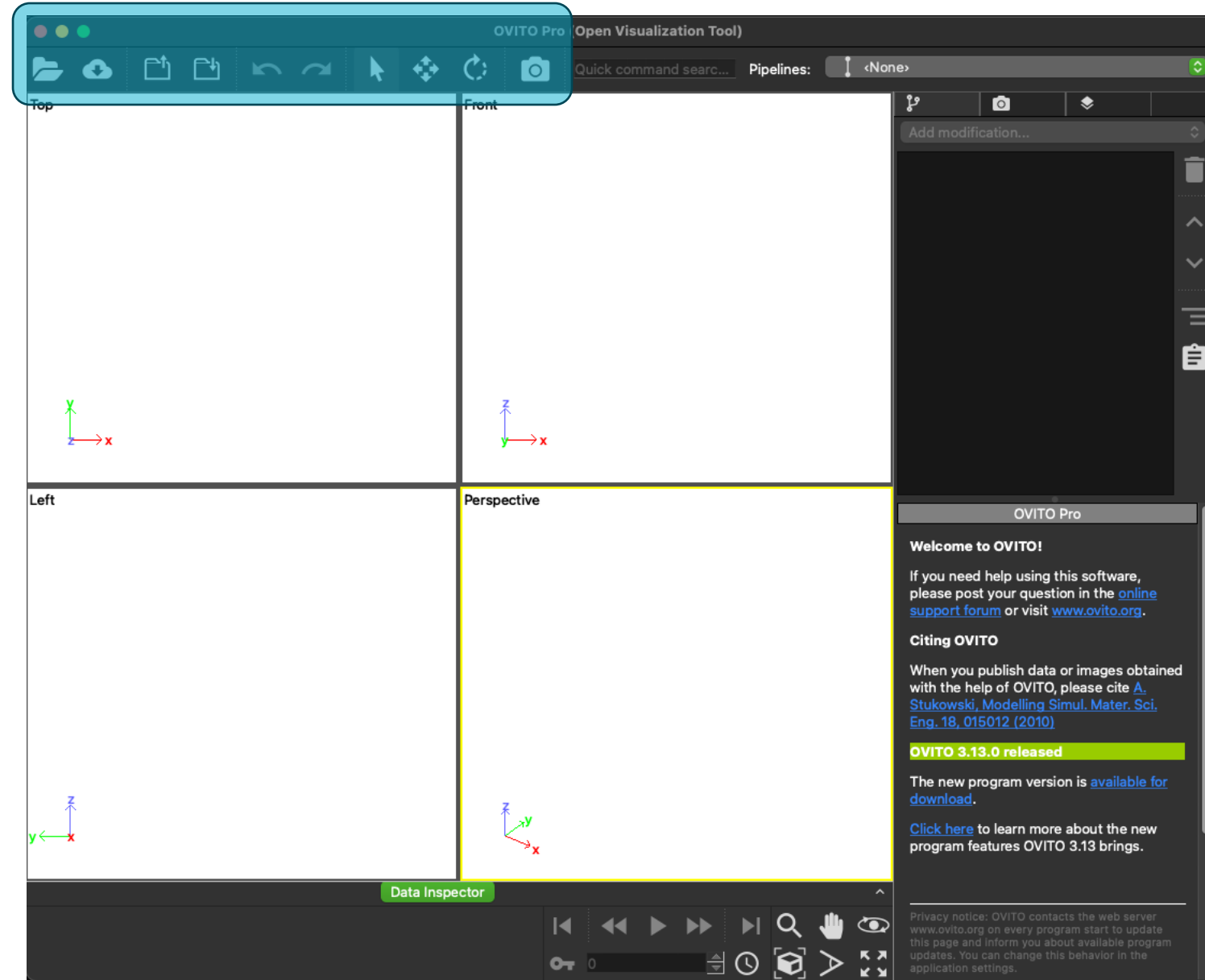
GUI Walkthrough

Save/Load an OVITO session



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

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



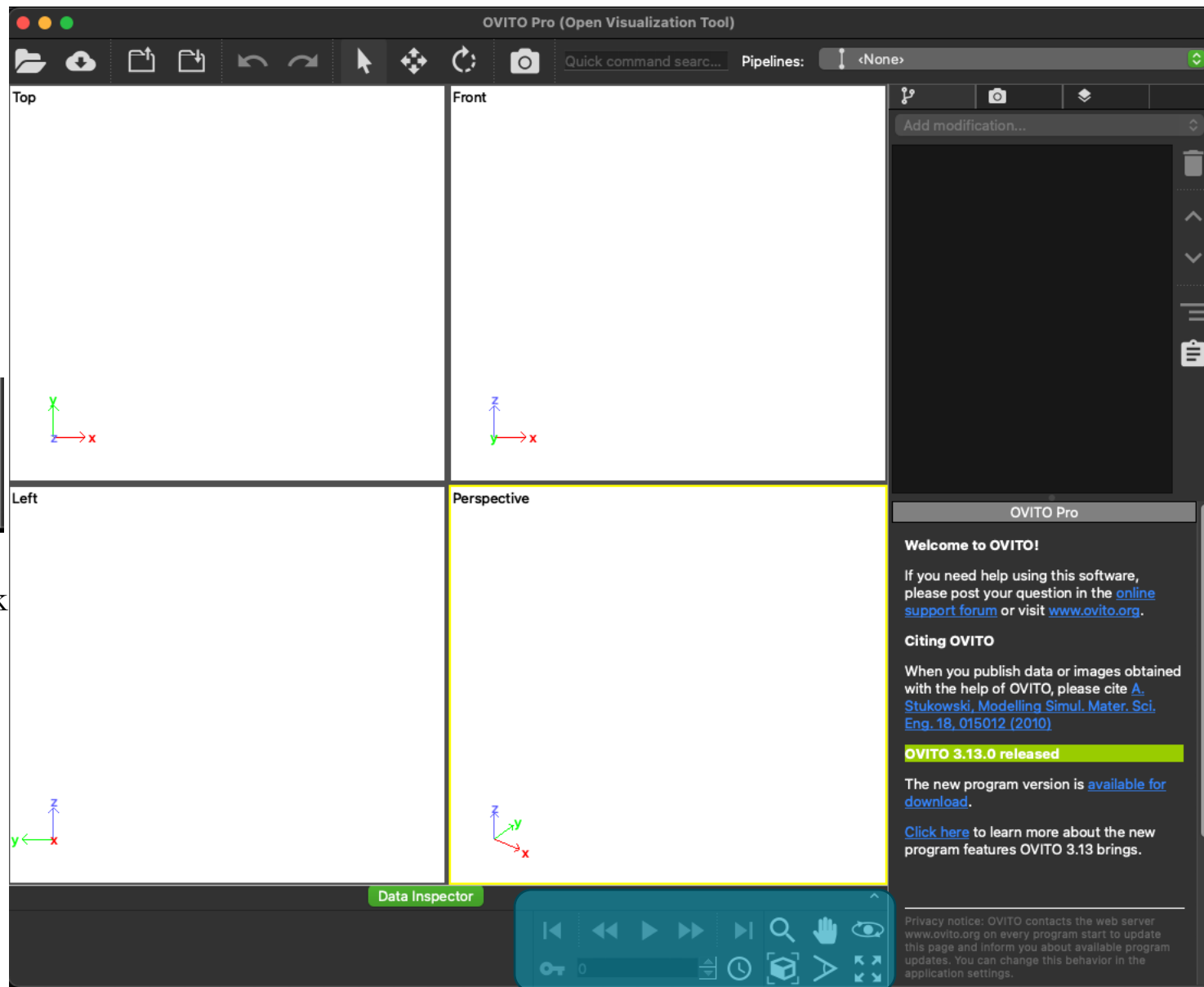


GUI Walkthrough

Focus on one viewing panel, click again to see all

Auto-Zoom to fit all atoms into the view

Adjust Zoom, left-click and drag up/down





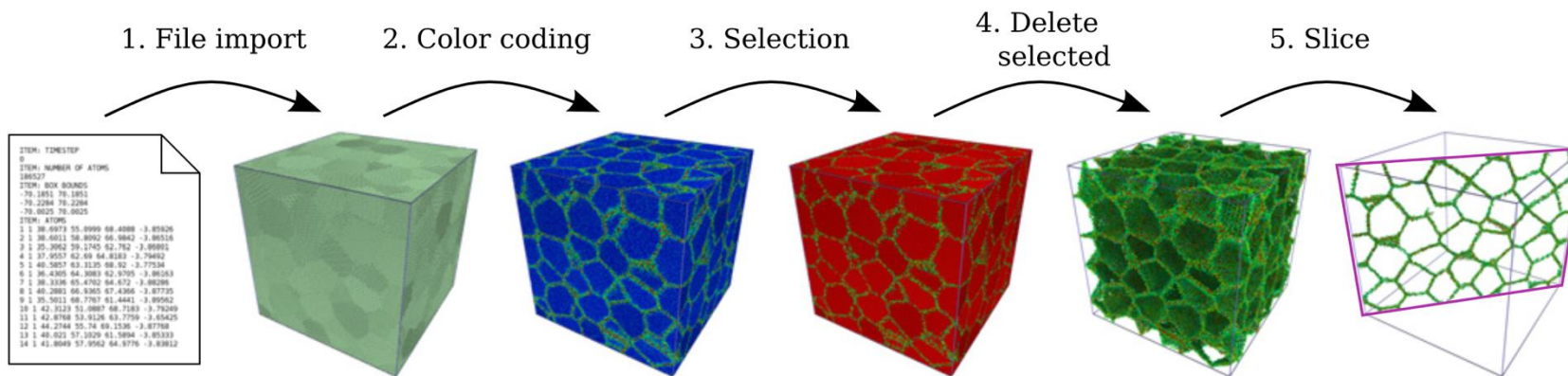
GUI Walkthrough

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

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GUI Walkthrough

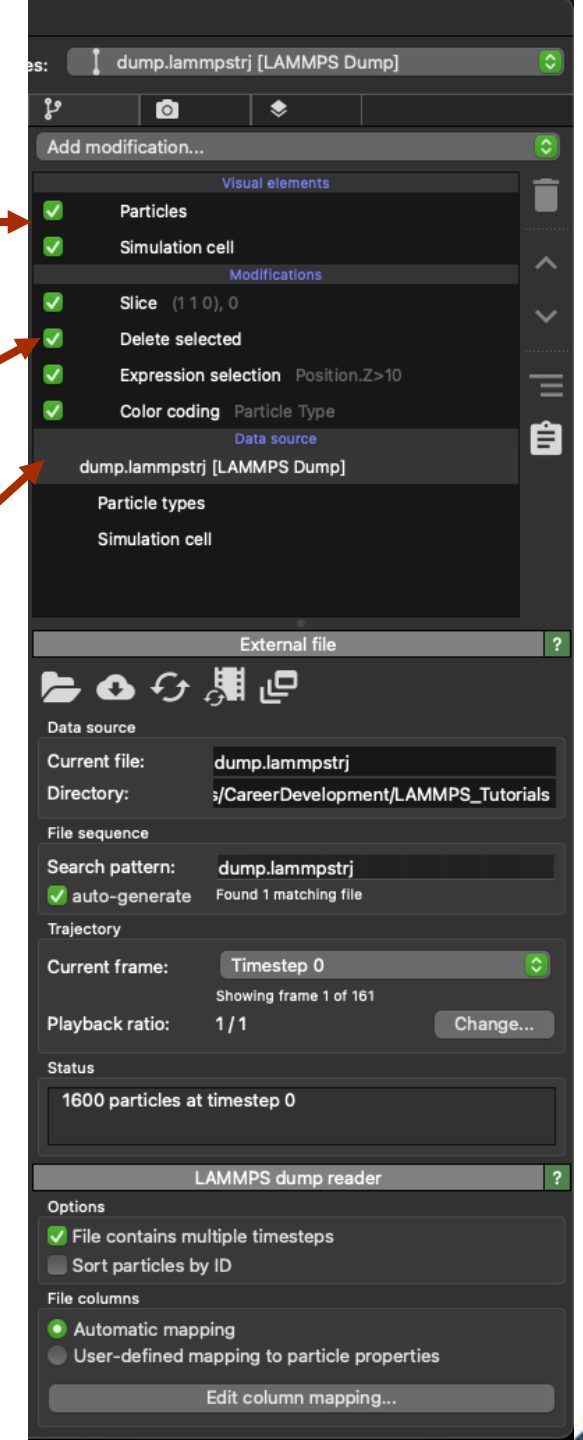
Building a Viz Workflow

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Visual Elements

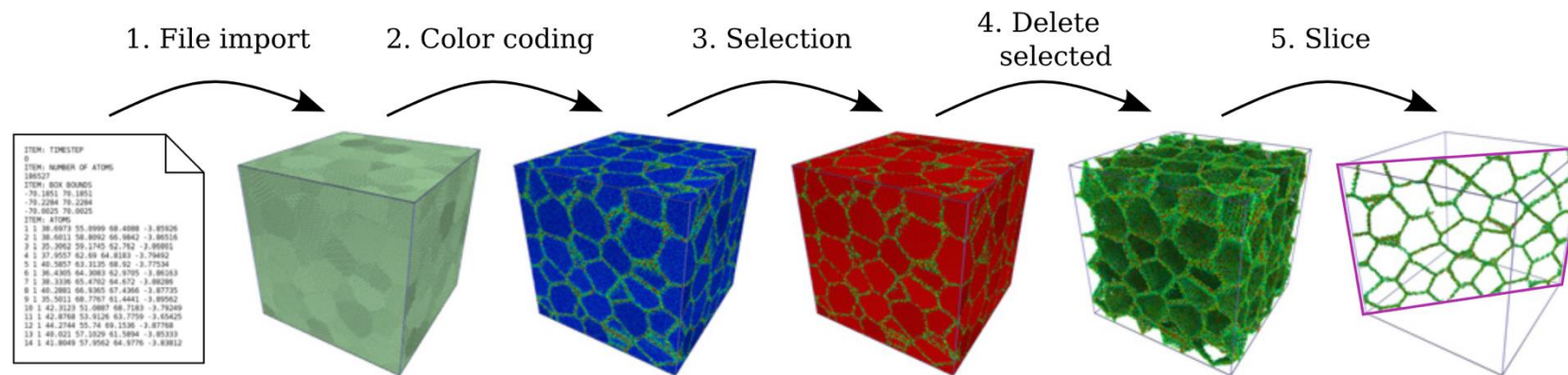
Active/Inactive modifications

File Imported



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GUI Walkthrough

From LAMMPS GUI :
LJ Fluid Example

See <https://lammptutorials.github.io/>

Make sure you have :
dump mydmp all atom 100 dump.lammpstrj

OVITO Pro (Open Visualization Tool)

Pipelines: dump.lammpstrj [LAMMPS Dump]

Quick command search (%P)

Top Front Left Perspective

Add modification...

Visual elements

- ✓ Particles
- ✓ Simulation cell

Modifications

- ✓ Coordination analysis
 - ☐ Slice (1 1 0), 0
 - ☐ Delete selected
 - ☐ Expression selection Position.Z>10
 - ☐ Color coding Particle Type

Data source

dump.lammpstrj [LAMMPS Dump]

Particle types

Simulation cell

External file ?

Data source

Current file: dump.lammpstrj

Directory: s/CareerDevelopment/LAMMPS_Tutorials

File sequence

Search pattern: dump.lammpstrj

✓ auto-generate Found 1 matching file

Trajectory

Current frame: Timestep 16000

Showing frame 161 of 161

Playback ratio: 1 / 1 Change...

Status

1600 particles at timestep 16000

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

0 20 40 60 80 100 120 140 160 / 160

160



GUI Walkthrough

Change left-click to inspect particles



Inspect properties of multiple particles (bond length, angles)



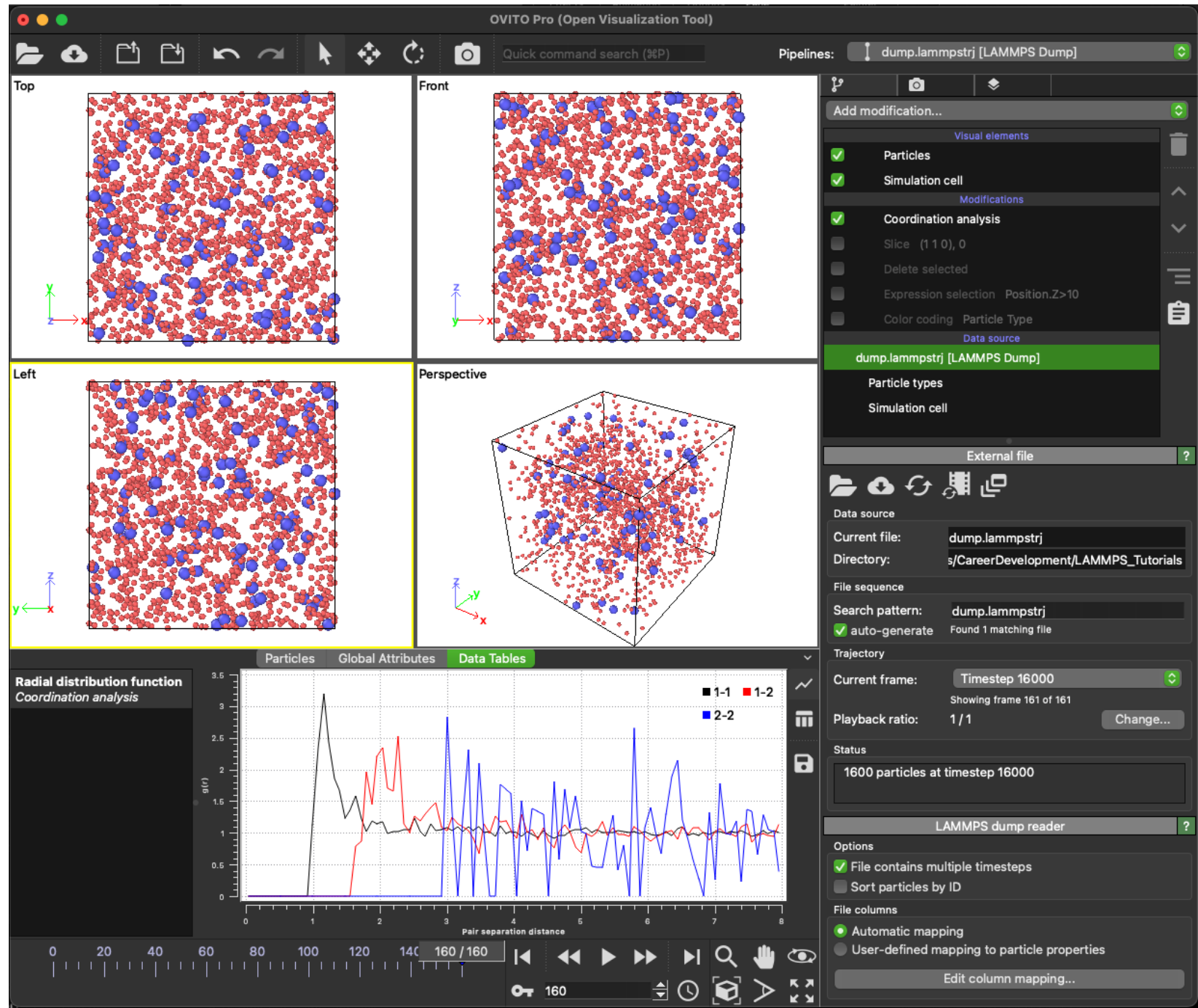
View plots generated by modifications



View data tables generated by modifications



Export data tables or plots generated by modifications



OVITO Pro (Open Visualization Tool)

Pipelines: dump.lammpstrj [LAMMPS Dump]

Top

Front

Left

Perspective

0 / 160 20 40 60 80 100 120 140 160

Particles Global Attributes

Quick command search (%P)

Add modification...

Simulation cell

Modifications

Clear selection

Compute property Transparency

Expression selection ParticleType==1

Clear selection

Compute property Particle Type

Expression selection Selection==1 && Partic...

Expand selection

Expression selection ParticleType==2

Data source

dump.lammpstrj [LAMMPS Dump]

Particle types

Expression selection ?

Operate on:

Particles

Boolean expression:

ParticleType==2

Variables ?

Available input variables:

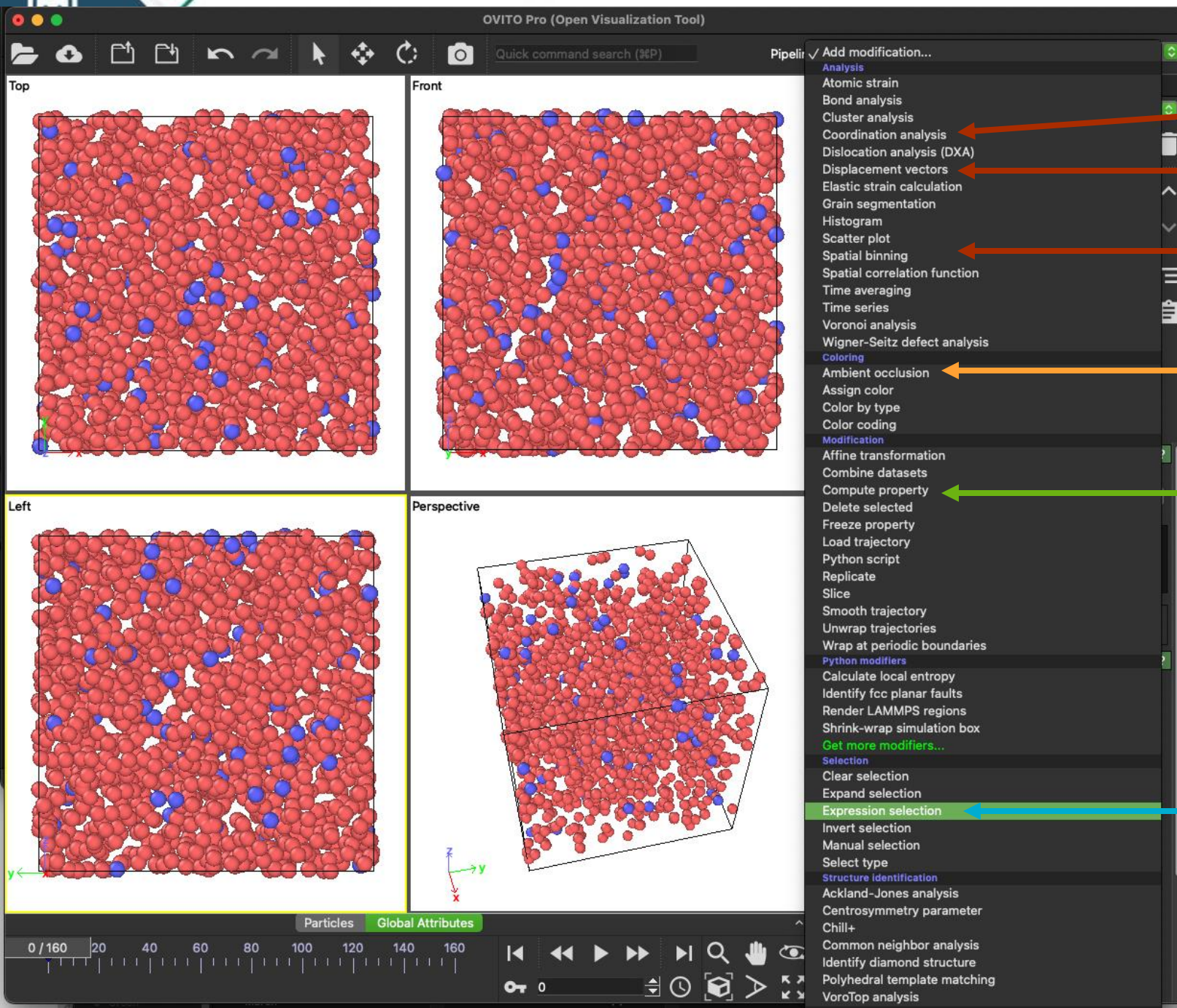
Properties:

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

Global values:

- N (total number of particles)
- Frame (animation frame number)
- SourceFile
- SourceFrame
- Timestep

Modifications to your scene are accessible here



Pair Distribution Function

Calculate how far things have moved

Locally Averaged Properties

Add Shadows

Manipulate per-atom data

The most powerful modification



LJ Fluid Example

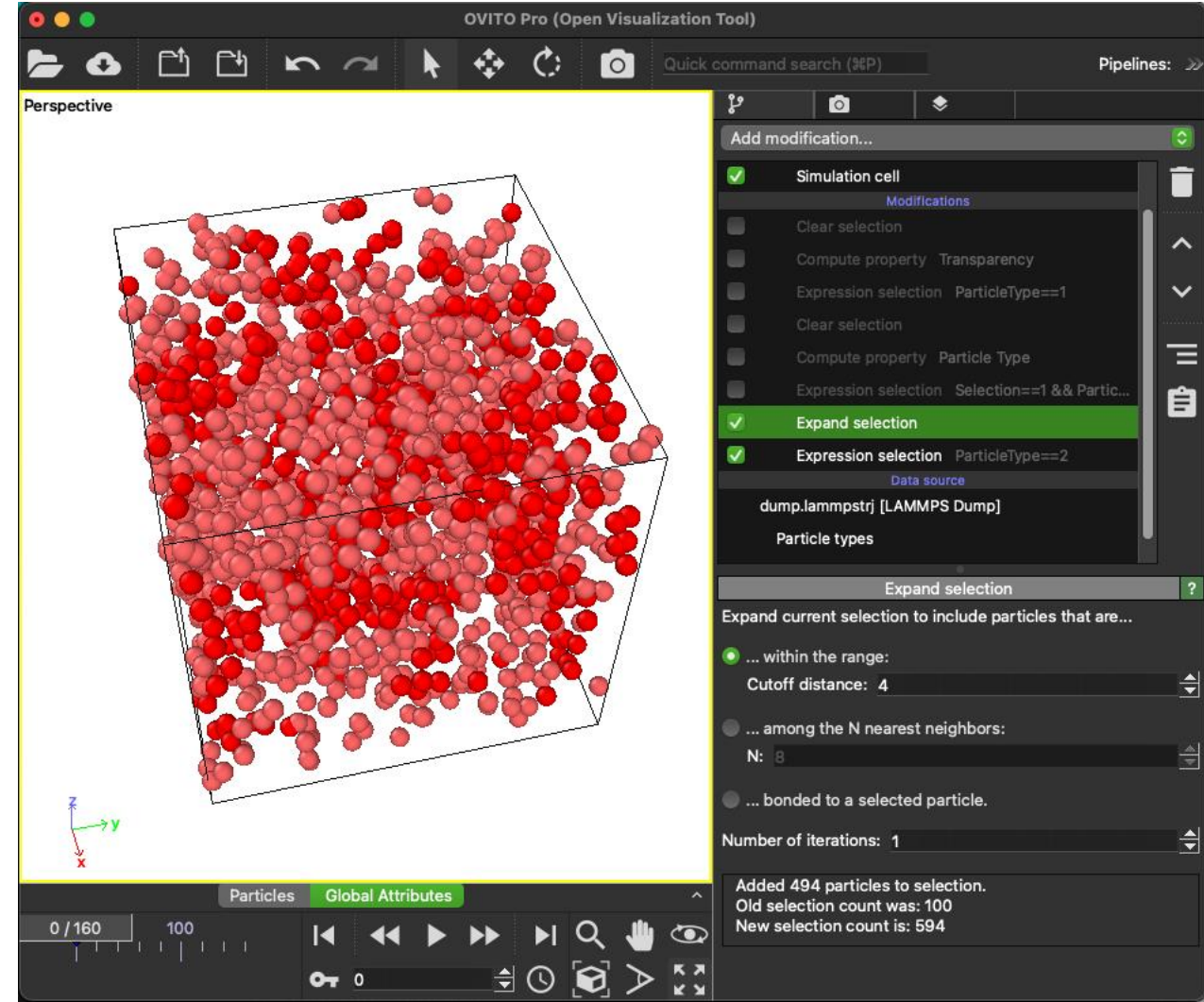
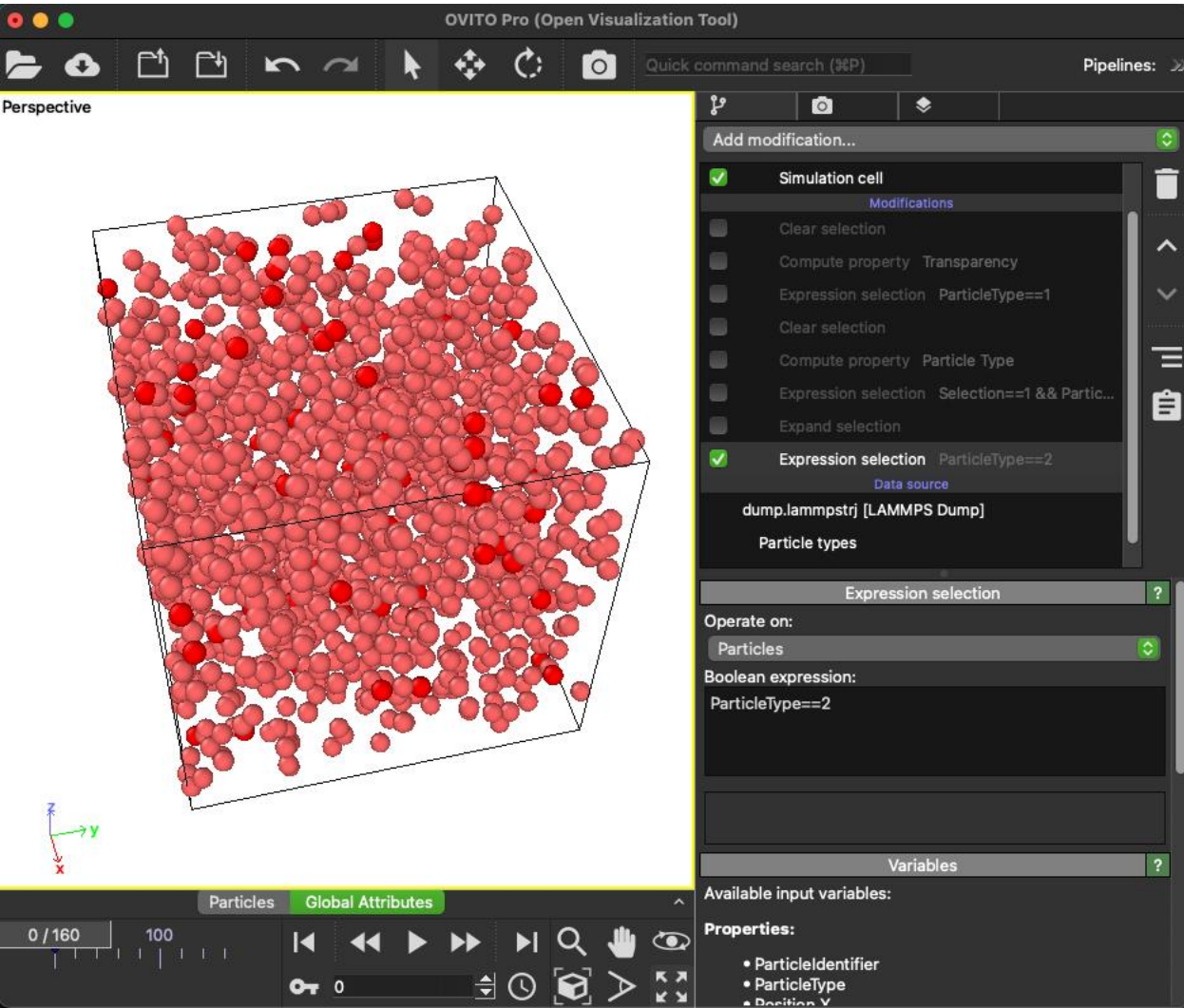
Expression Selection

"ParticleType==2"

Expand Selection

...within the range

Cutoff Distance 4

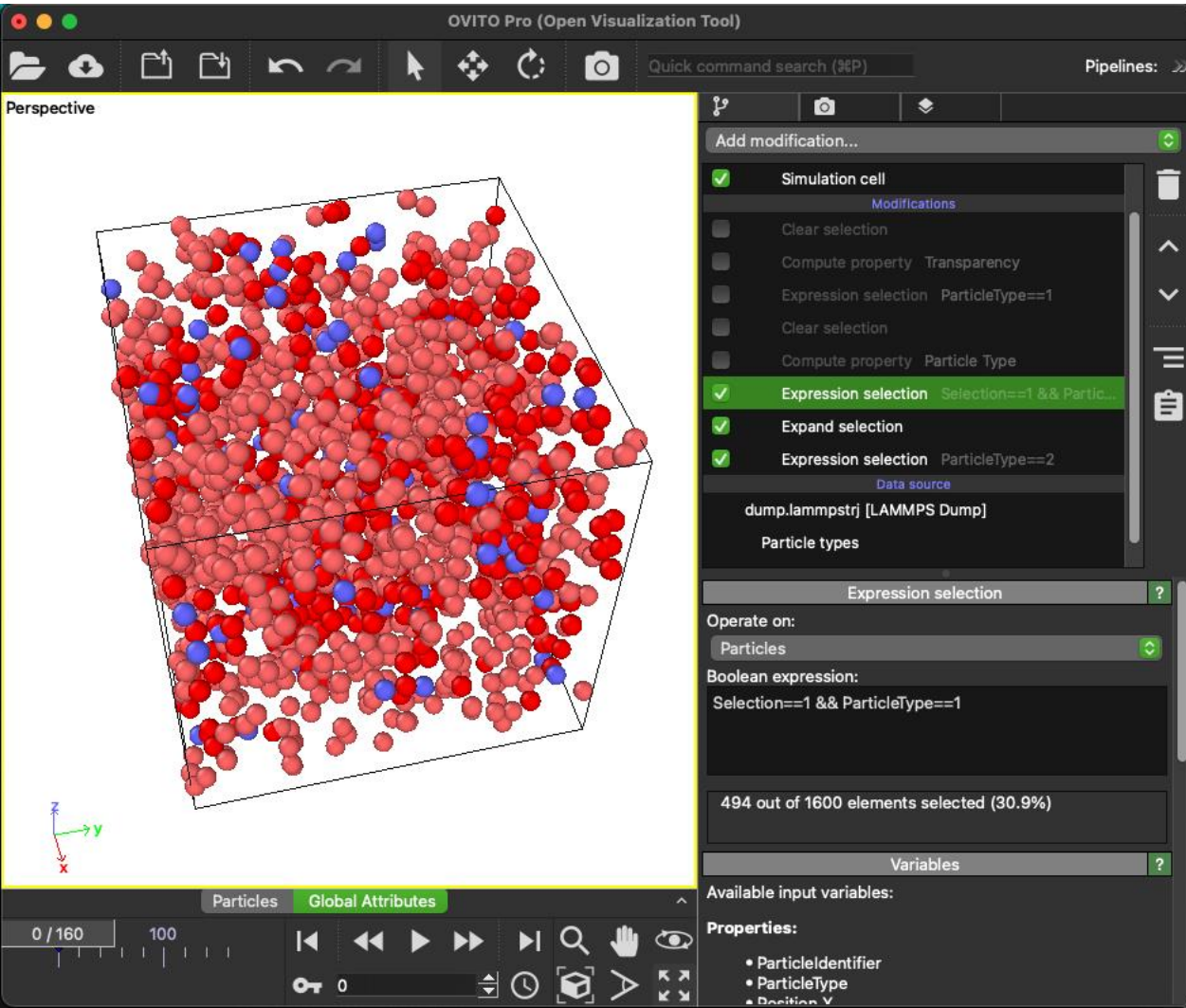




LJ Fluid Example

Expression Selection

"Selection==1 && ParticleType==1"

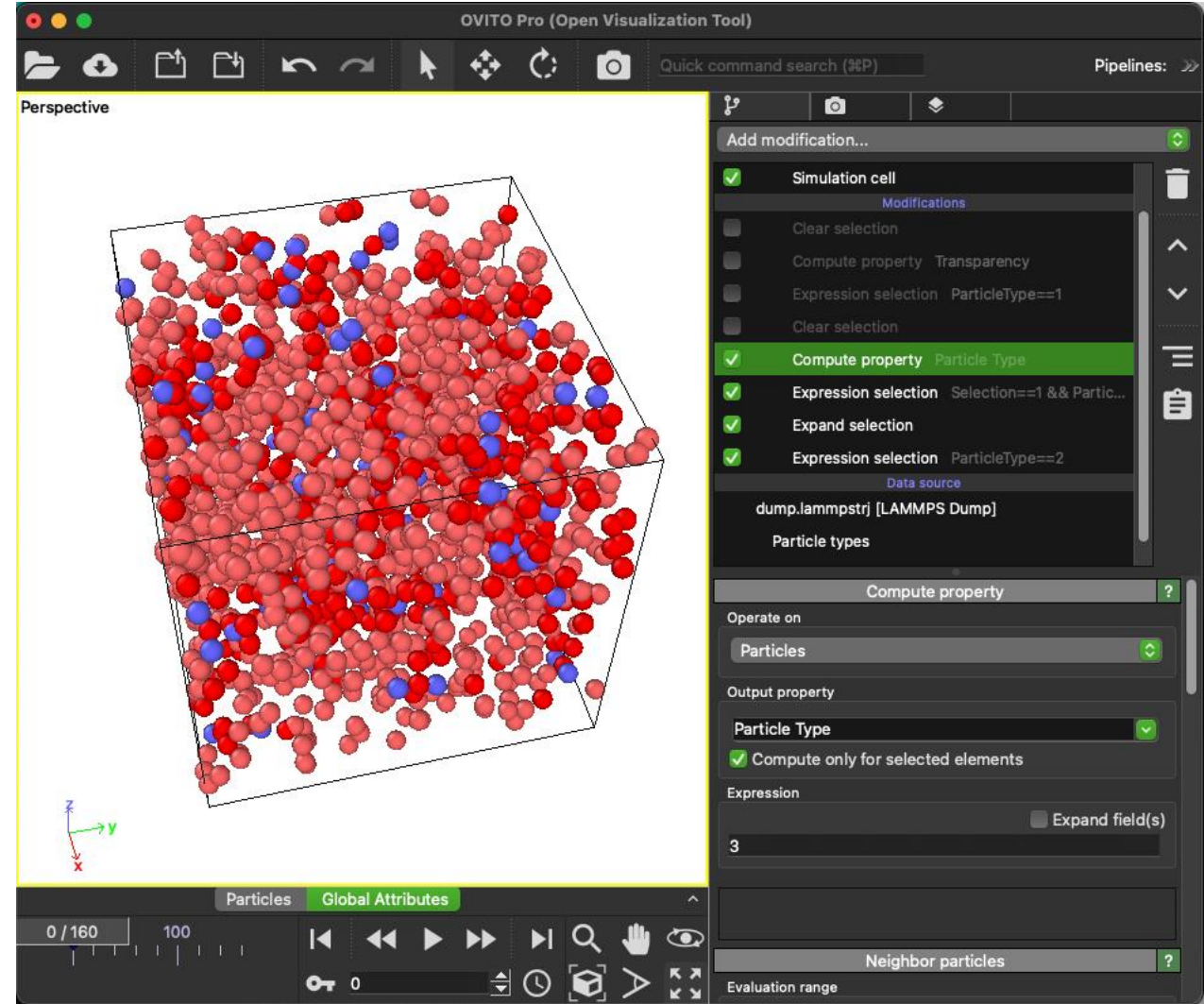


Compute Property

Output Property : ParticleType

✓ Compute only for selected elements

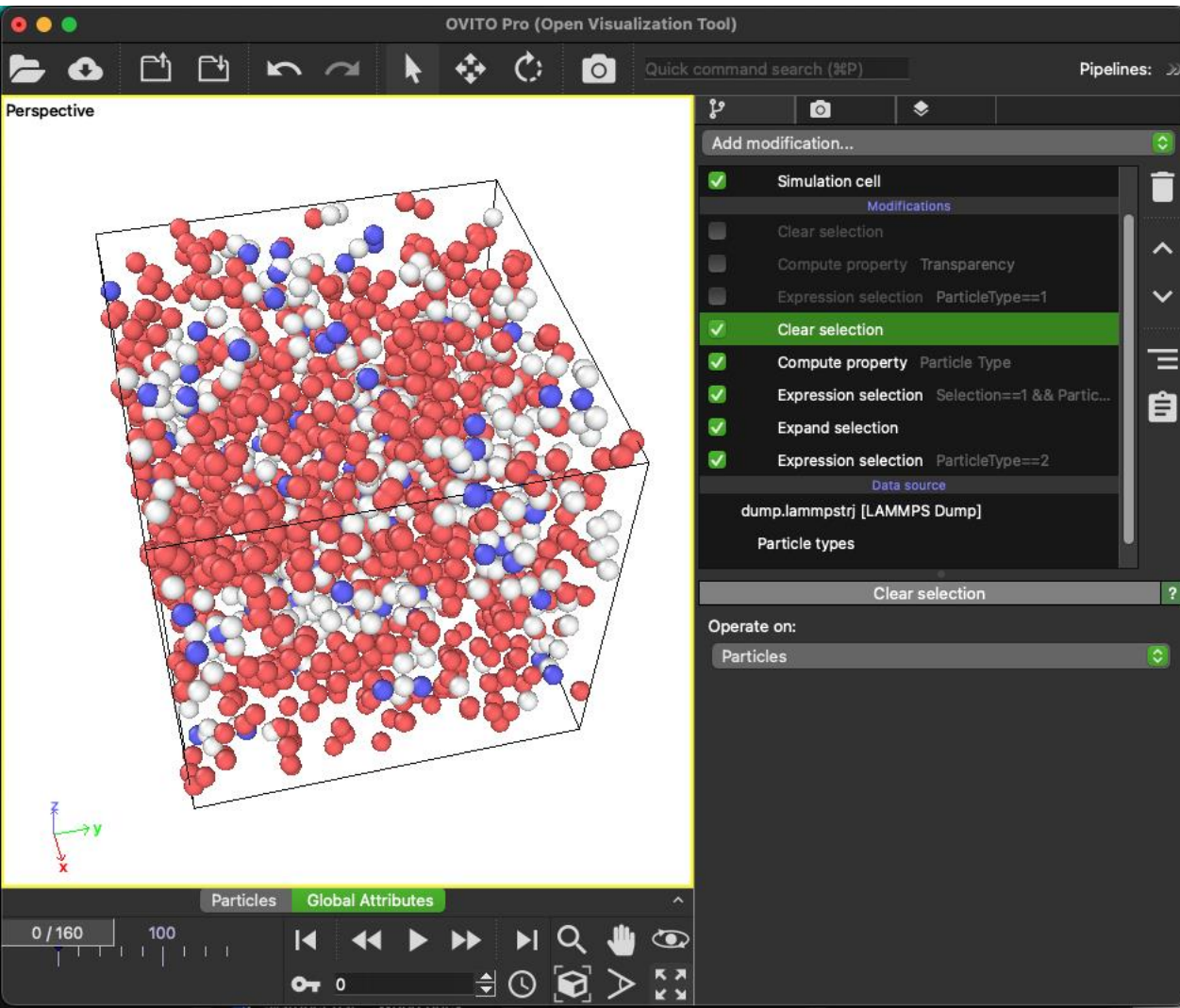
Expression : 3



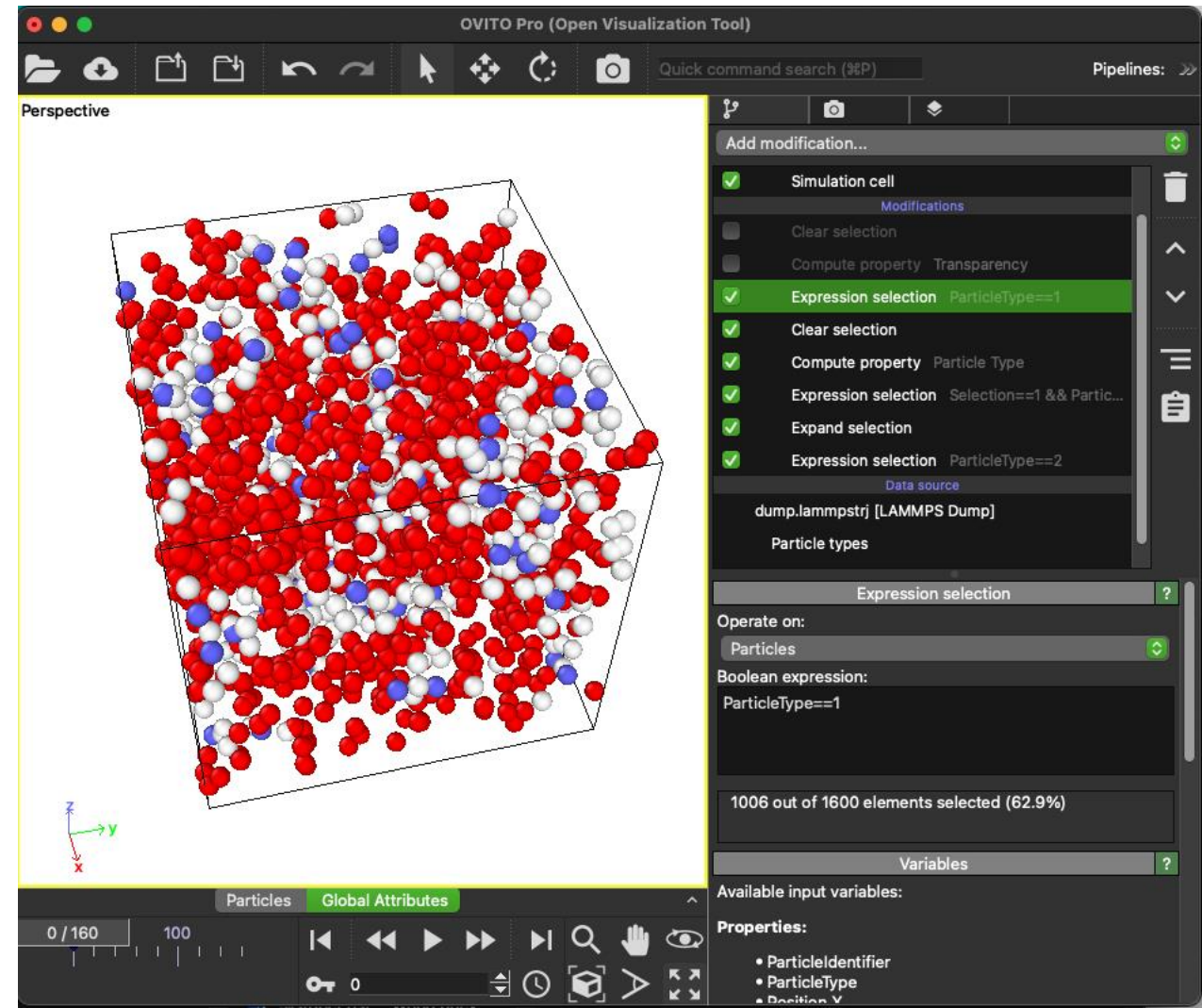


LJ Fluid Example

Clear Selection



Expression Selection
"ParticleType==1"

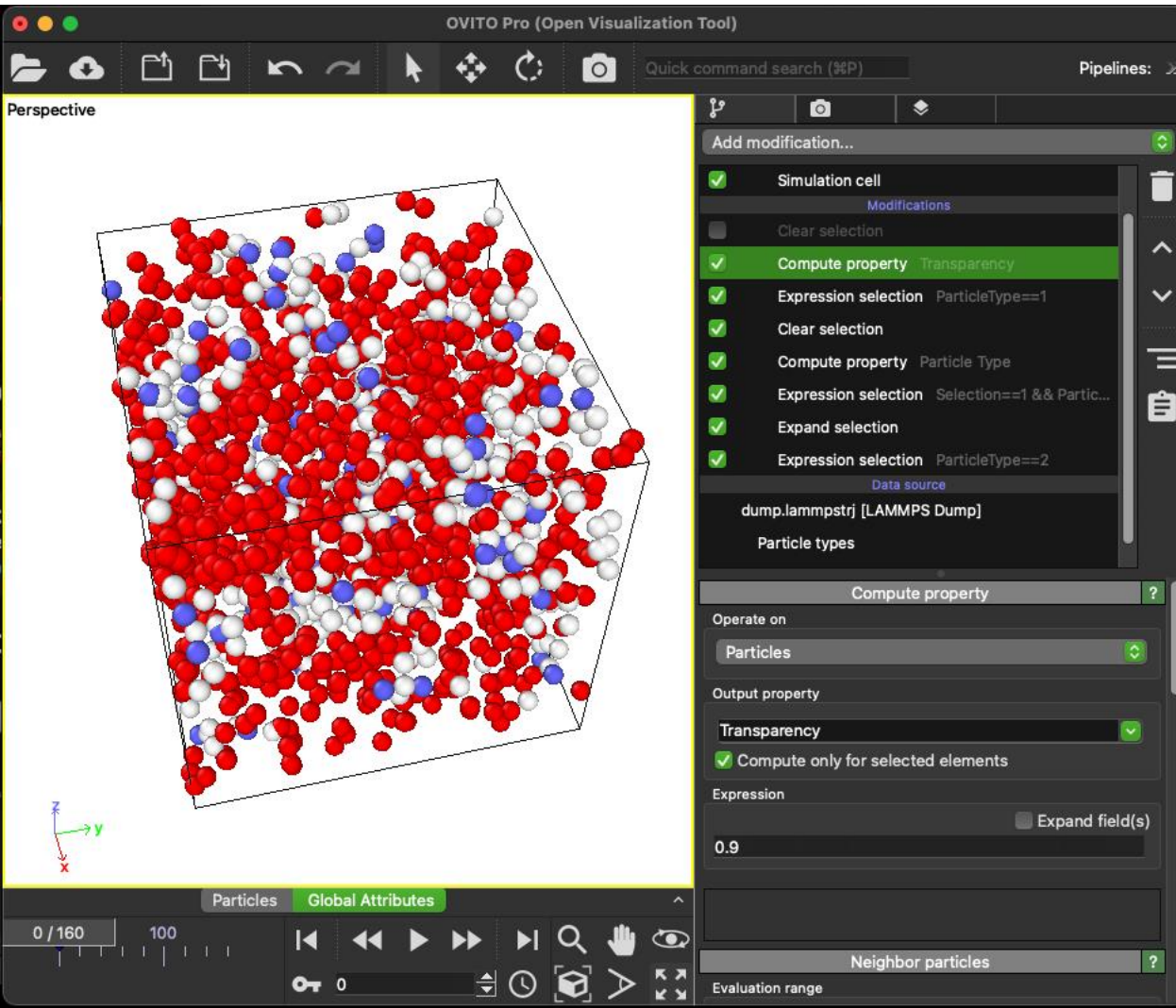


Compute Property

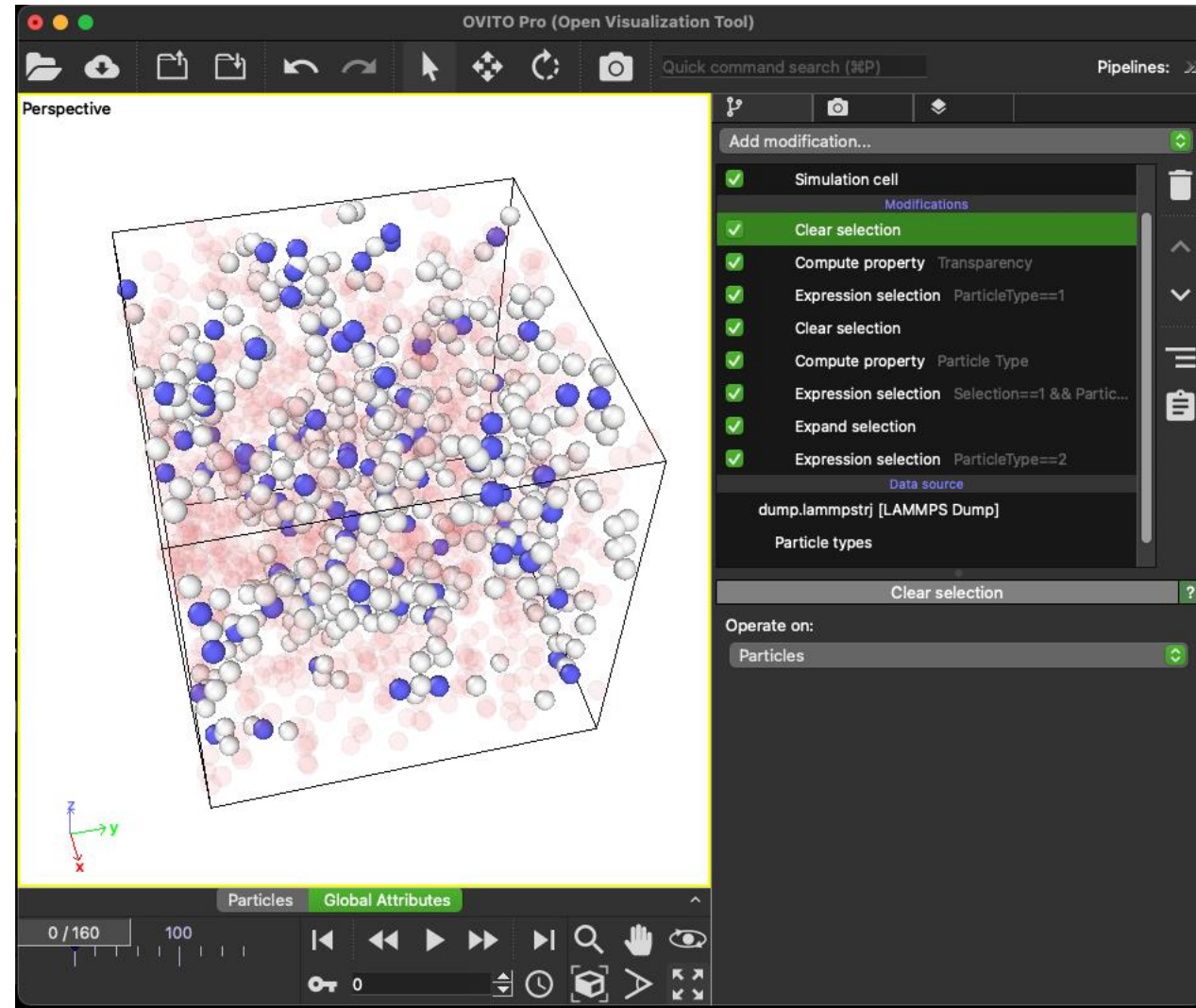
Output Property : Transparency

✓ Compute only for selected elements

Expression : 0.9



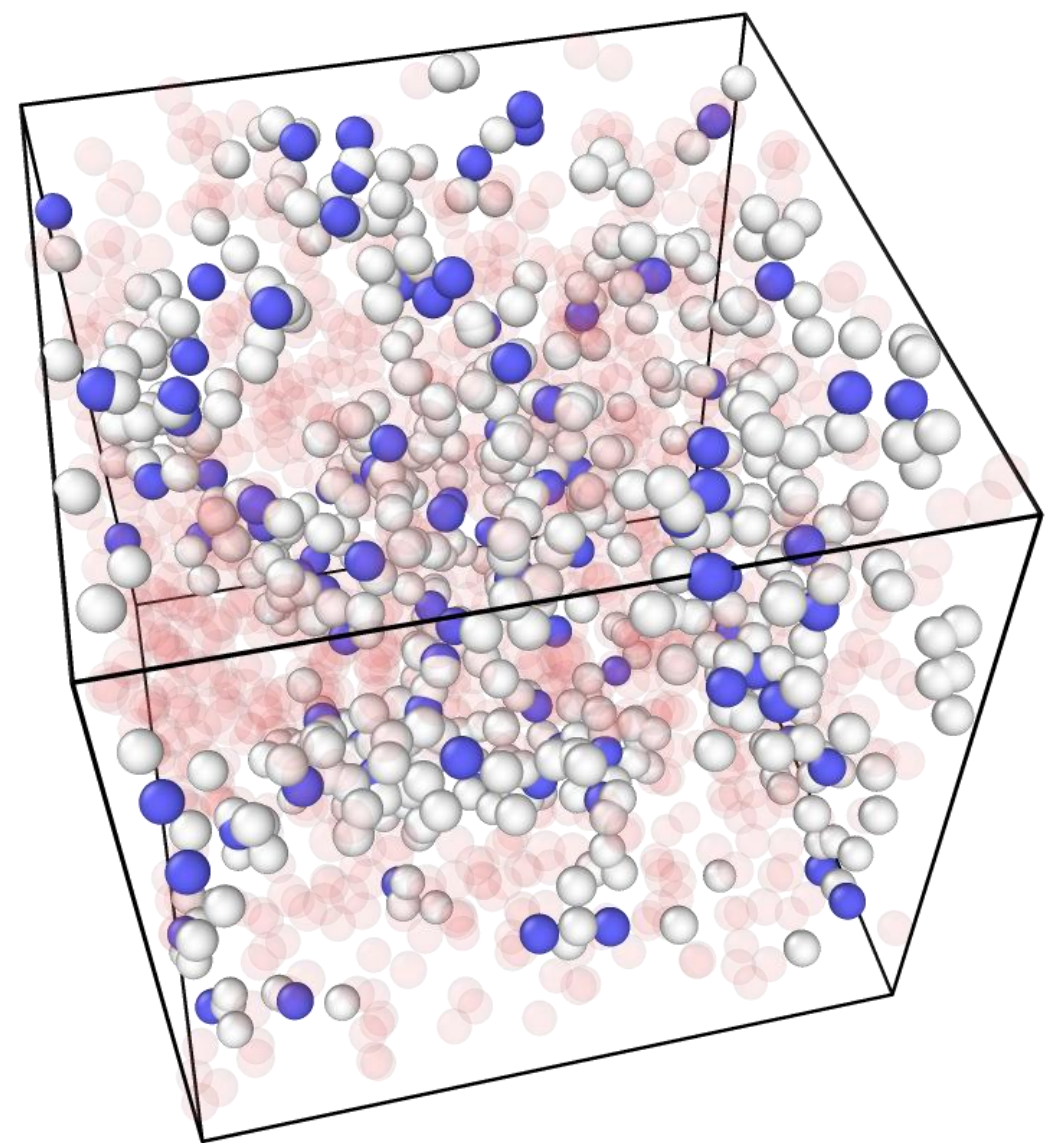
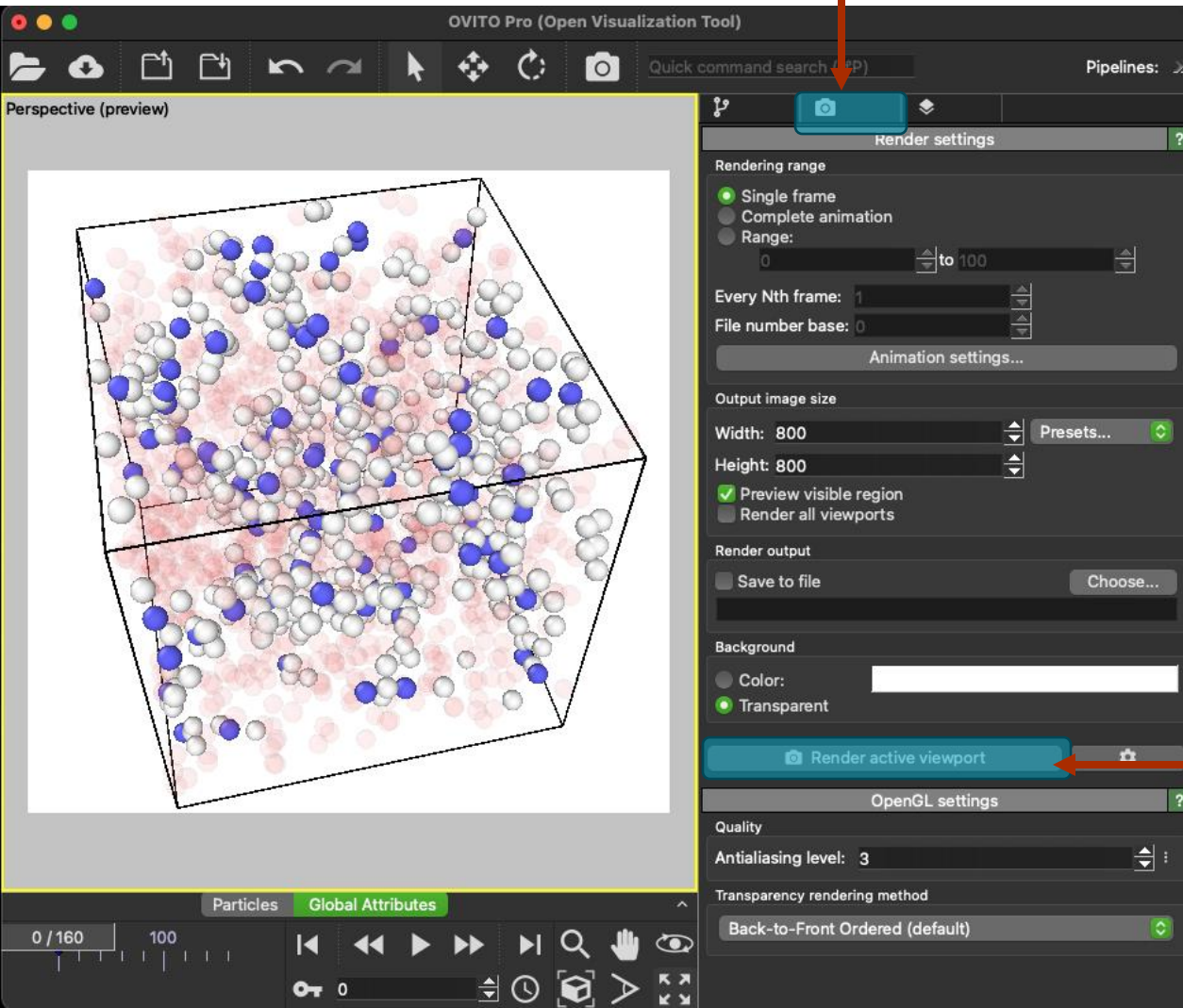
Clear Selection





LJ Fluid Example

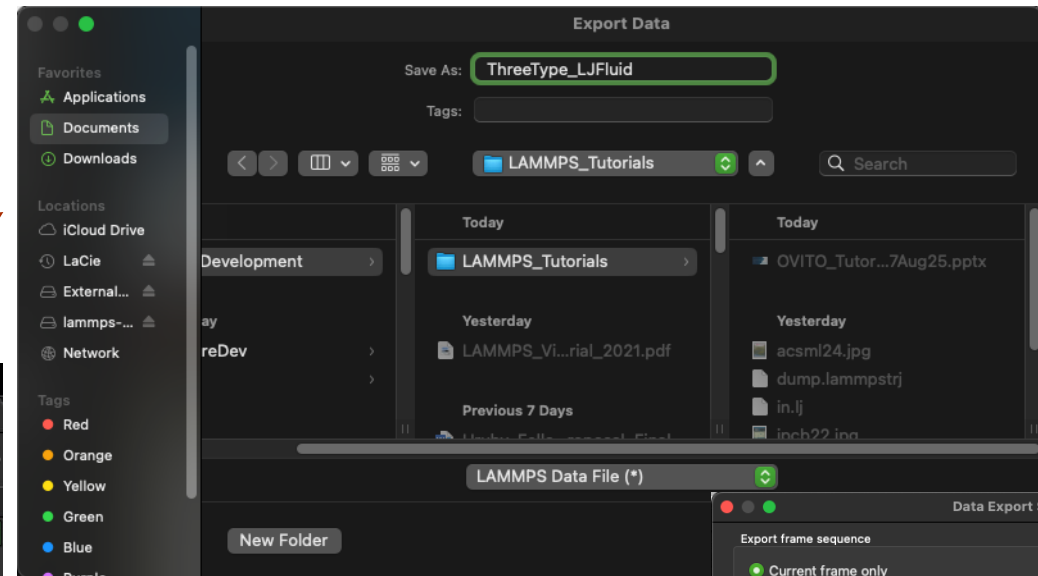
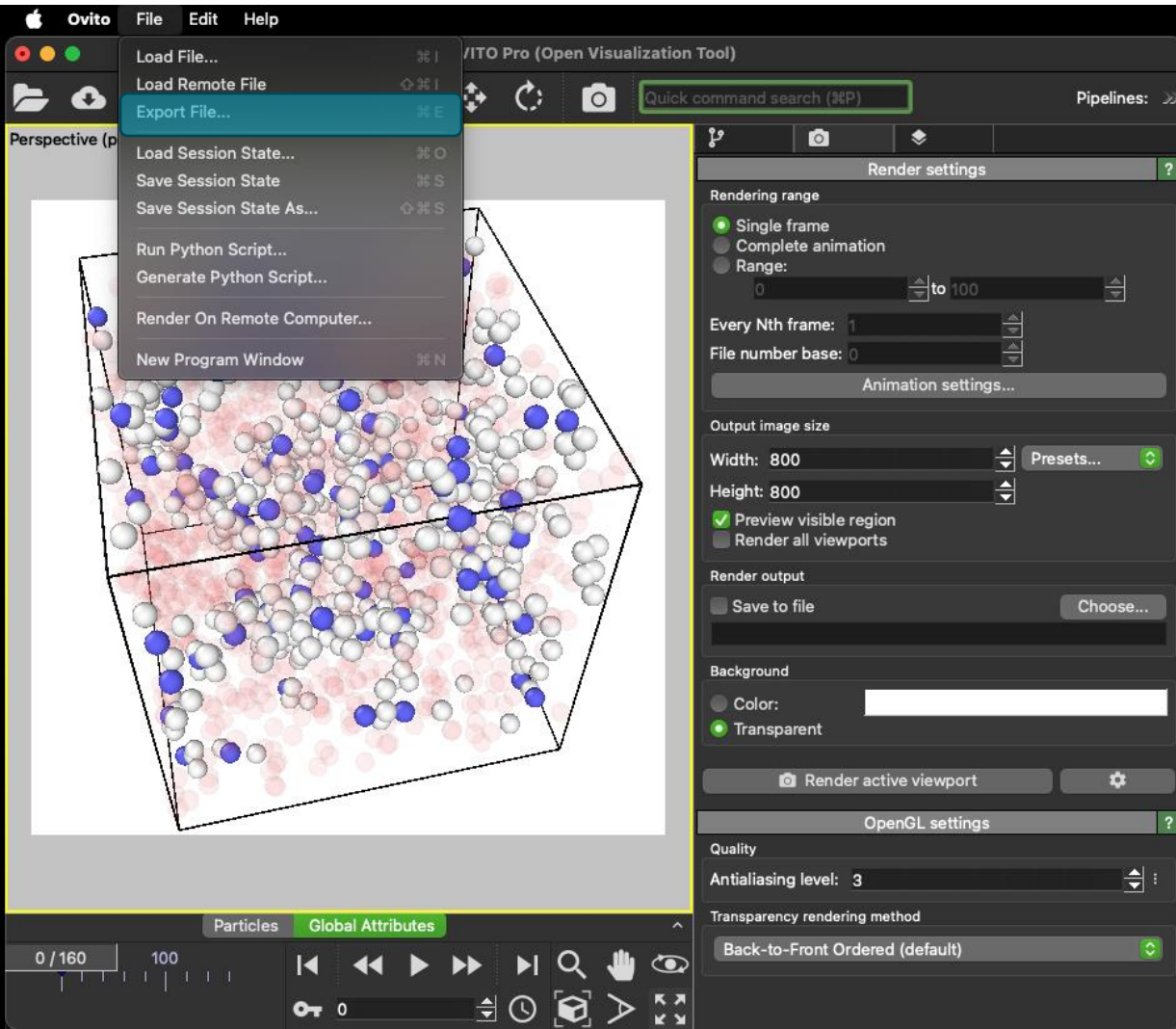
Move over to the Rendering tab



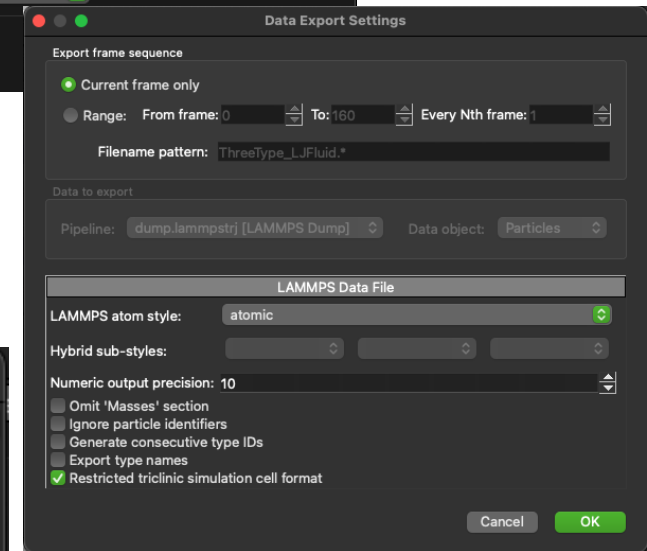
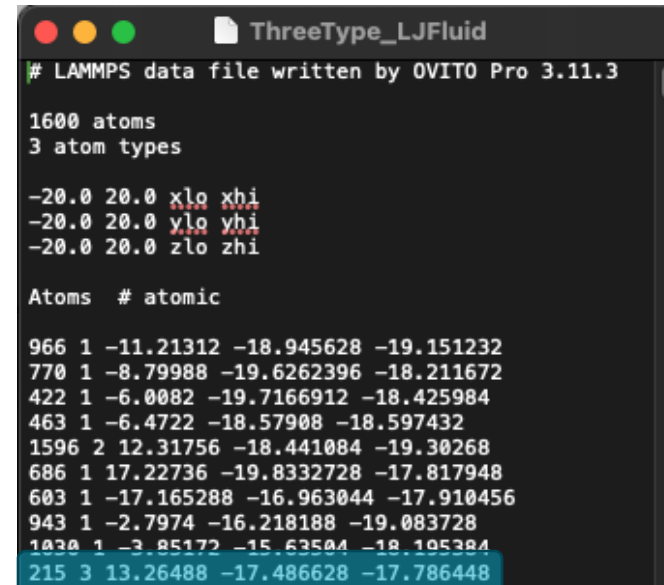
Change any setting here you like, including the angle and zoom in the left panel, then render!



Exporting Structures



Any modifications made
will be reflected in the
new data file

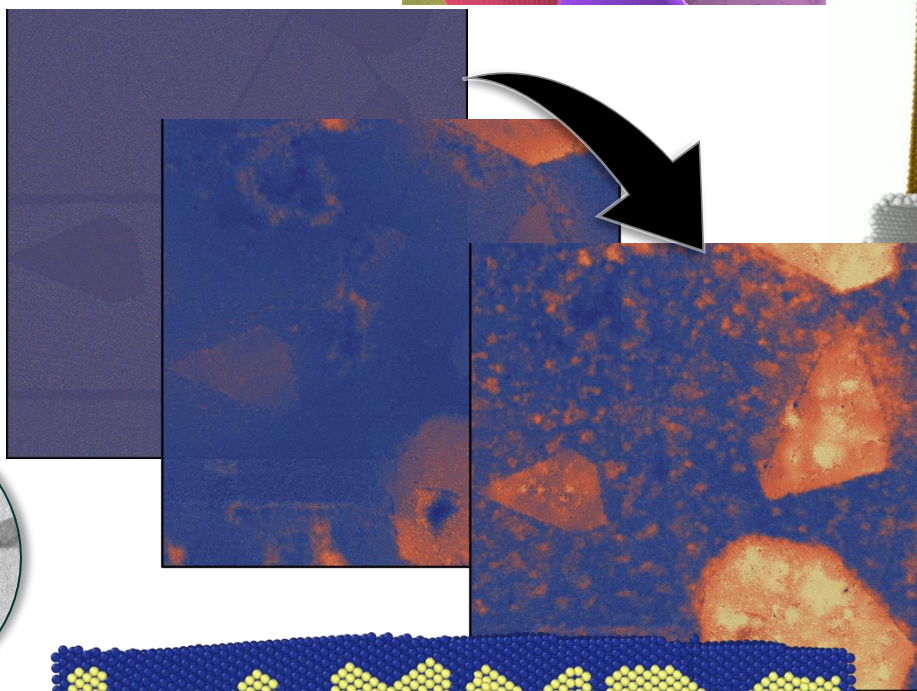
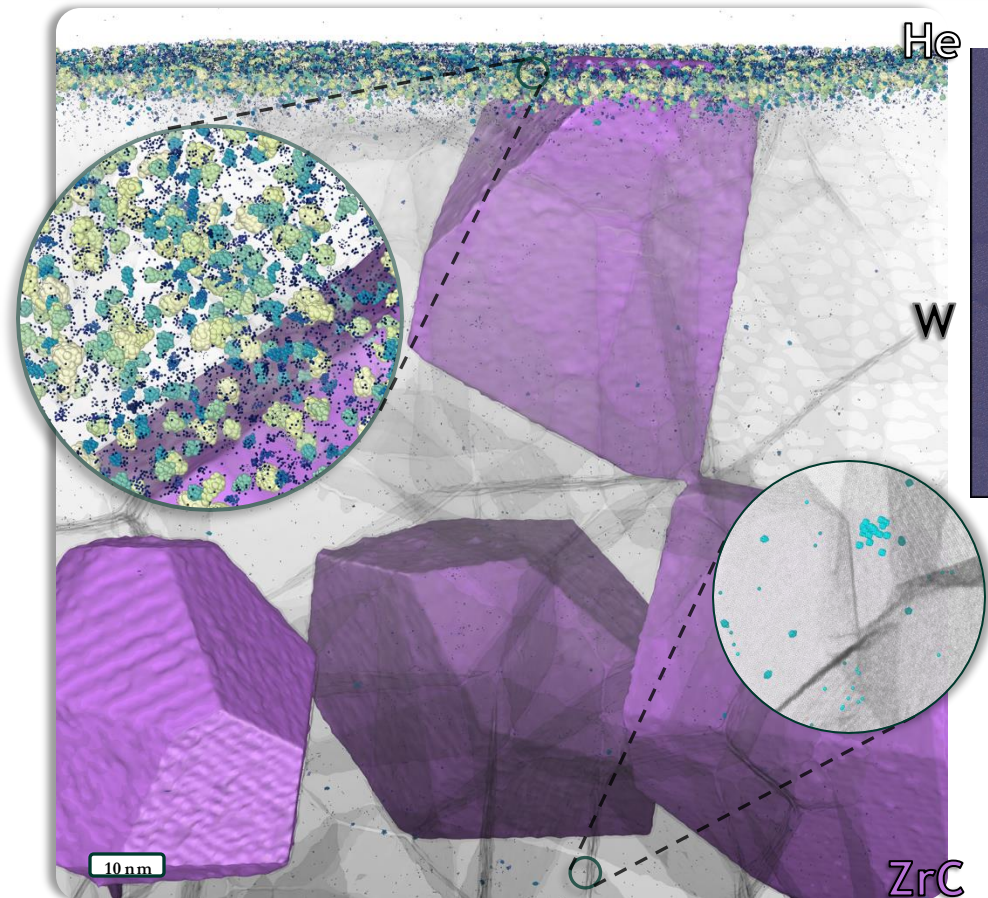
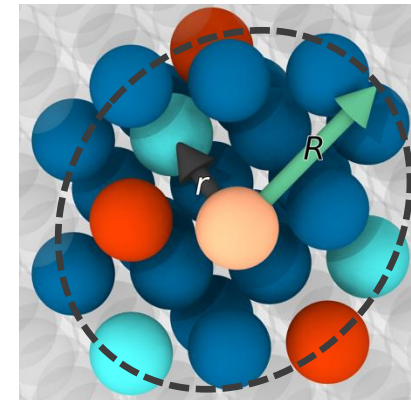
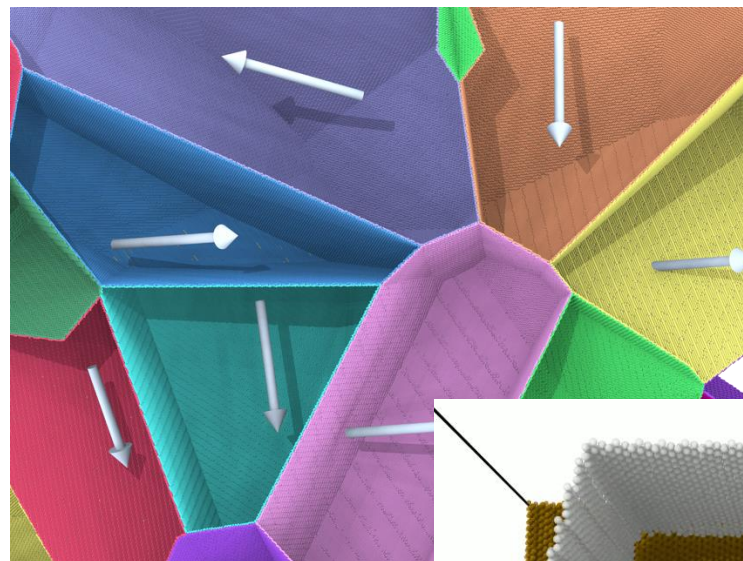




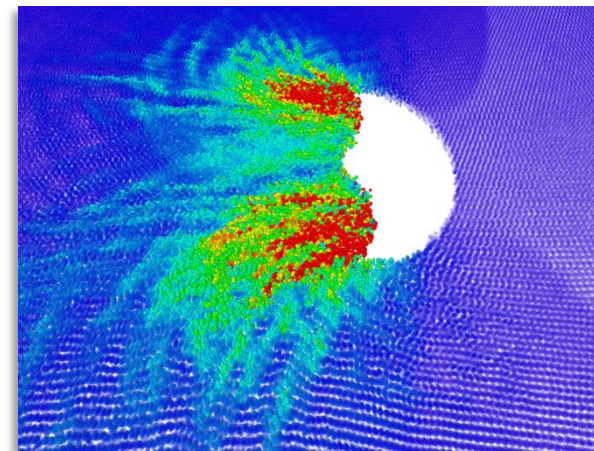
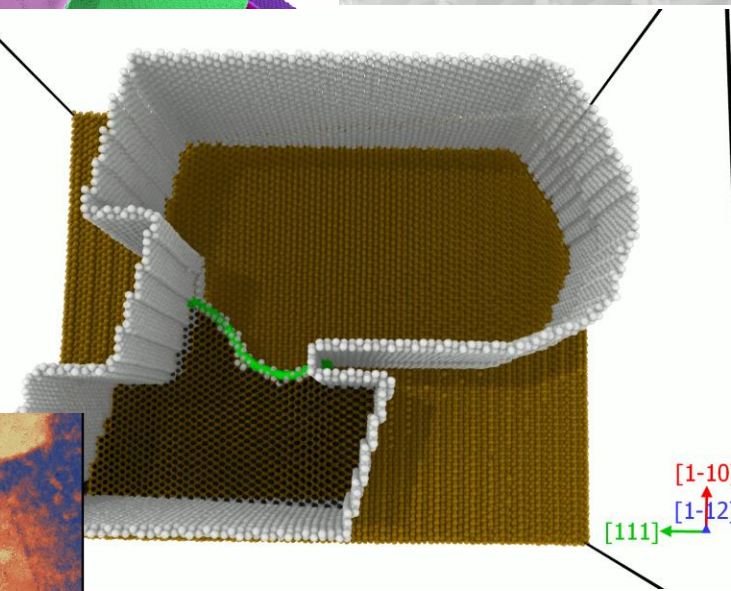
PMMA Short Chains, $\lambda = 24\text{nm}$

$U_p = 2.25\text{ km/s}$, $S_{\text{Fac}} = 1.0$

Time 1ps



LAMMPS



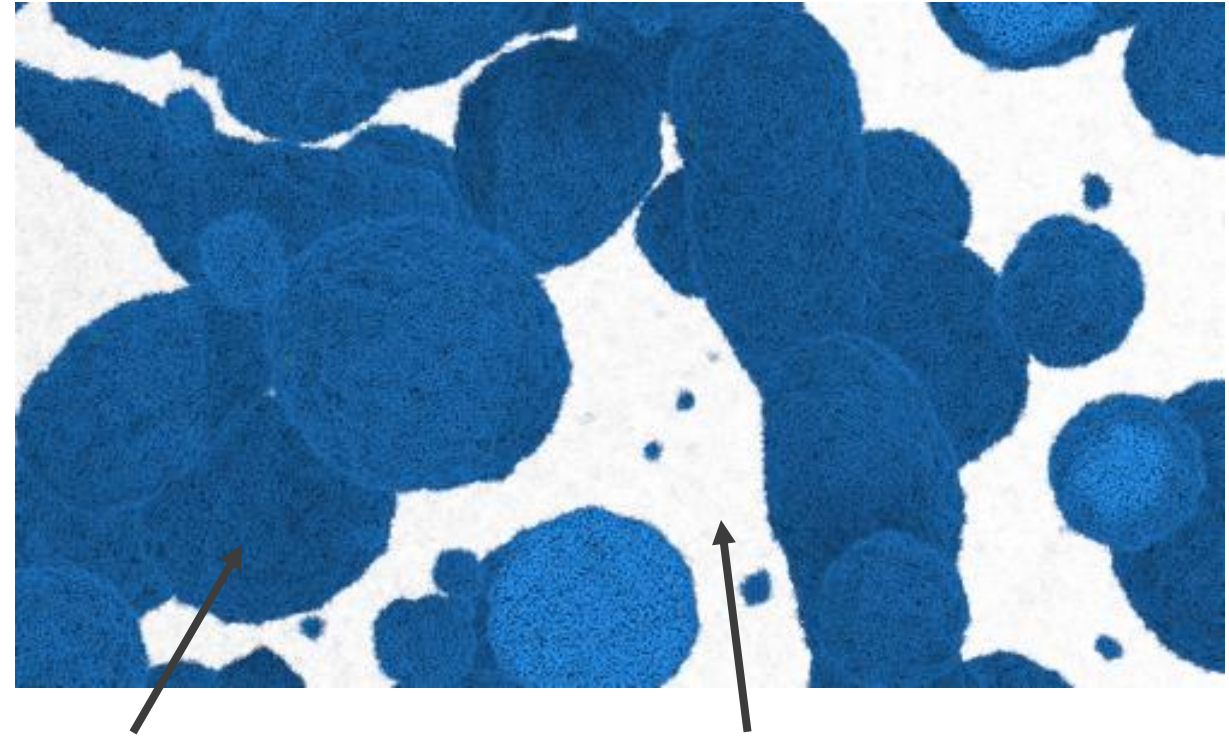


Advanced Features



Analyzing Large Simulations

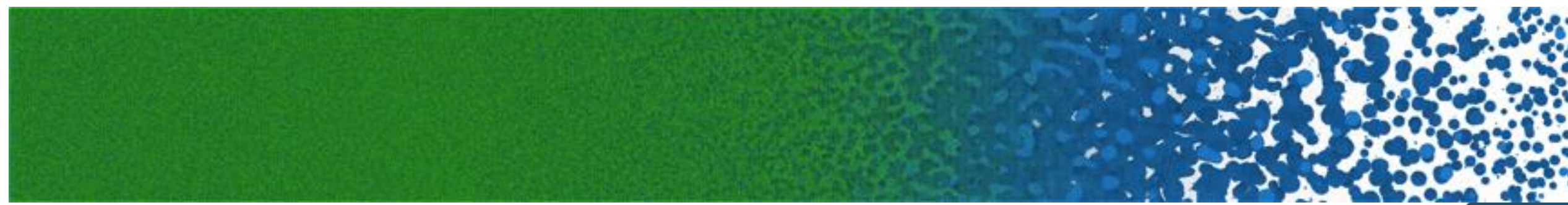
- If you really enjoy the features of OVITO, there is a paid version that will enable python scripting
- This also allows for batch processing on a cluster computing resource
- Highly scriptable with Python and useful for data post-processing and analysis in general (in addition to rendering images)



Visual size of an atom is scaled by local density

Green : Above T_c

Blue : Below T_c





Support Forum

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



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CONTACT

General questions

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

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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