# OVITO Visualization for LAMMPS Users

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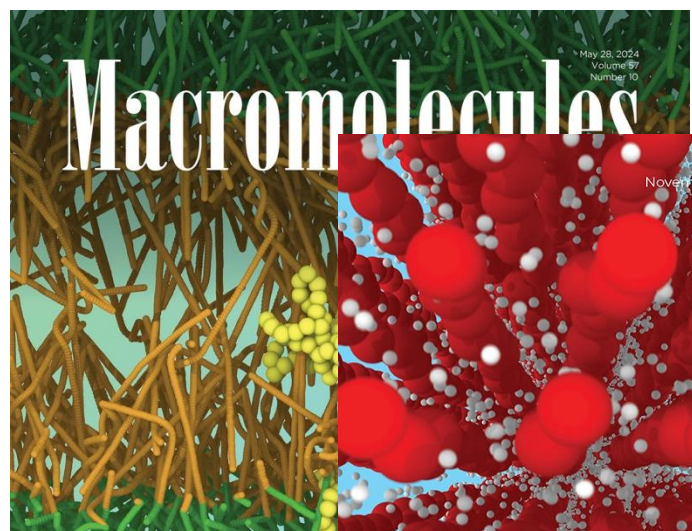
LAMMPS Workshop, Albuquerque, 2025

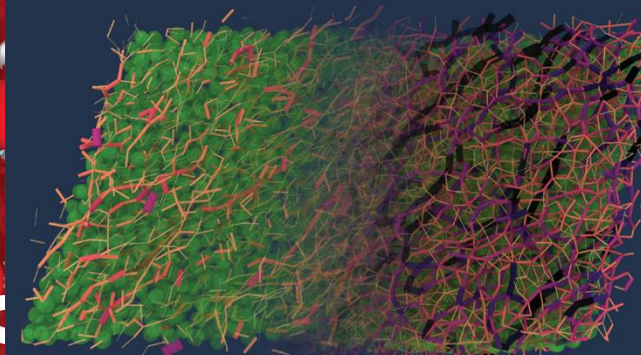*Follow along by downloading at ovito.org !*

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…
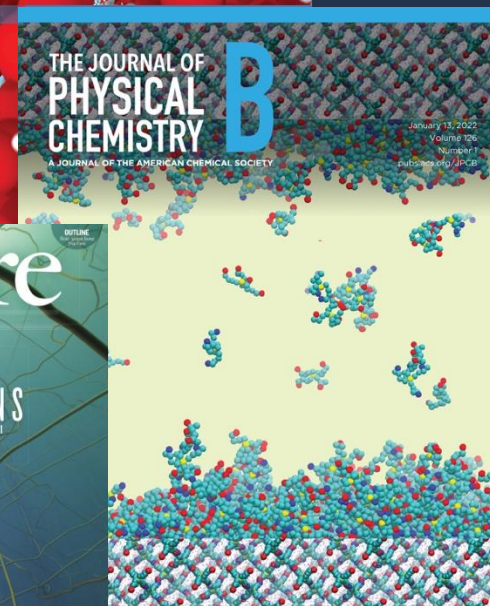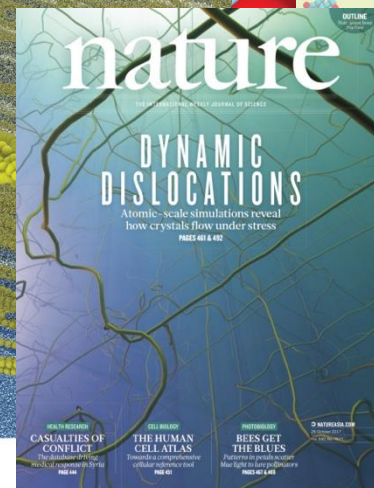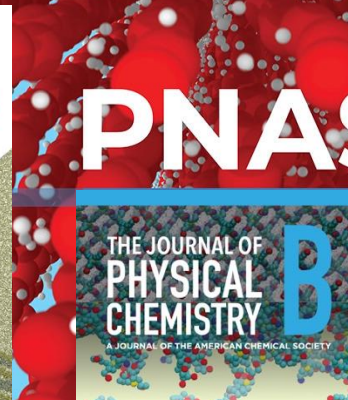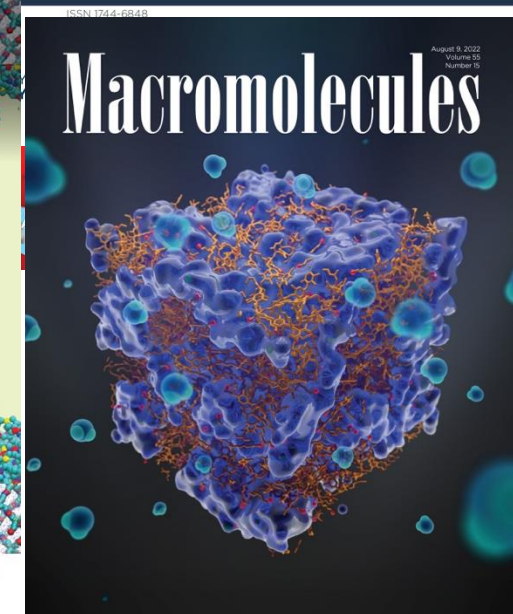
- Art?

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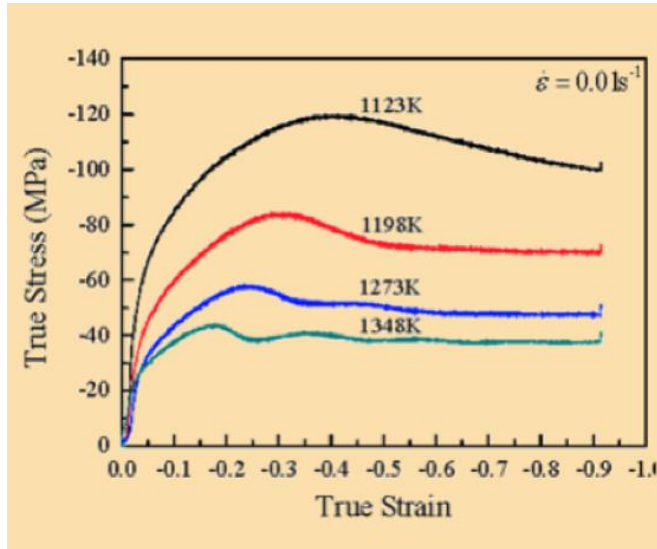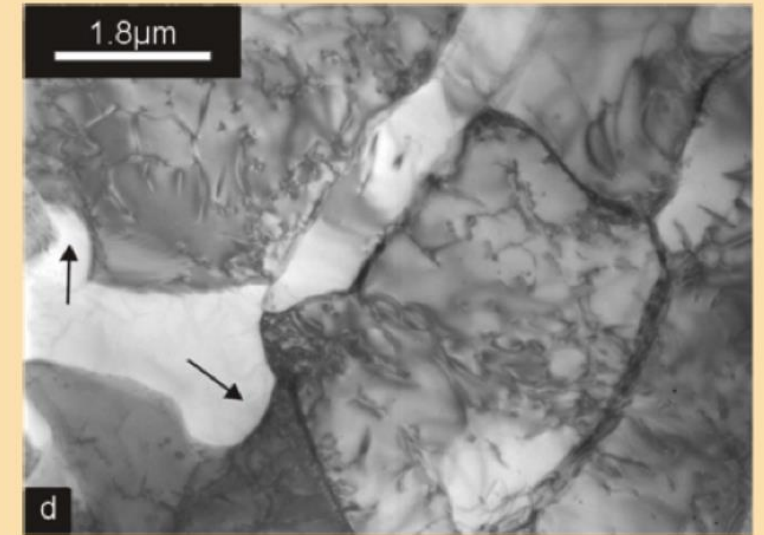
Microscopy & Imaging

Raw output data

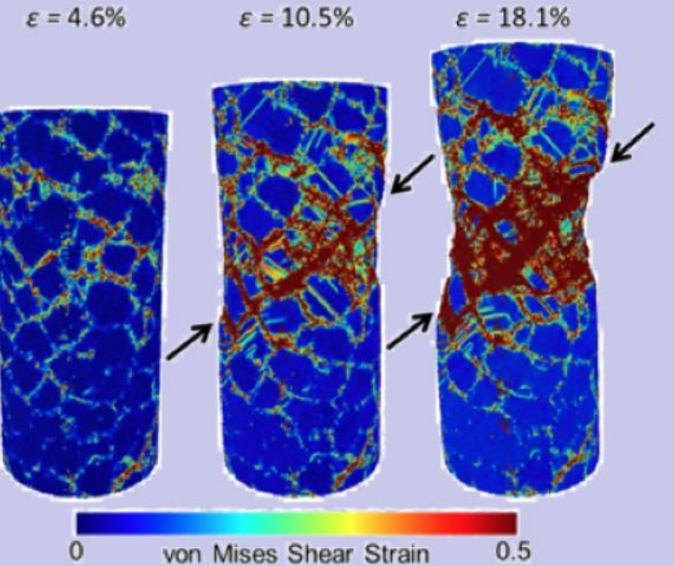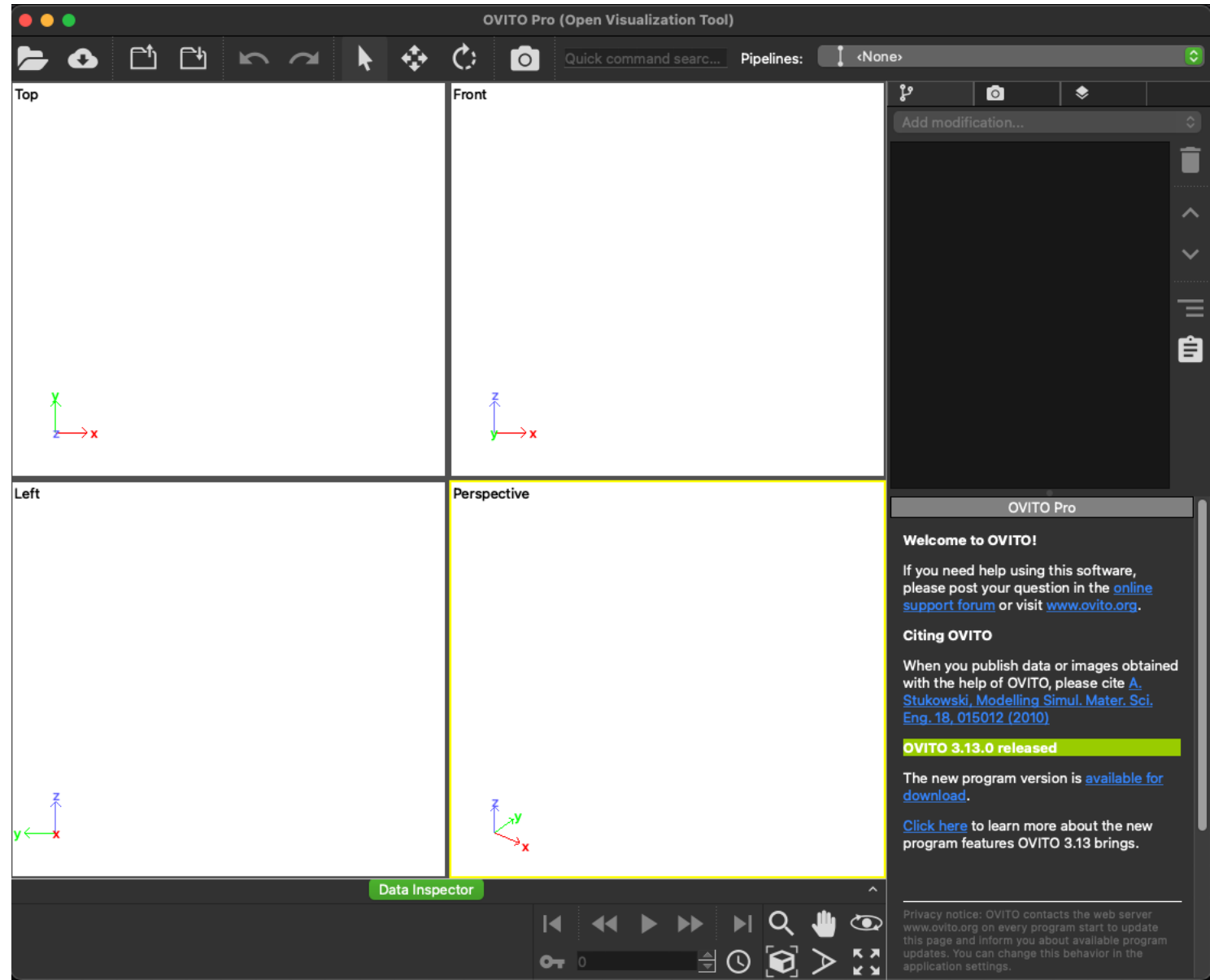Data analysis & Visualization
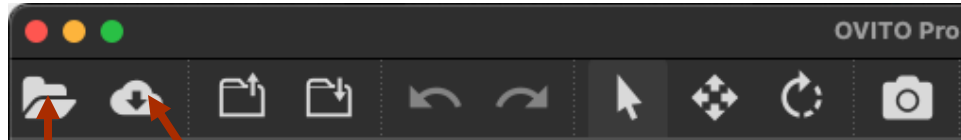
"in-silico microscopy"

von Mises Shear Strain

(Credit A. Stukowski LAMMPS Users Meeting 2019)
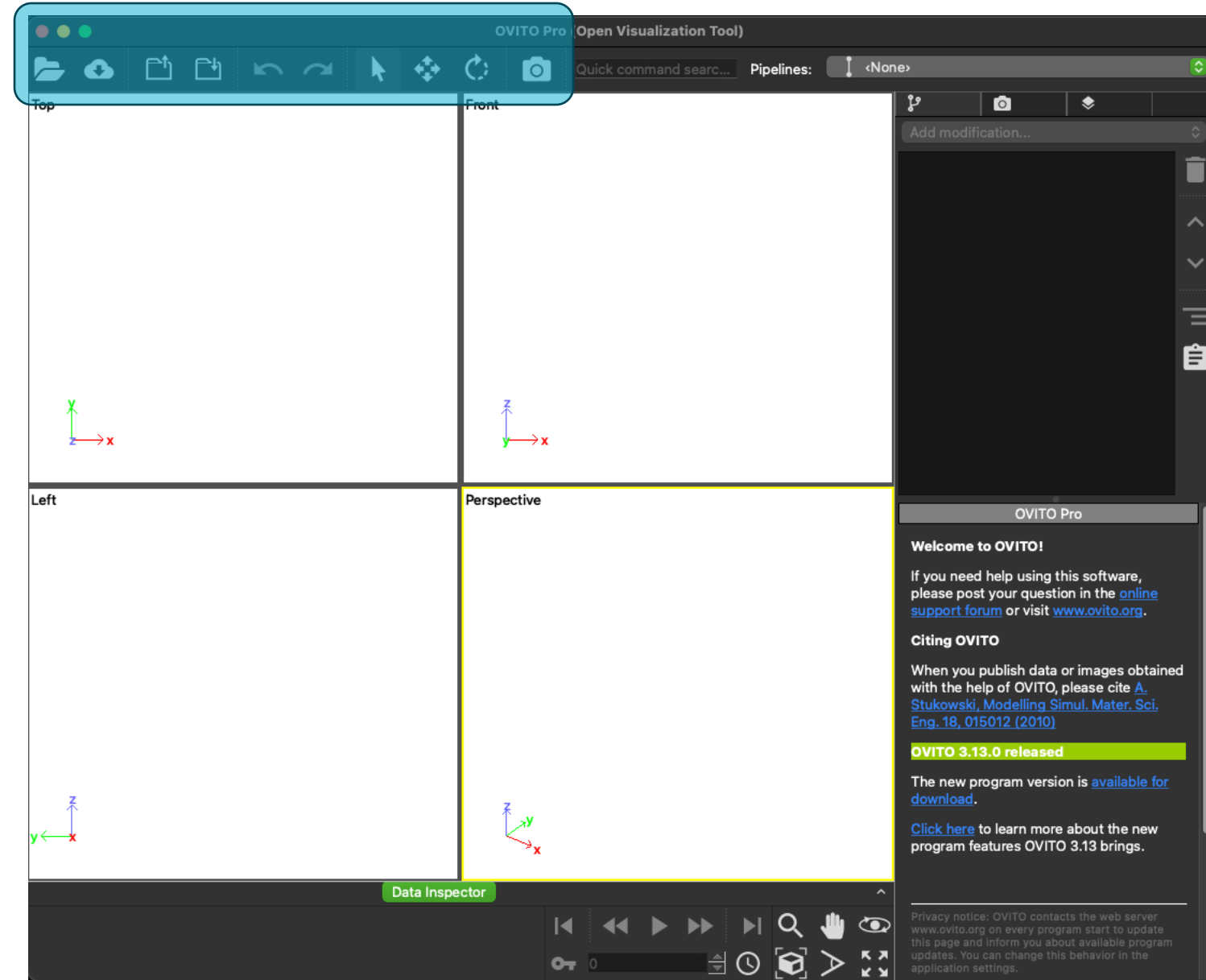
# GUI Walkthrough

# GUI Walkthrough



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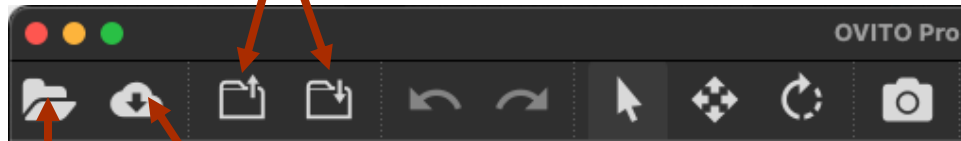sftp://user@machine//Path/To/
The/LAMMPS.data
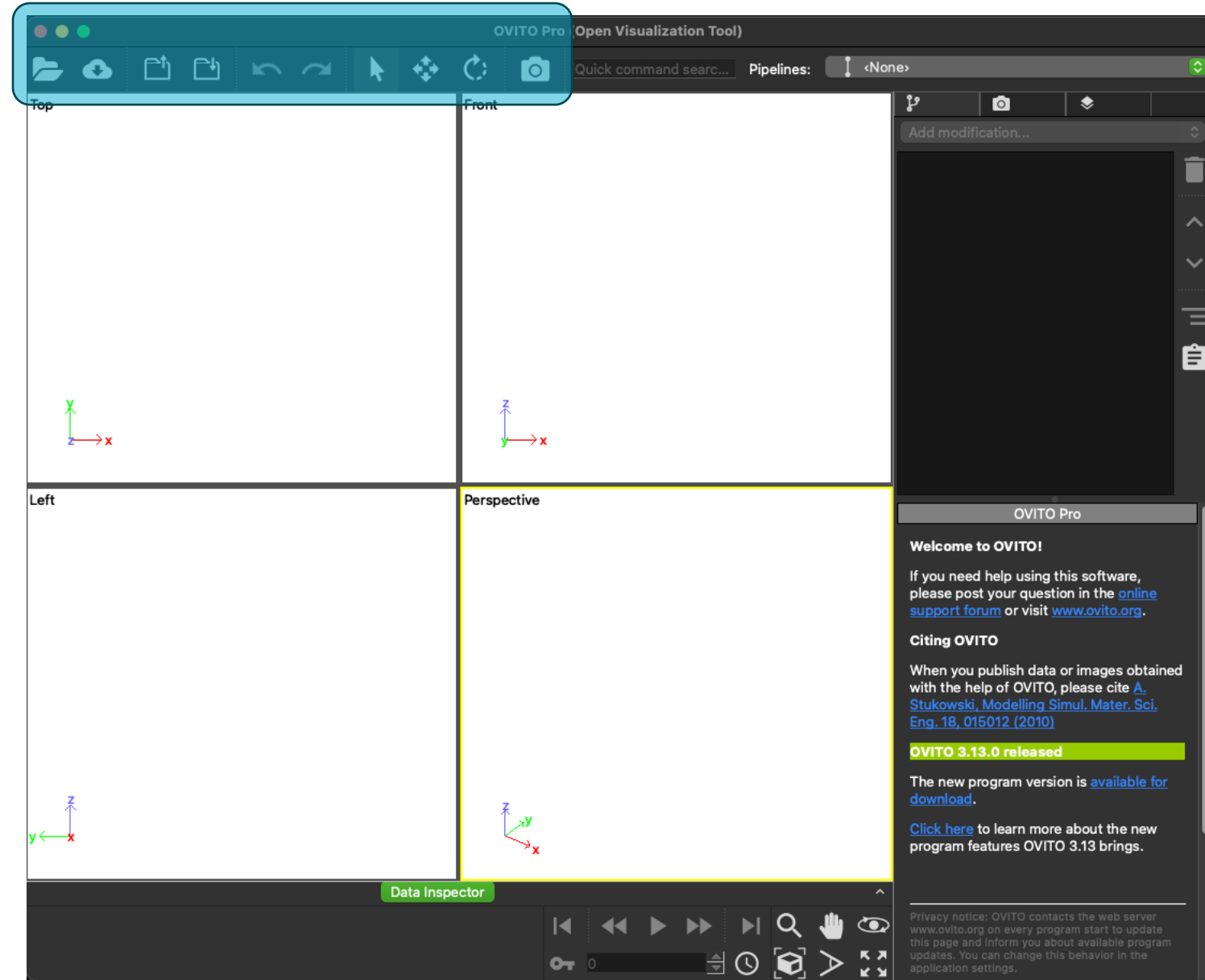
Load a local file on
your machine

# GUI Walkthrough

Save/Load an OVITO session

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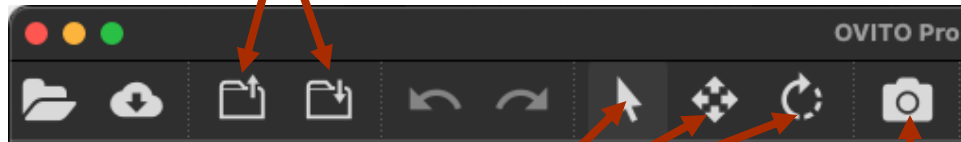sftp://user@machine//Path/To/
The/LAMMPS.data
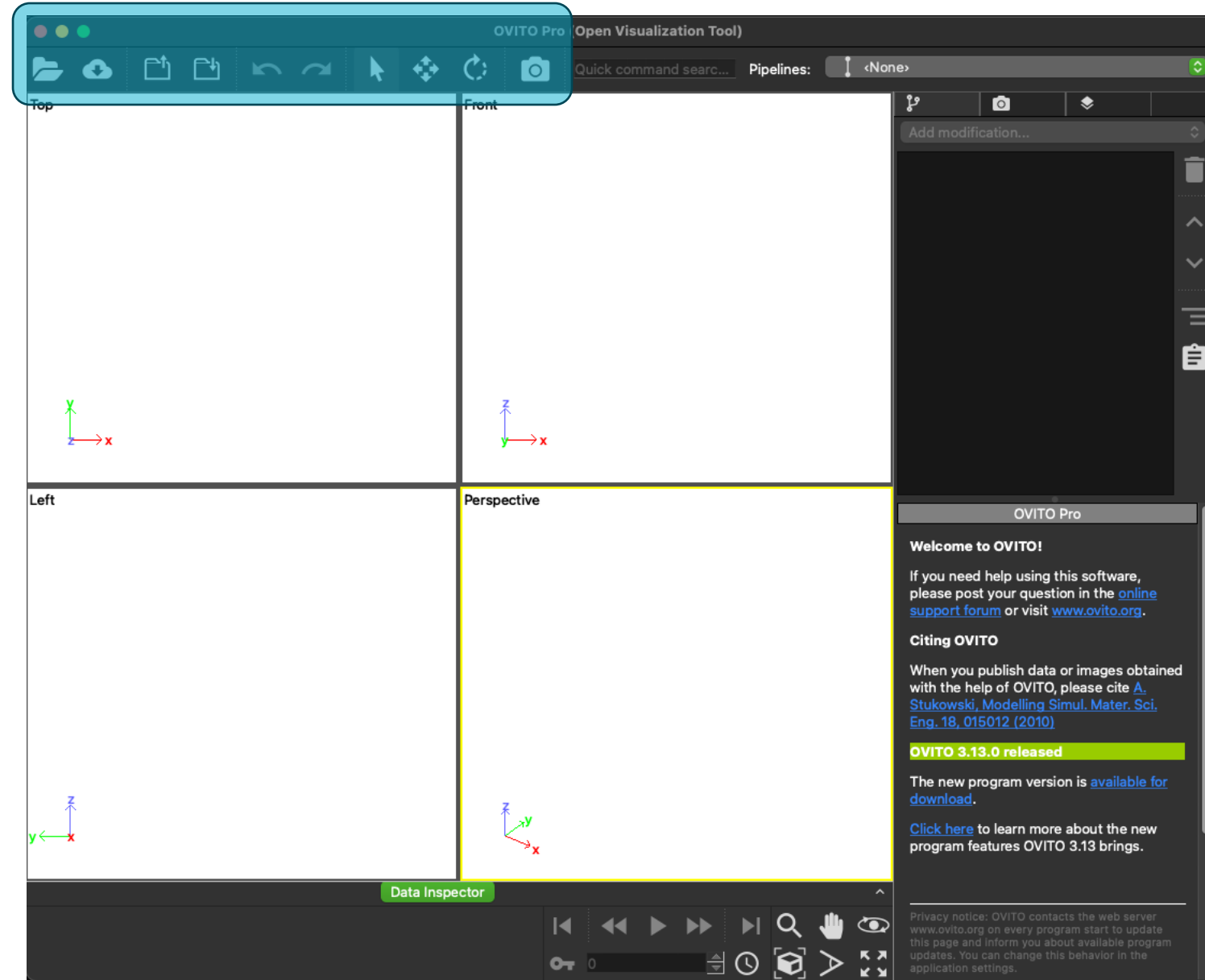
Load a local file on
your machine

# 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
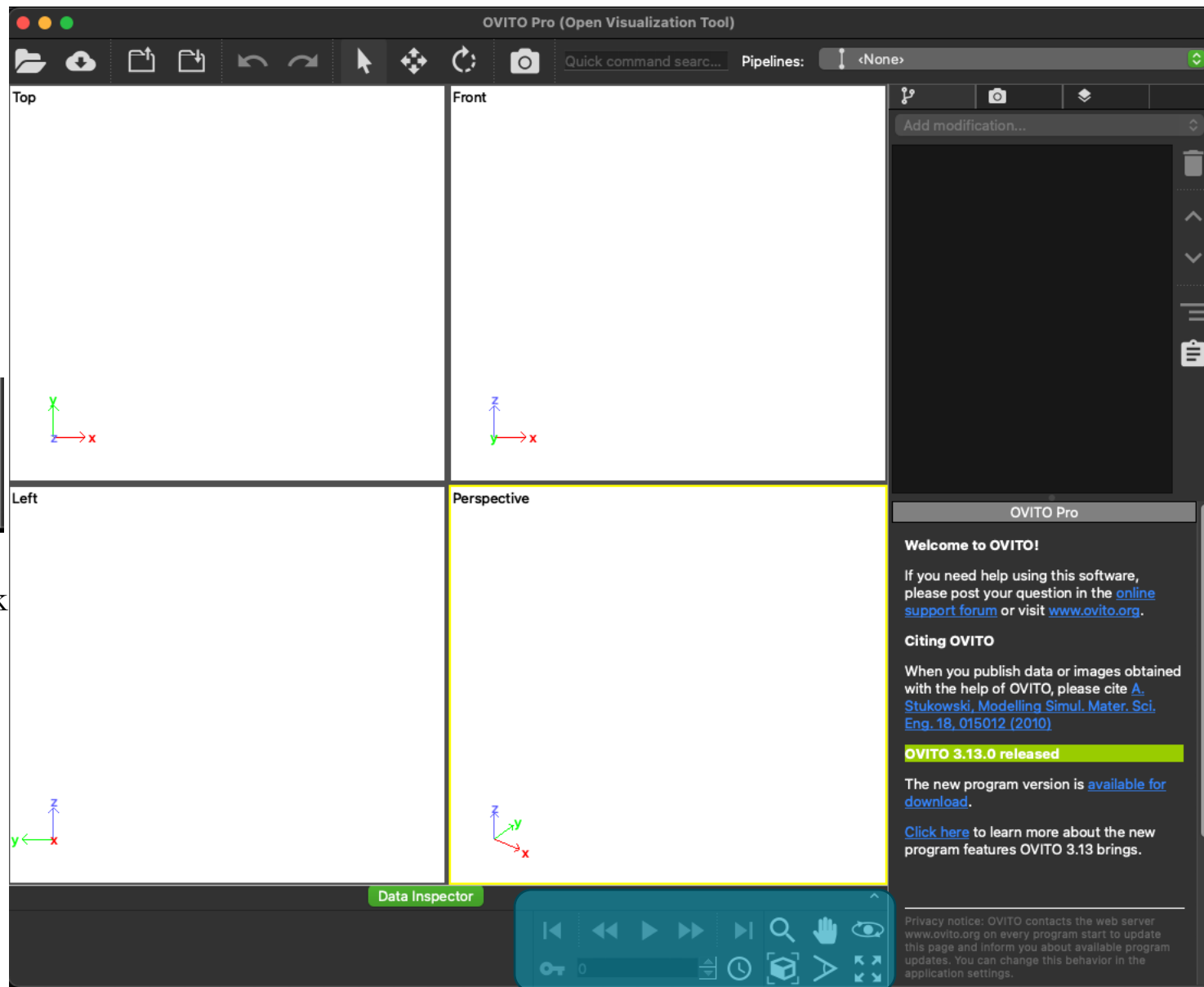of four panels highlighted in yellow

# GUI Walkthrough



Play a movie of your simulation trajectory

Select a particular frame to view

Move one frame forward, jump to end.

# GUI Walkthrough

Focus on one viewing panel, click again to see all

Auto-Zoom to fit all atoms into the view
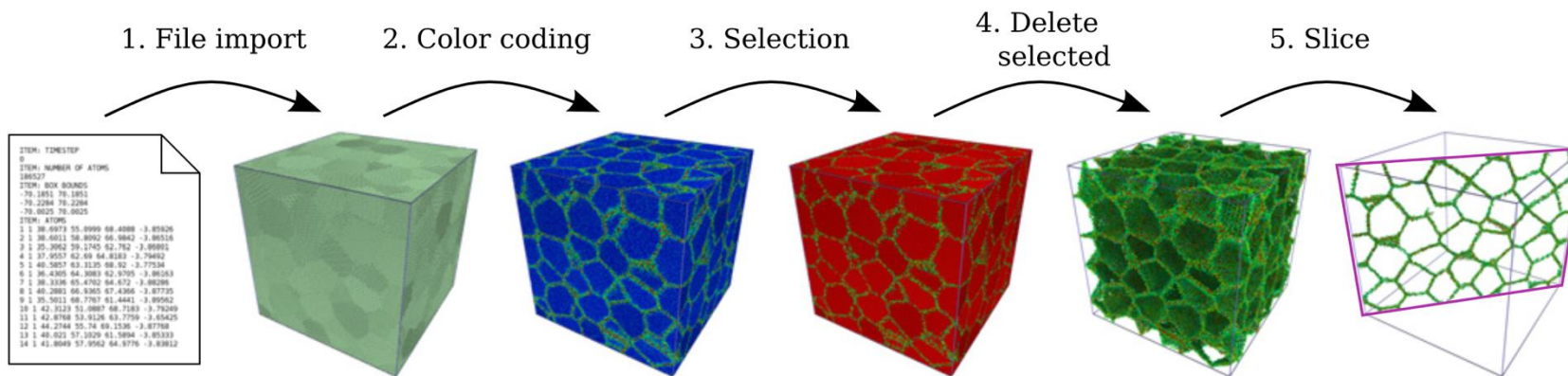
Adjust Zoom, left-click and drag up/down
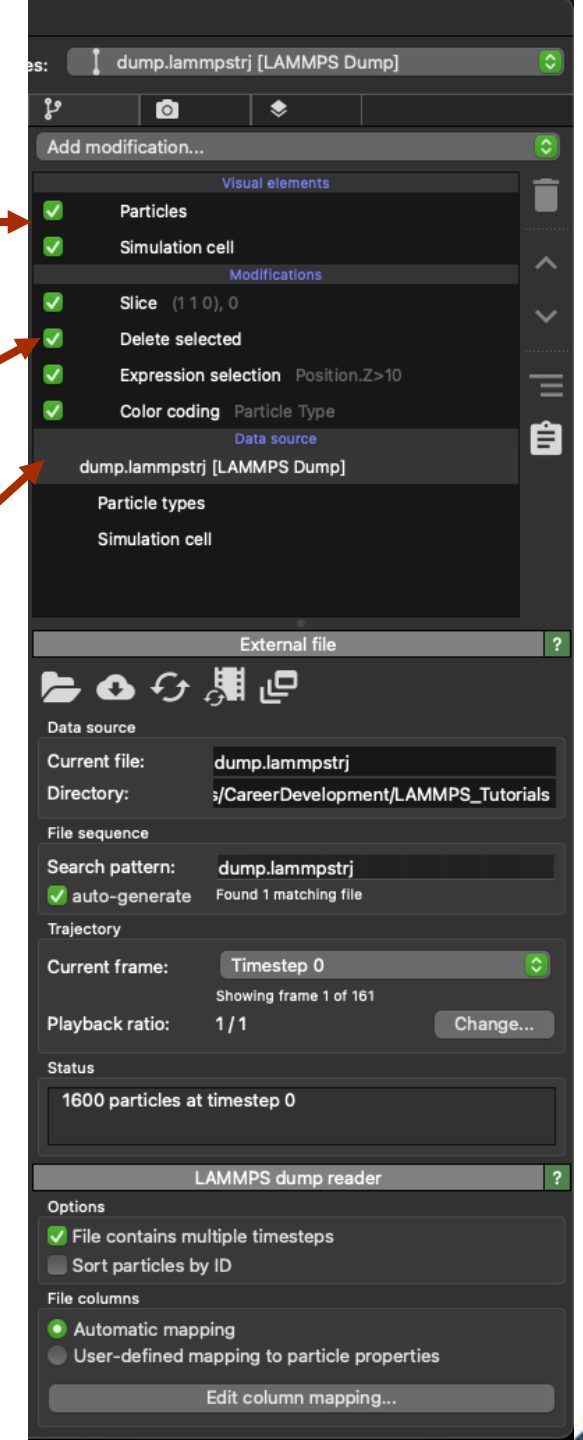
# GUI Walkthrough

## 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        A Stukowski



1. File import    2. Color coding    3. Selection    4. Delete selected    5. Slice

# GUI Walkthrough

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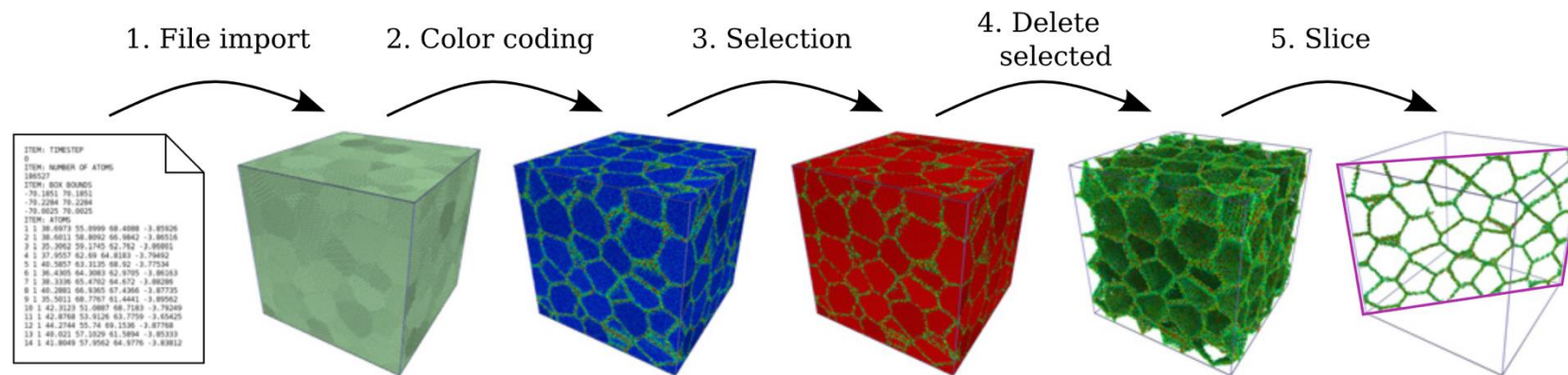
Visual Elements

Active/Inactive modifications

File Imported

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

1. File import → 2. Color coding → 3. Selection → 4. Delete selected → 5. Slice

# GUI Walkthrough

From LAMMPS GUI :
LJ Fluid Example

See https://lammpstutorials.github.io/

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

# GUI Walkthrough



Change left-click to inspect particles
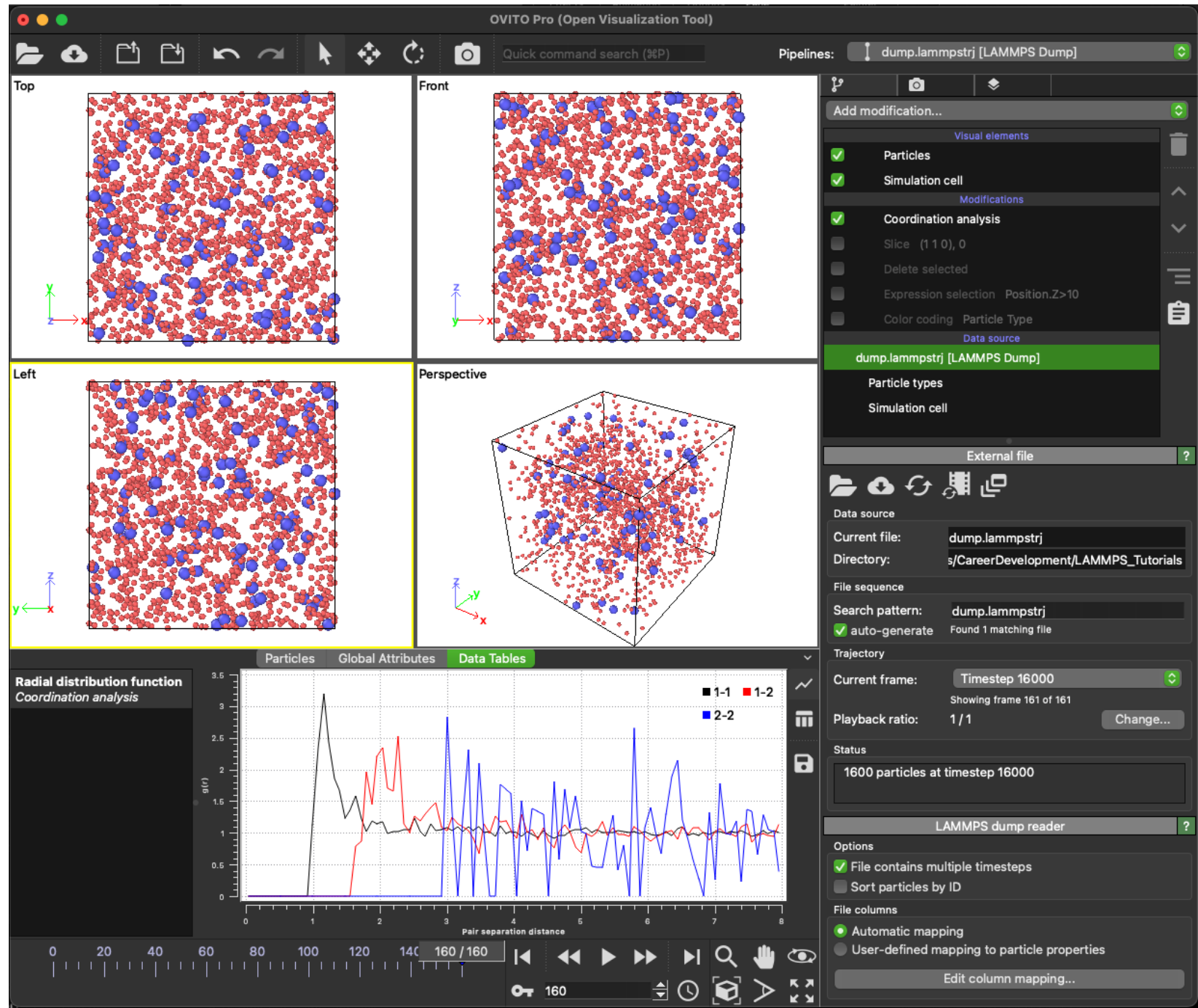
Inspect properties of multiple particles (bond length, angles)

View plots generated by modifications

View data tables generated by modifications

Export data tables or plots generated by modifications

Modifications to your scene are accessible here
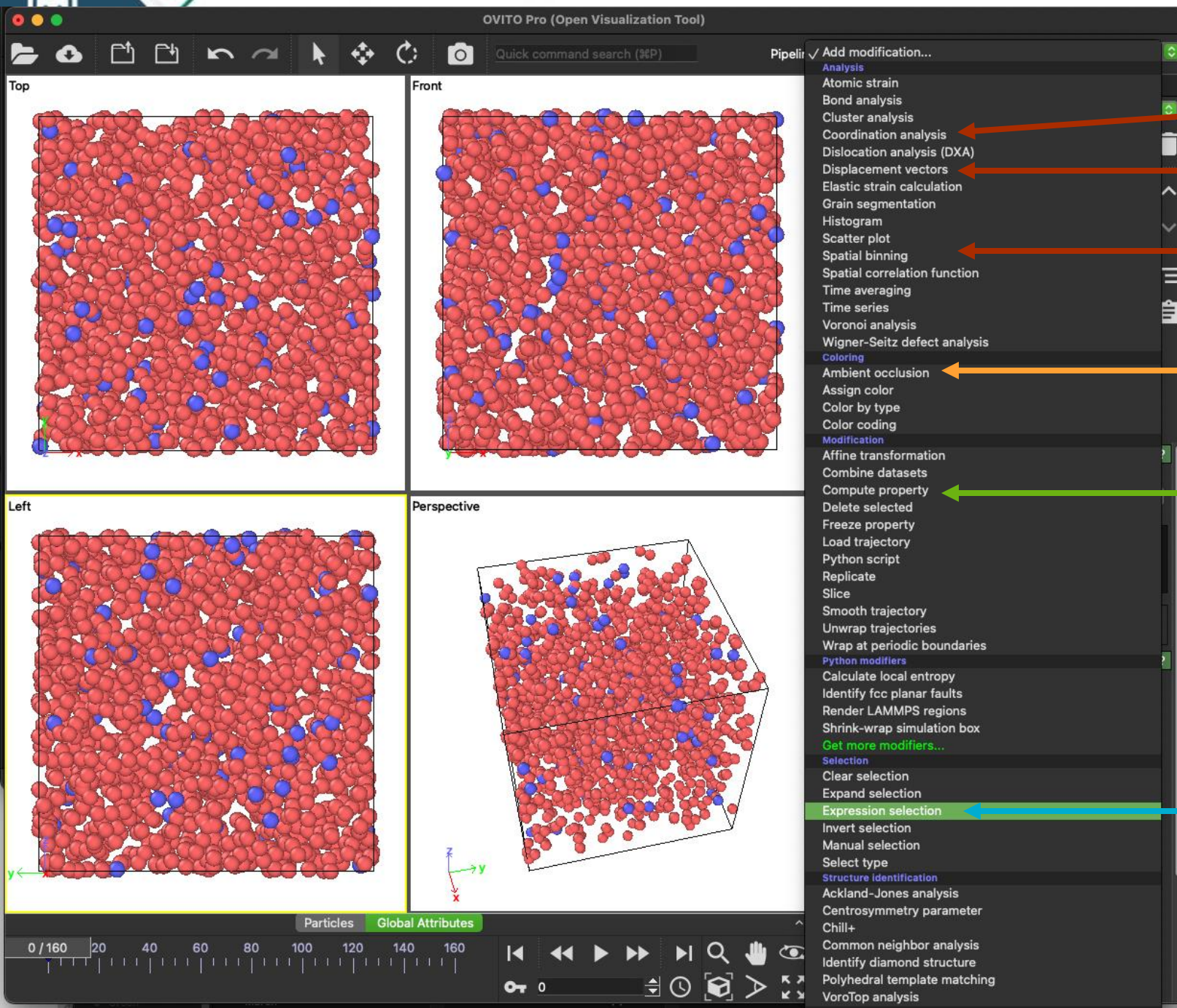
Pair Distribution Function

Calculate how far things have moved

Locally Averaged Properties
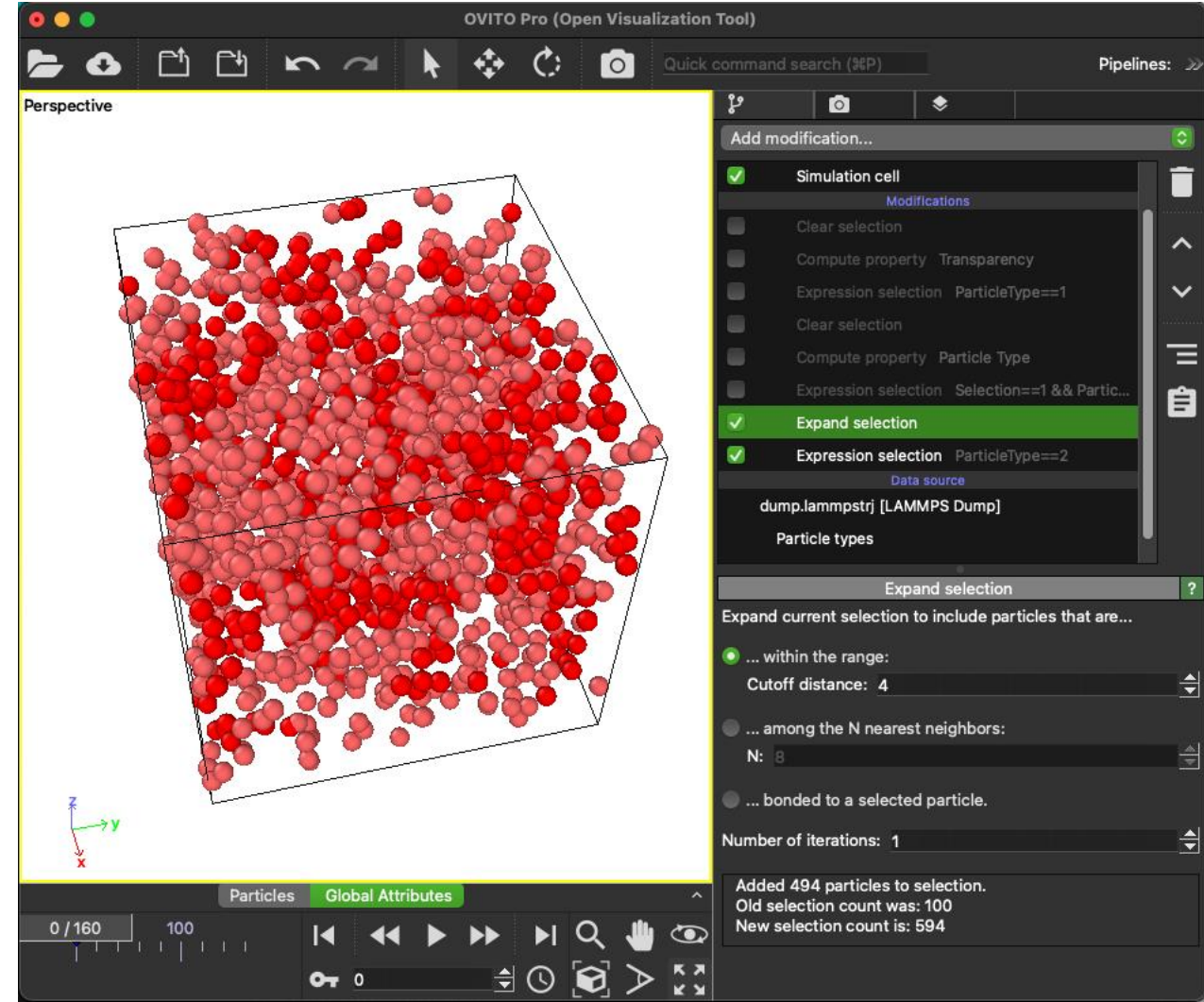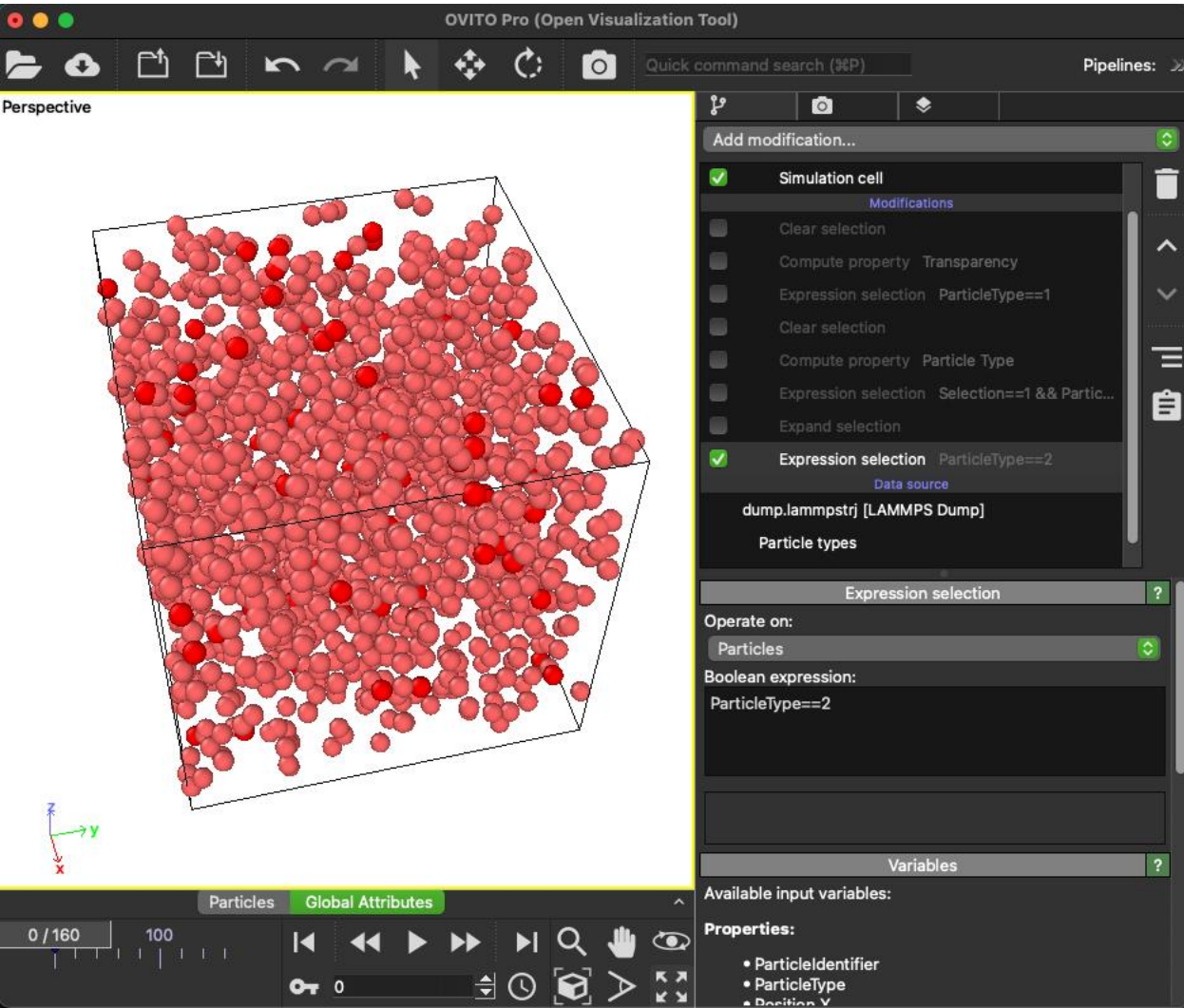
Add Shadows

Manipulate per-atom data

The most powerful modification

# LJ Fluid Example

**Expression Selection**
"ParticleType==2"

**Expand Selection**
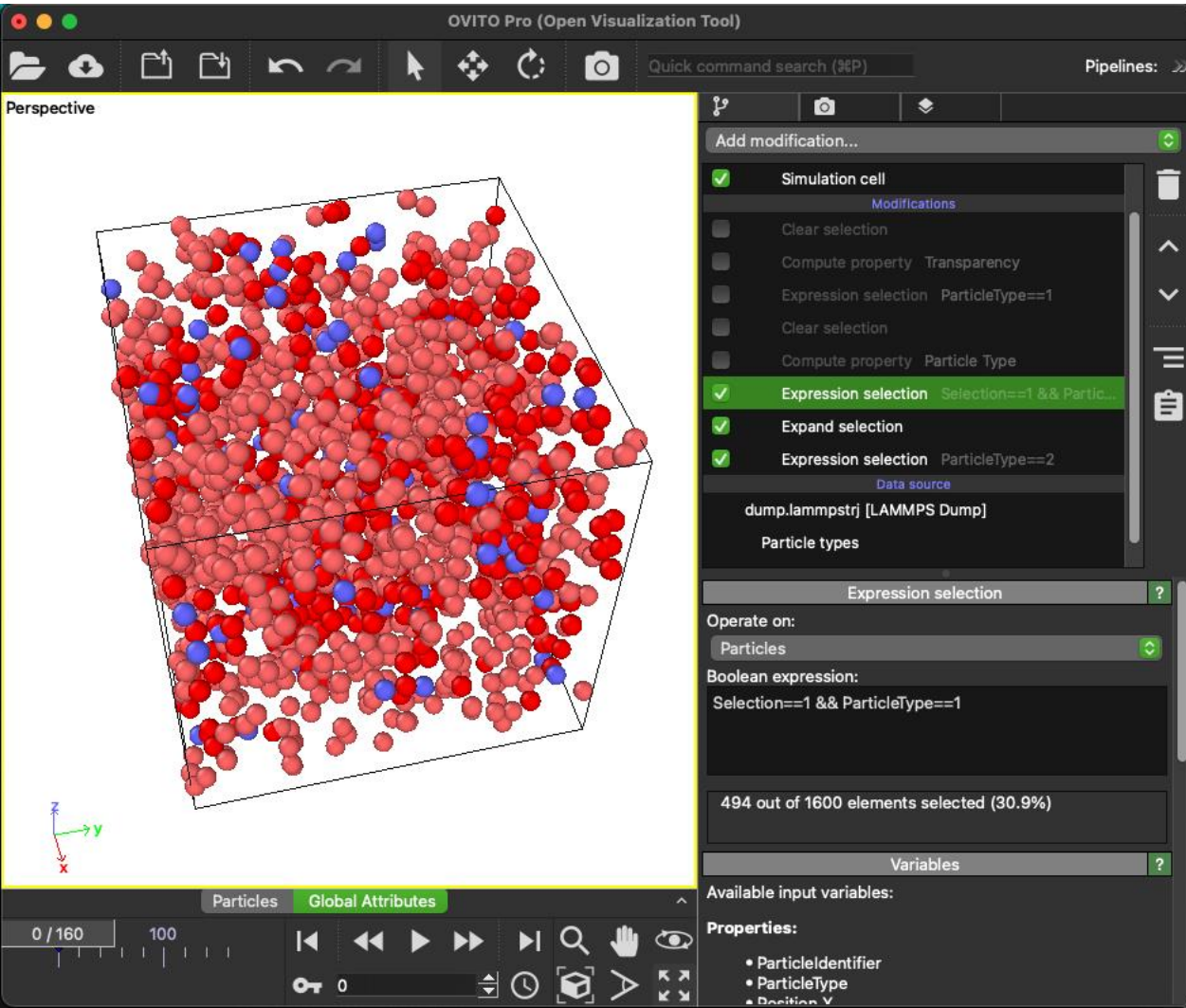...within the range
Cutoff Distance 4

# LJ Fluid Example
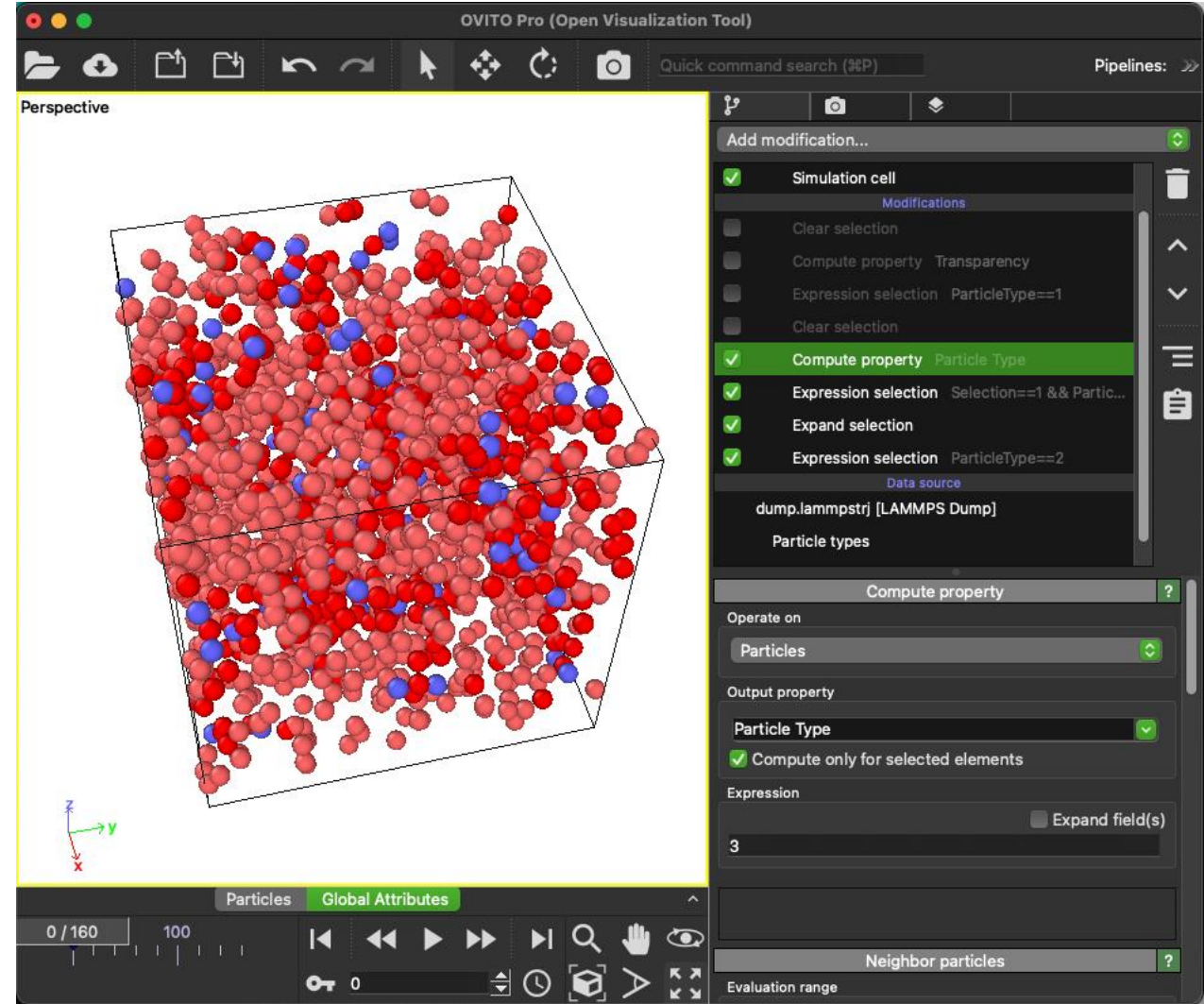
## Expression Selection
"Selection==1 && ParticleType==1"
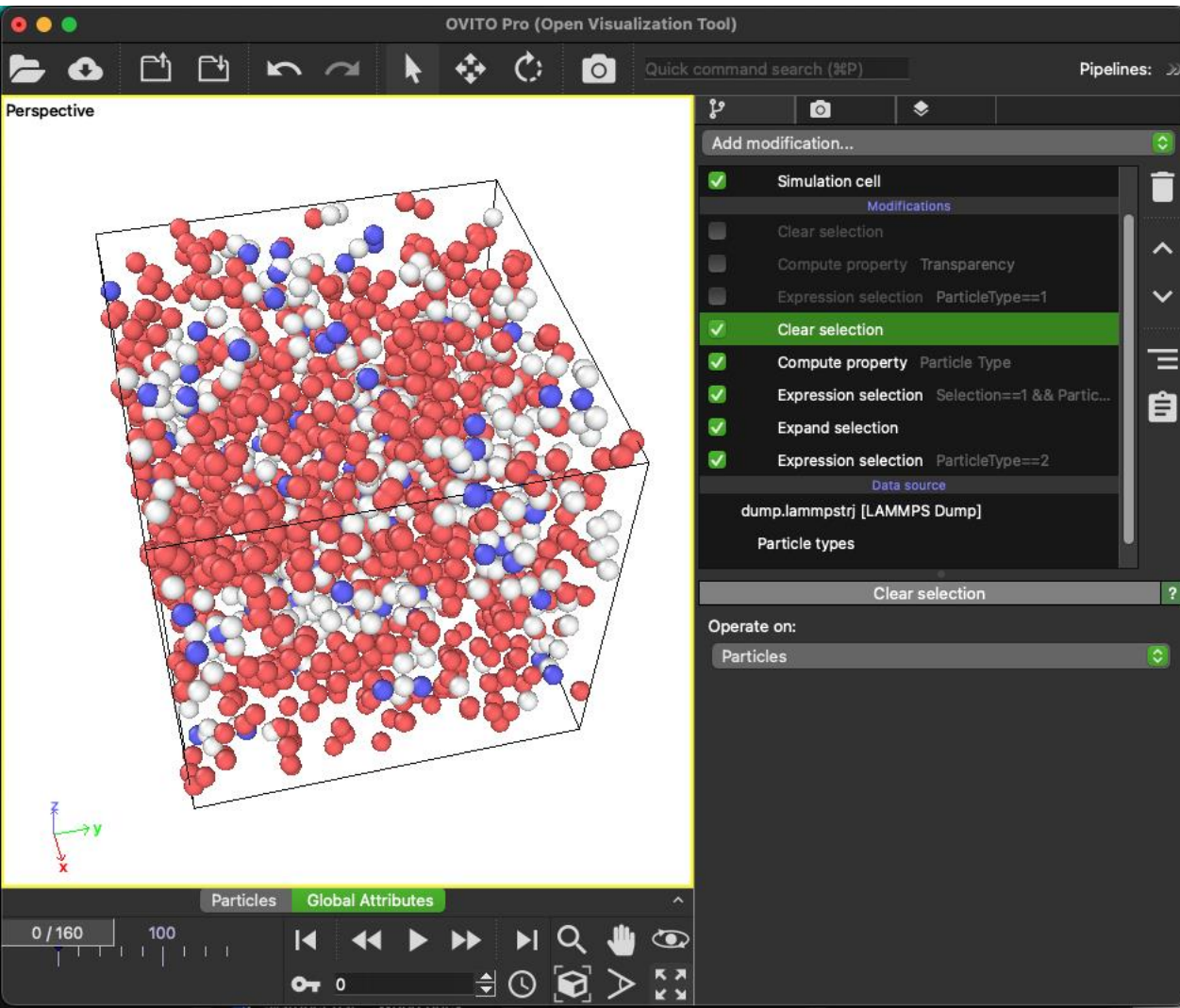
## Compute Property
Output Property : ParticleType
☑ Compute only for selected elements
Expression : 3

# LJ Fluid Example

Clear Selection
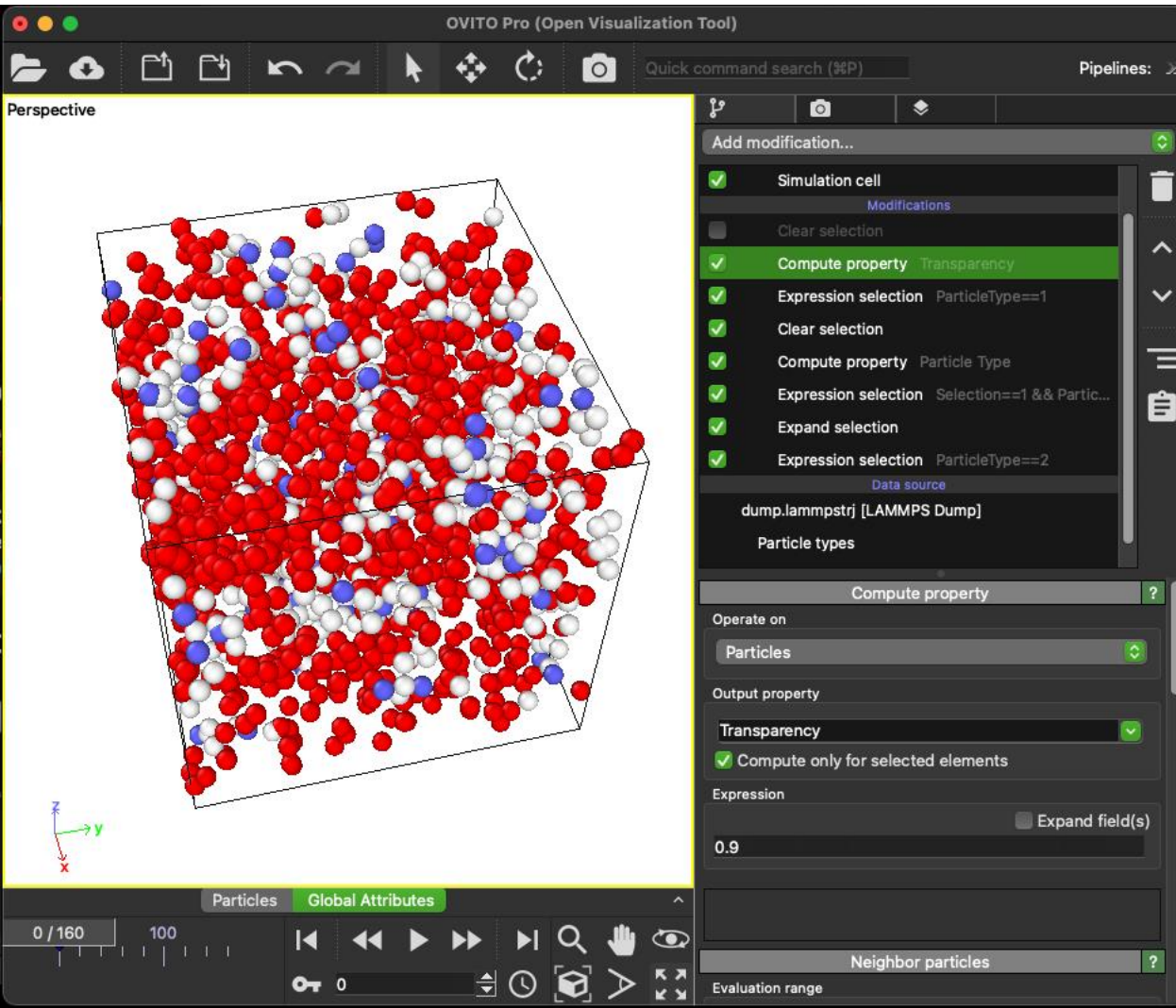
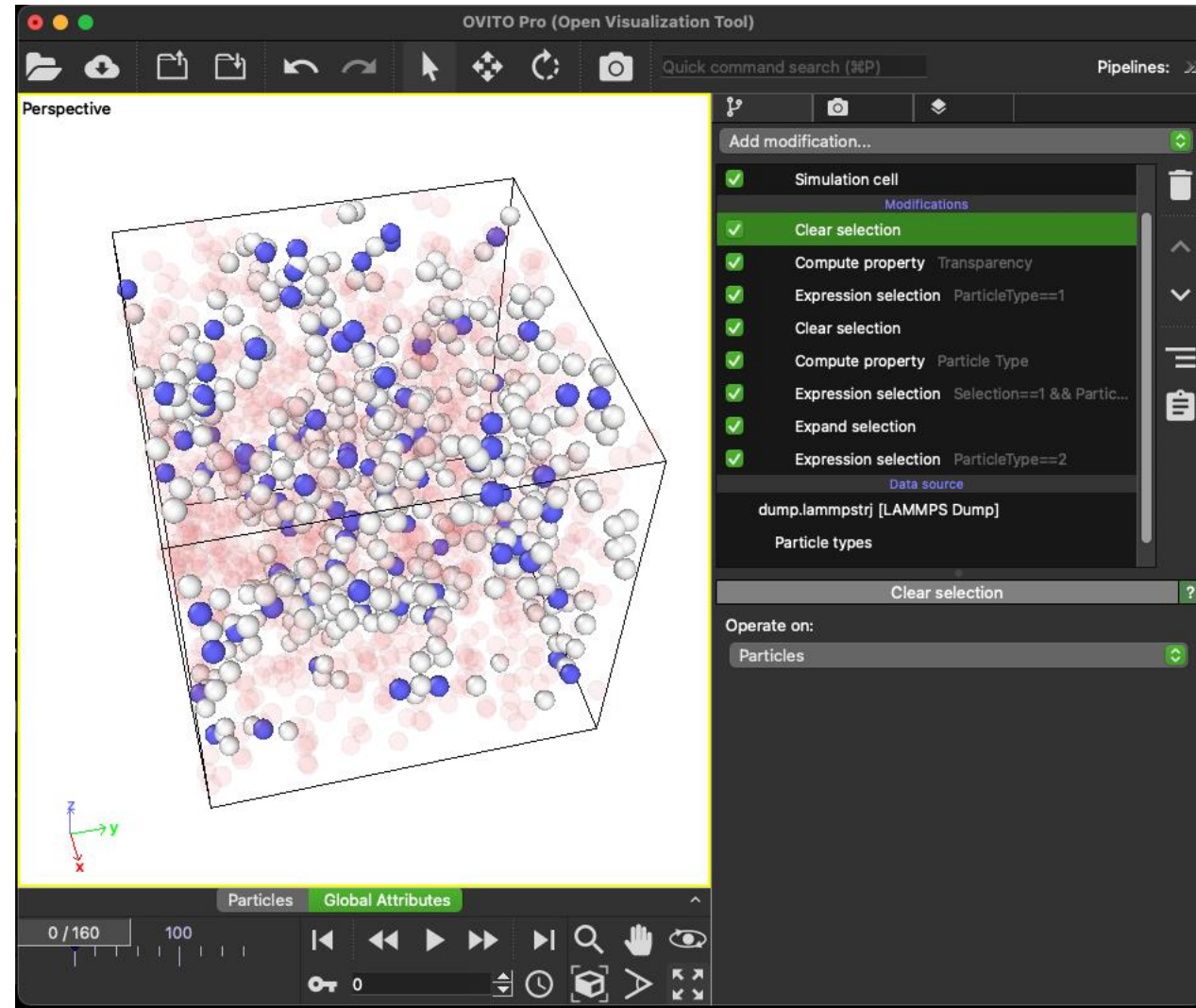Expression Selection
"ParticleType==1"
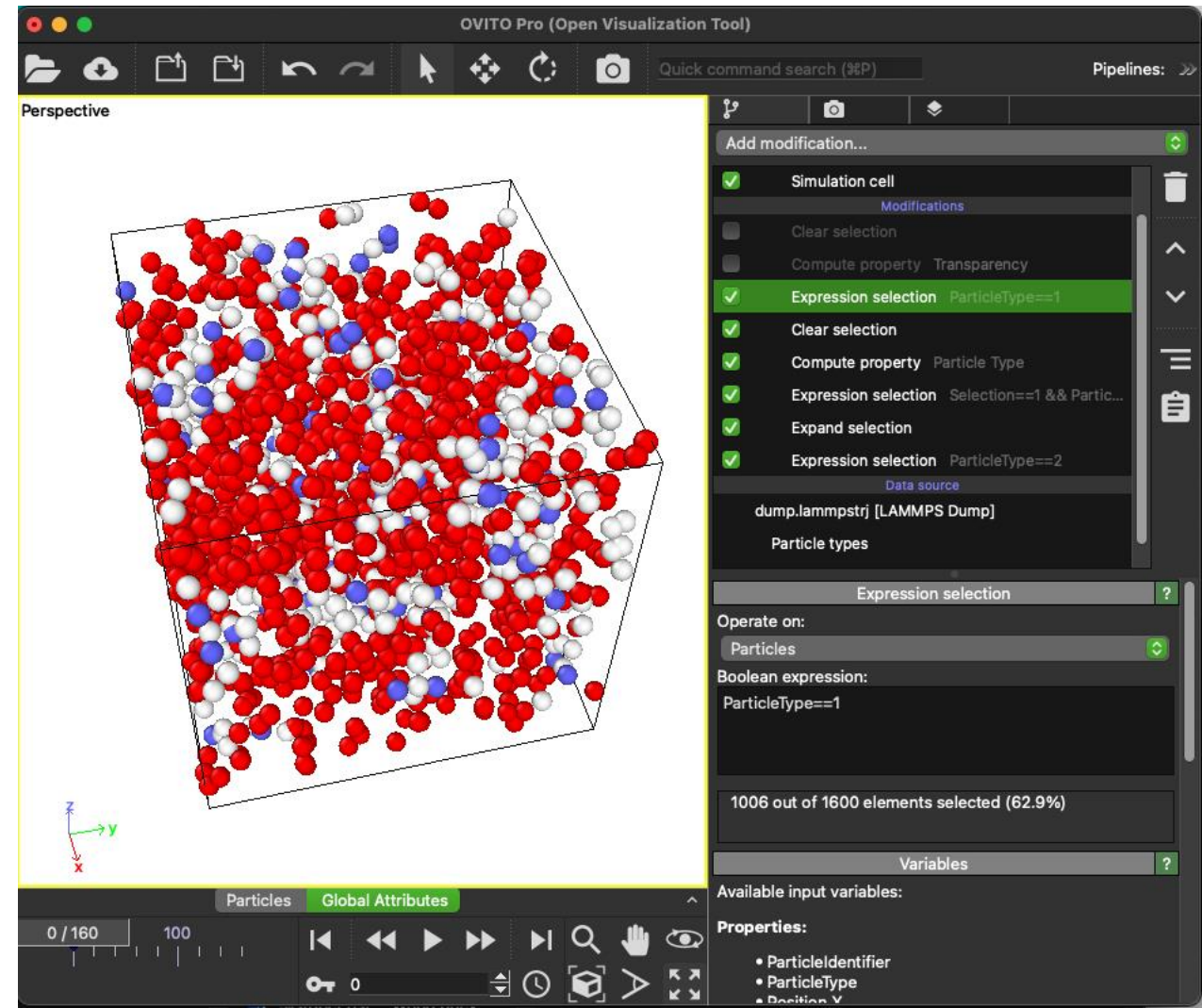
# Compute Property
Output Property : Transparency
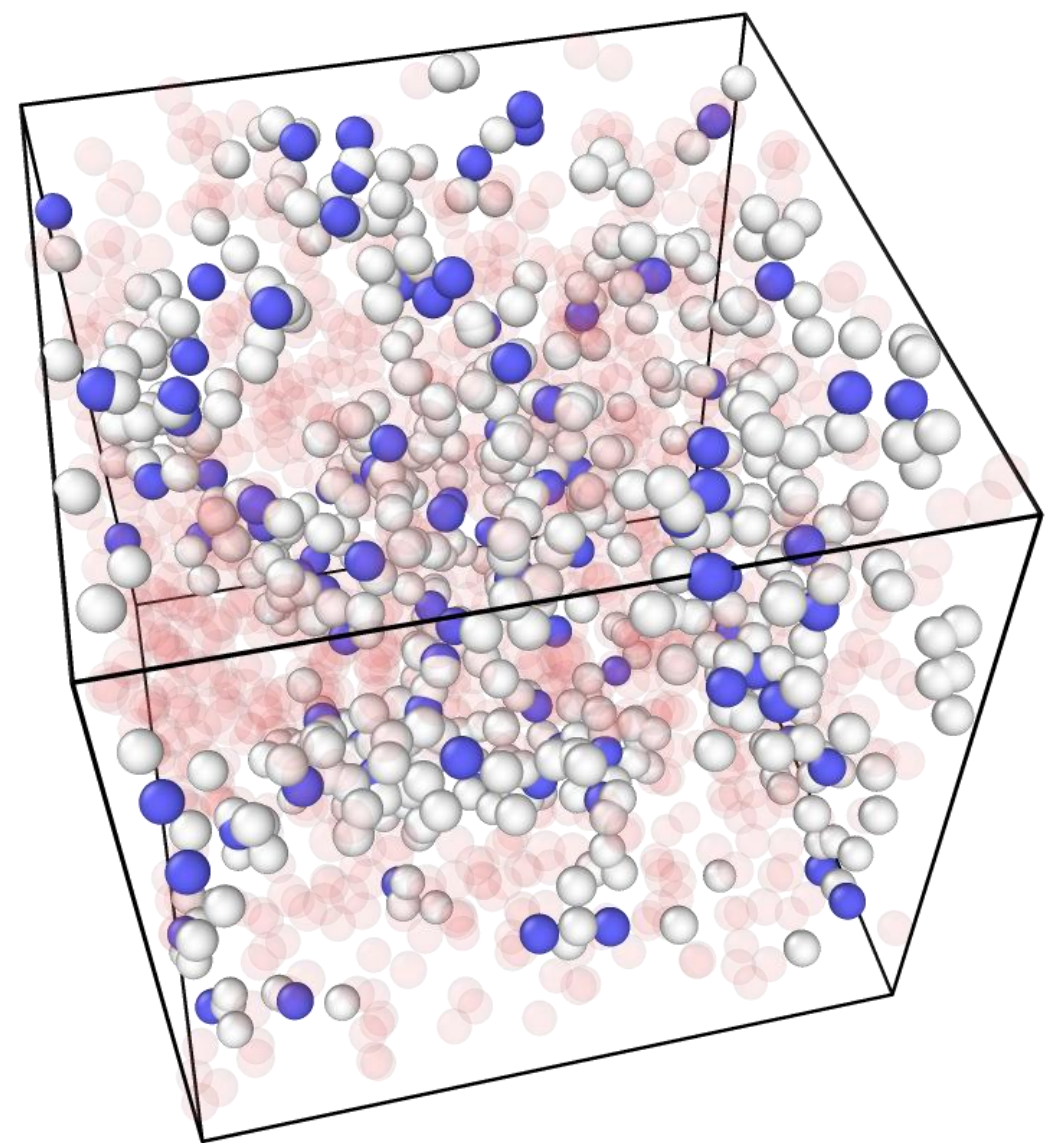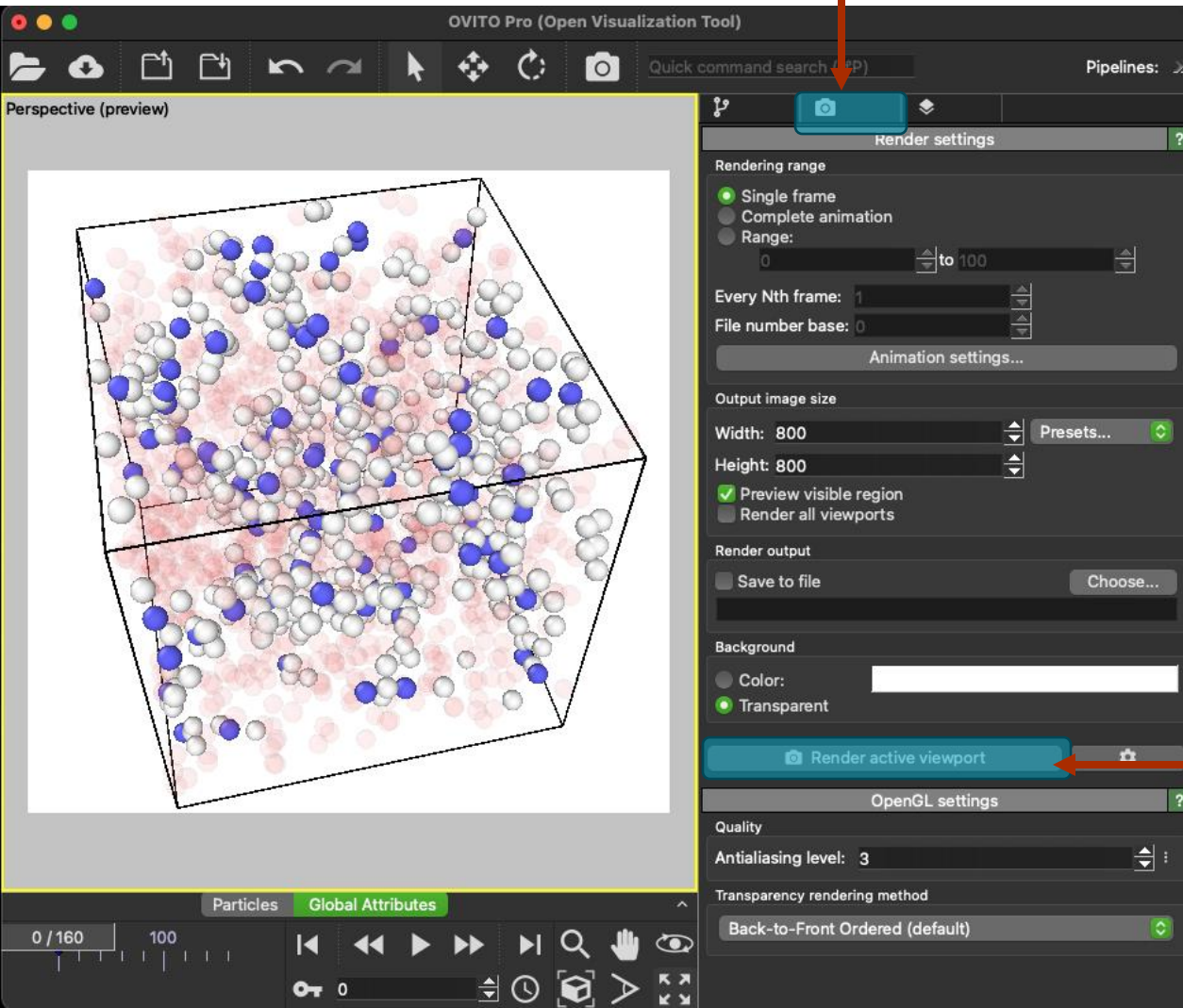☑ Compute only for selected elements
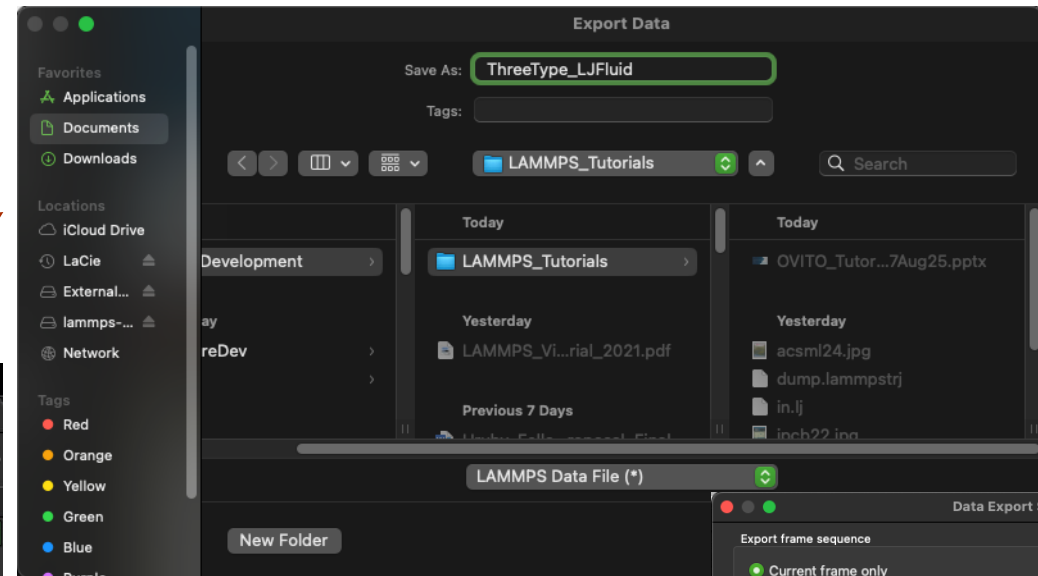Expression : 0.9

# Clear Selection
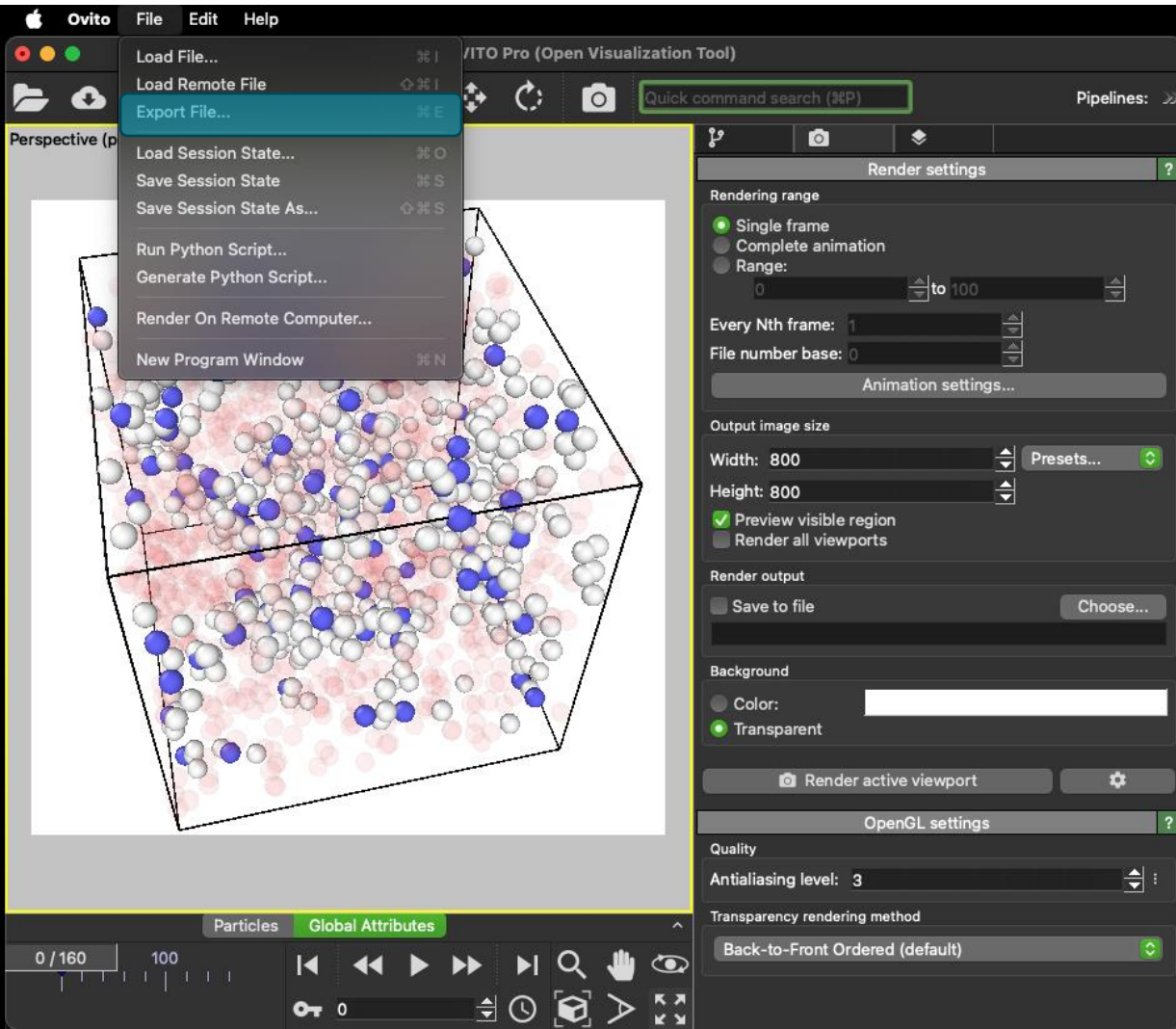
# LJ Fluid Example

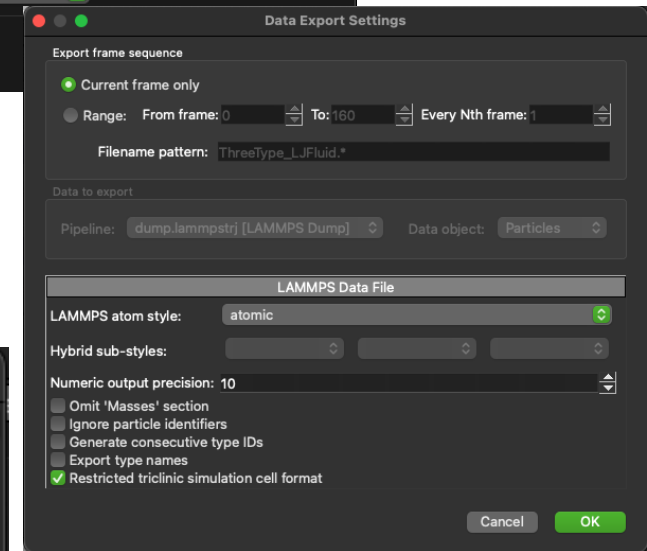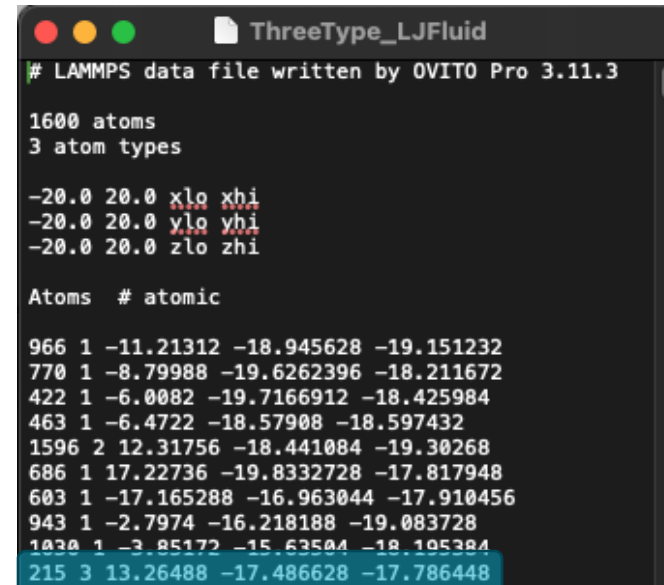Move over to the Rendering tab



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

# Exporting Structures



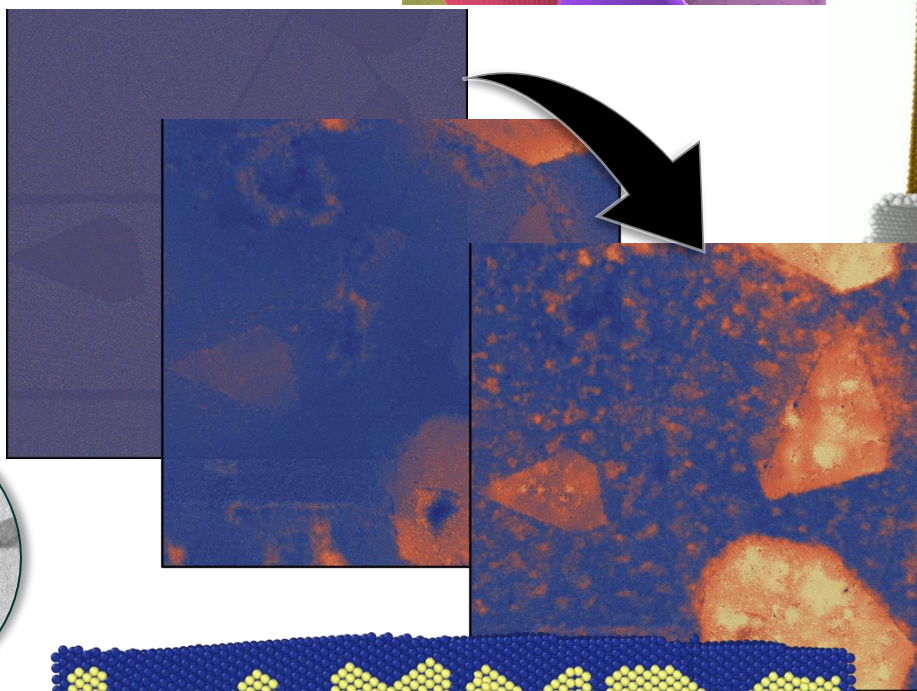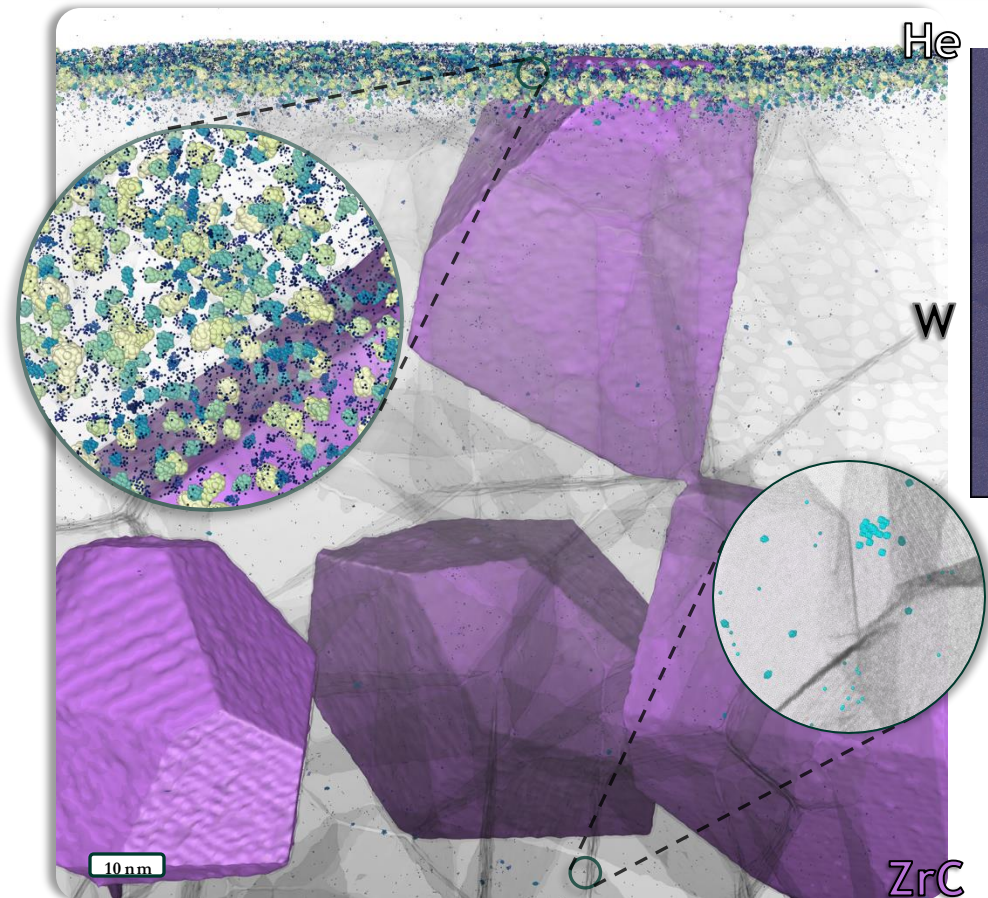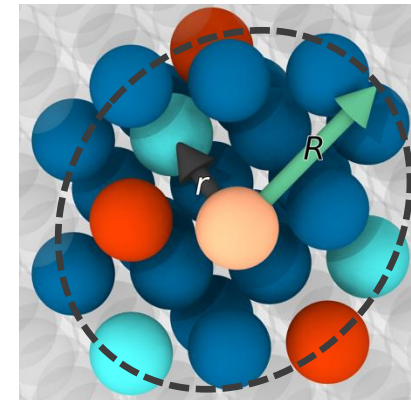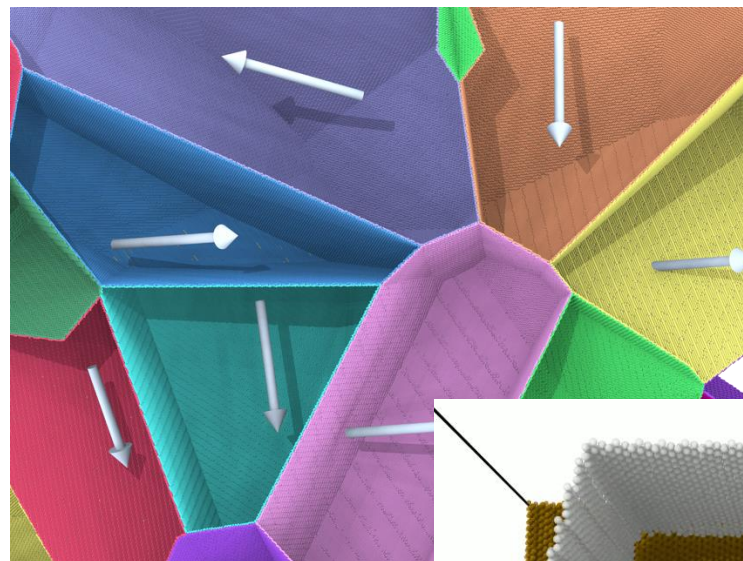Any modifications made will be reflected in the new data file

PMMA Short Chains, lambda = 24nm        Up = 2.25 km/s, SFac = 1.0        Time 1ps

He

W

ZrC

10 nm

R

r

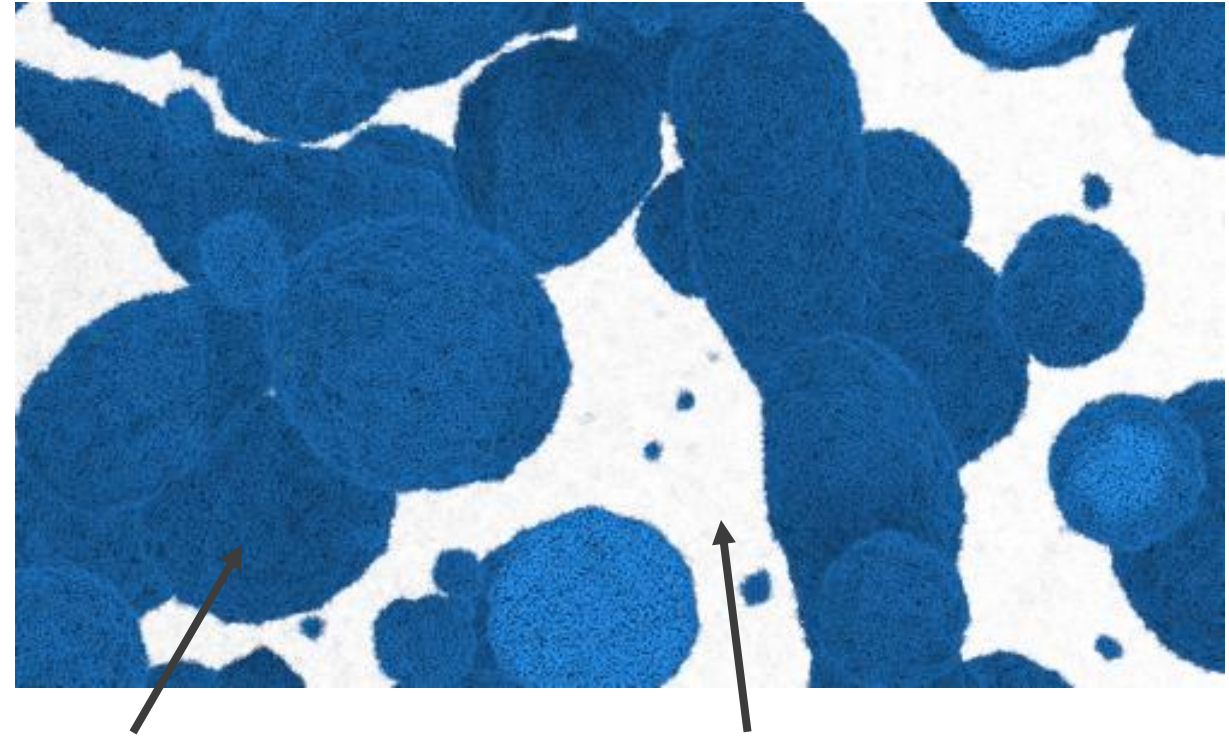[1-10]
[1-12]
[111]

LAMMPS
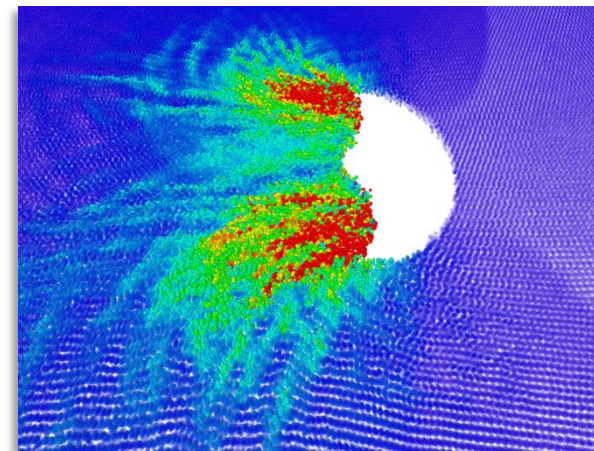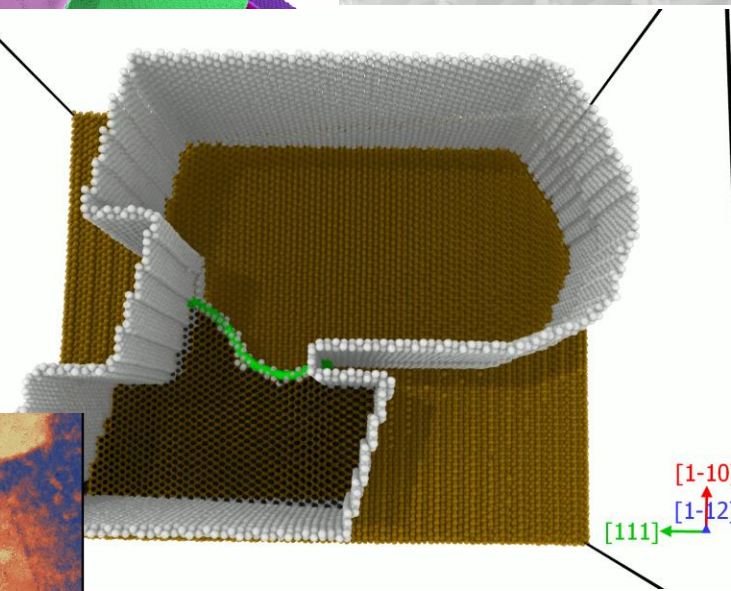
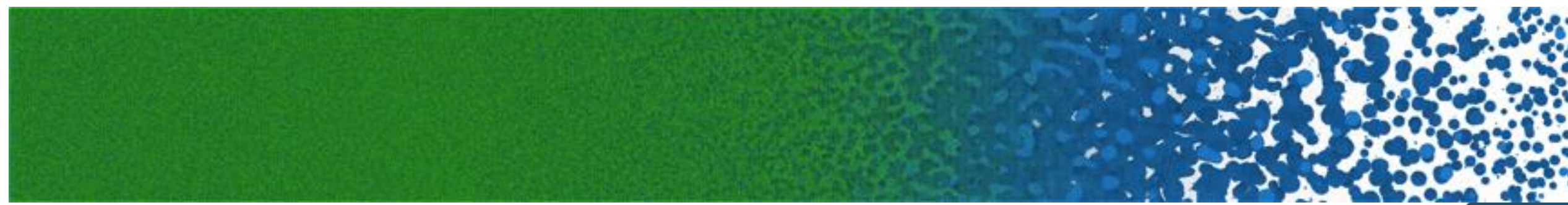# Advanced Features

## 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