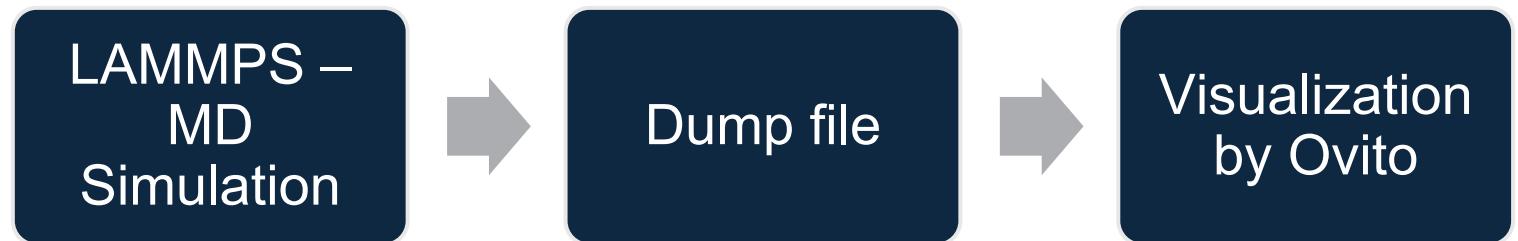


OVITO

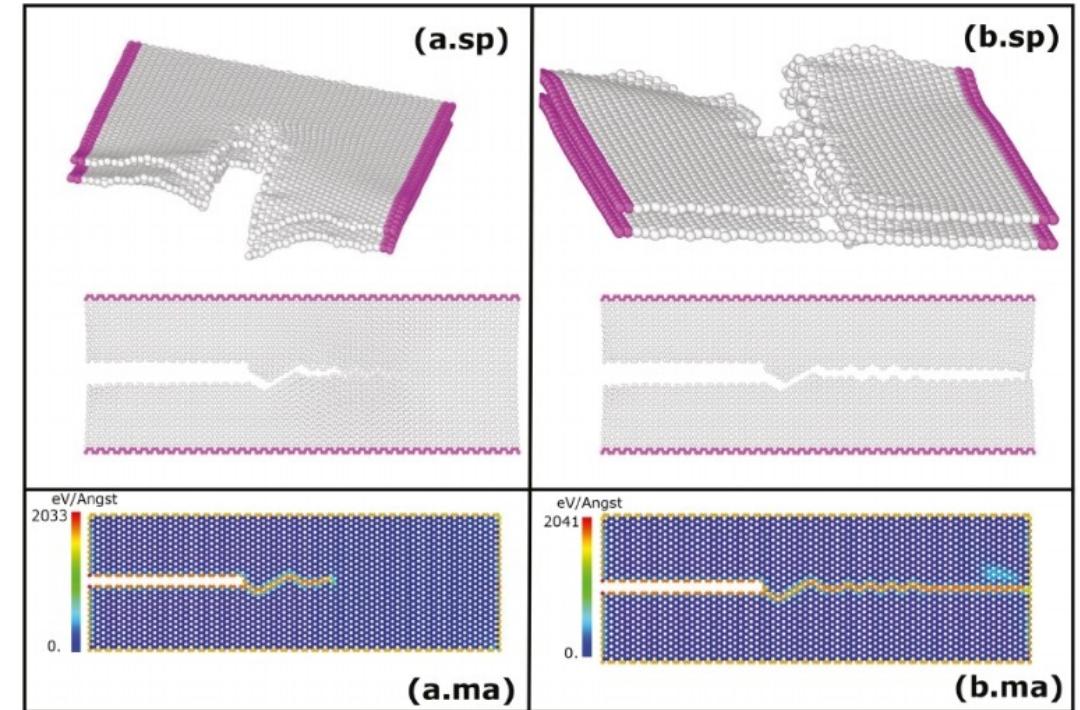
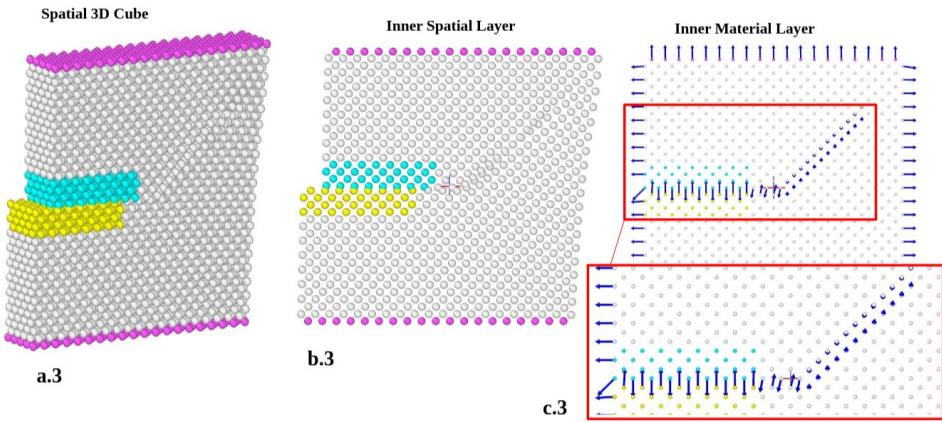


The Open Visualization Tool

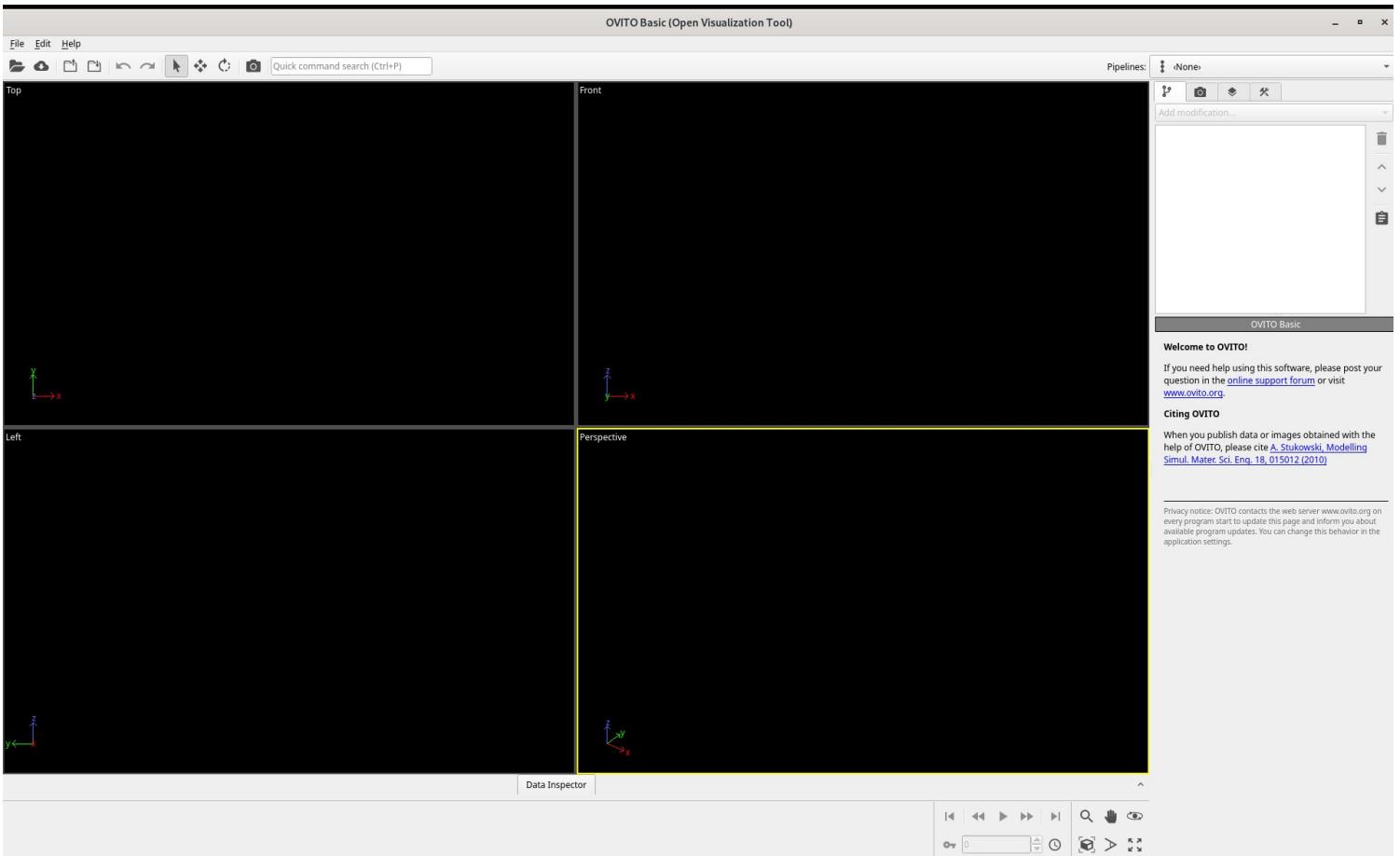
<https://www.ovito.org/>

Main features

- Visualize and explore particle simulations of any kind and size. From ab initio to large-scale models with 100M+ atoms or particles.
- Many features are available free of charge under an open source license.
- Additional analysis, visualization, and automation functions are available on OVITO Pro version.
- <https://www.ovito.org/> is the home- page of software, it includes user-friendly installation steps.



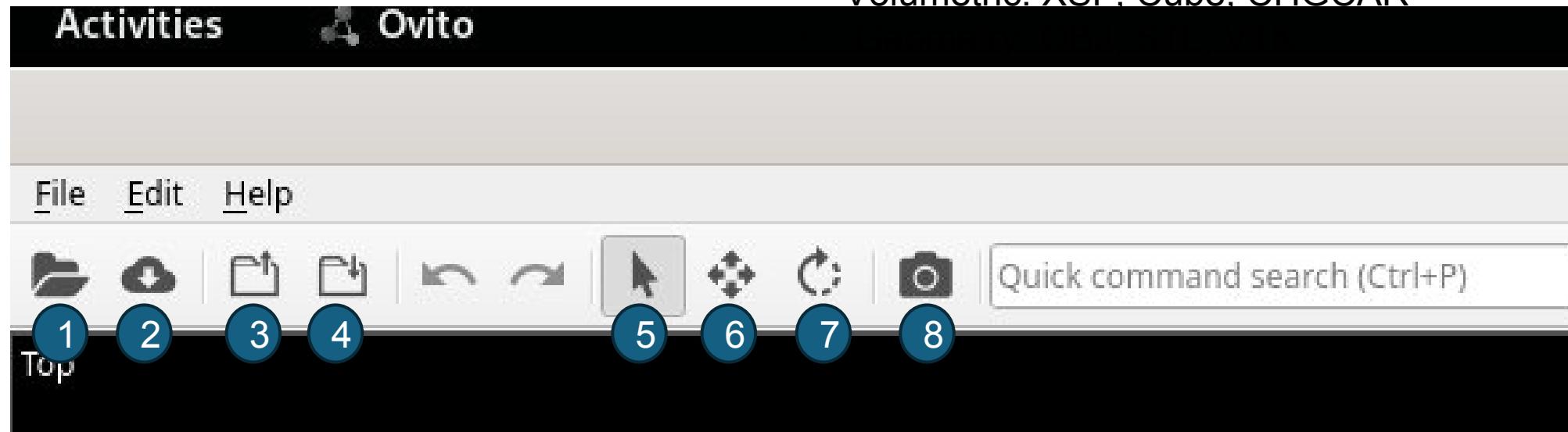
Introduction to GUI



Data Input/Output

Supported input file formats

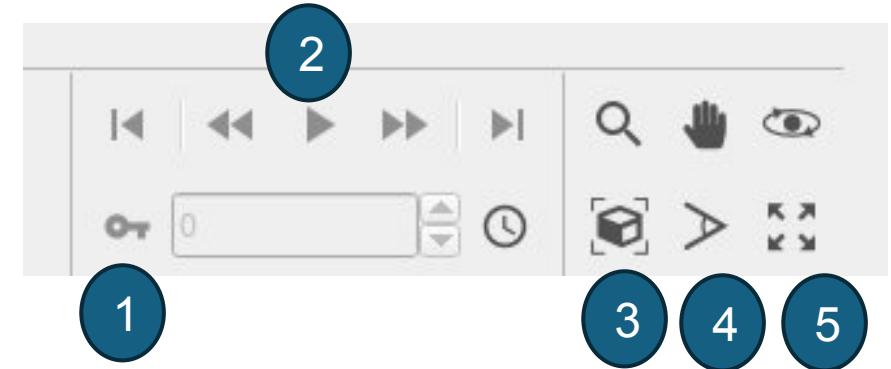
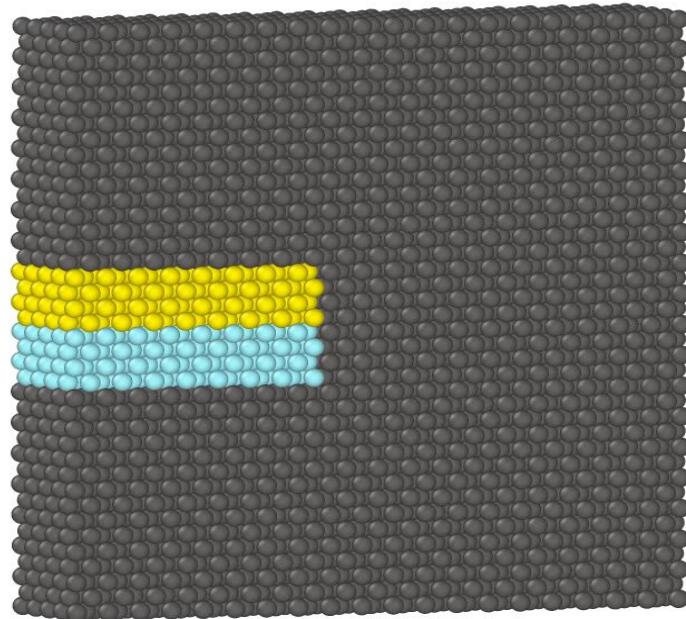
- XYZ (basic and extended variants)
- NetCDF (written with ‘dump netcdf’ command)
- CFG, GSD/HOOMD, IMD, PDB, GALAMOST, DL_POLY
- Ab initio codes: POSCAR, FHI-aims, QE, CASTEP
- Volumetric: XSF, Cube, CHGCAR



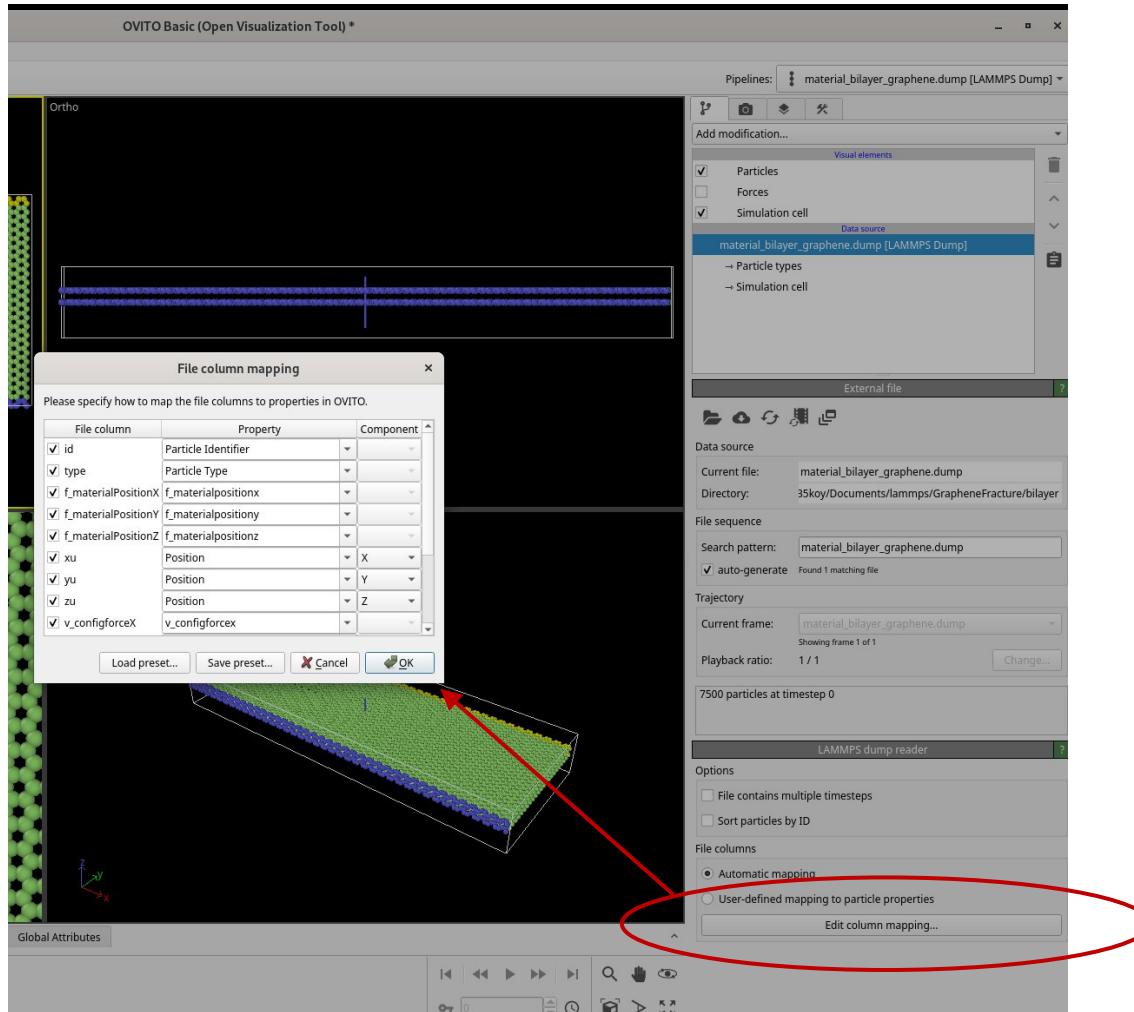
1. Load a file from local machine
2. Load a file from remote machine using OpenSSH
3. Save the current session
4. Load the saved session
5. Make mouse left-click button to Select
6. Make mouse left-click button to Move
7. Make mouse left-click button to Rotate
8. Render active view-point

Movie and Zoom

1. Enter frame number
2. Play all frames as multiple files can be loaded at once and make a movie from it
3. Fit view
4. Adjust zoom
5. See one view-panel, re-click to exit



Customized file mapping



Visualization elements

Visual elements are *graphical representations of data*.

Particles, Bonds, Vector arrows, Simulation cell, Surface meshes, Polyhedra Trajectory lines, Dislocation lines, ...

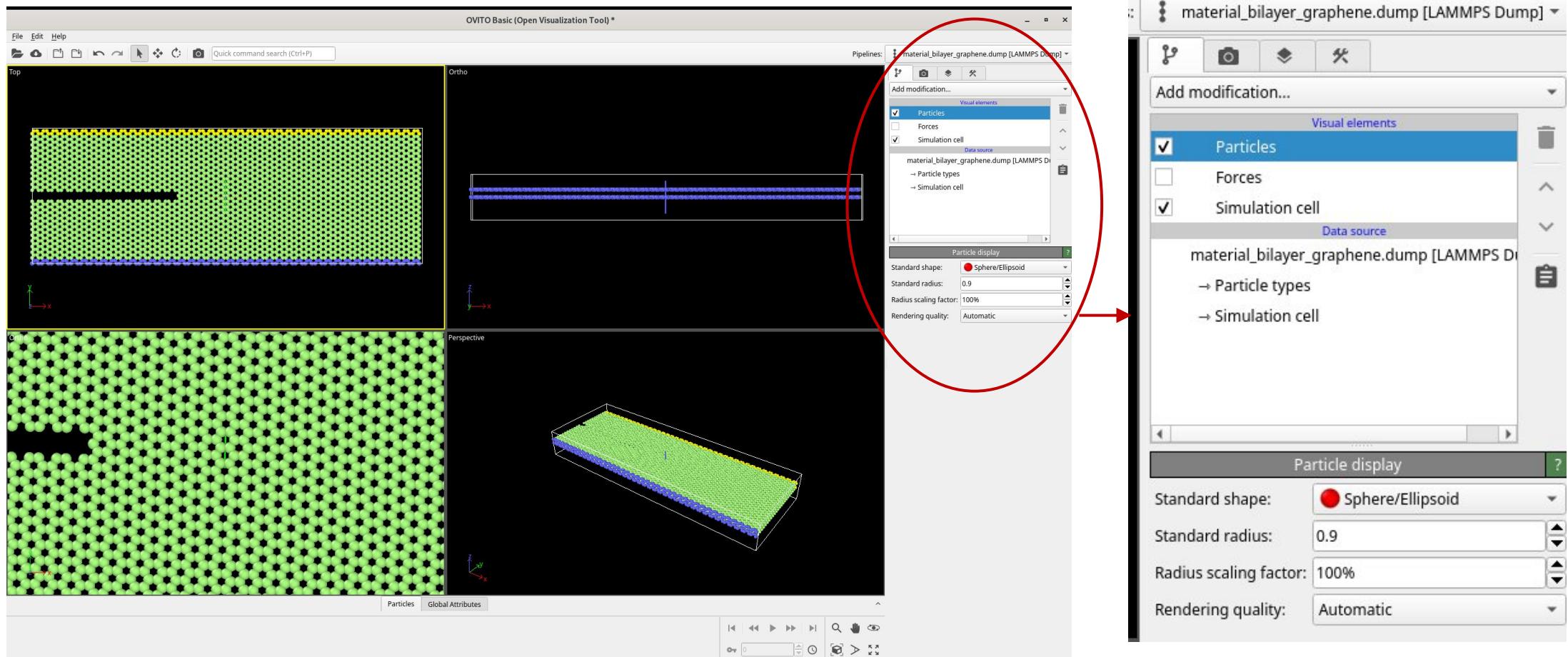


Image Export

OVITO Basic (Open Visualization Tool) *

Pipelines: material_bilayer_graphene.dump [LAMMPS Dump]

File Edit Help

Ortho

Top

Particles

Forces

Simulation cell

Visual elements

Add modification...

Particle display

Standard shape: Sphere/Ellipsoid

Standard radius: 0.9

Radius scaling factor: 100%

Rendering quality: Automatic

Ortho

Perspective

Particles Global Attributes

Render settings

Pipelines: material_bilayer_graphene.dump [LAMMPS Dump]

Single frame

Complete animation

Range:

0 to 100

Every Nth frame: 1

File number base: 0

Animation settings...

Output image size

Width: 640 Presets...

Height: 480

Preview visible region

Render all viewports (OVITO Pro)

Render output

Save to file Choose...

Background

Color:

Transparent

Render active viewport Switch renderer...

OpenGL settings

Quality

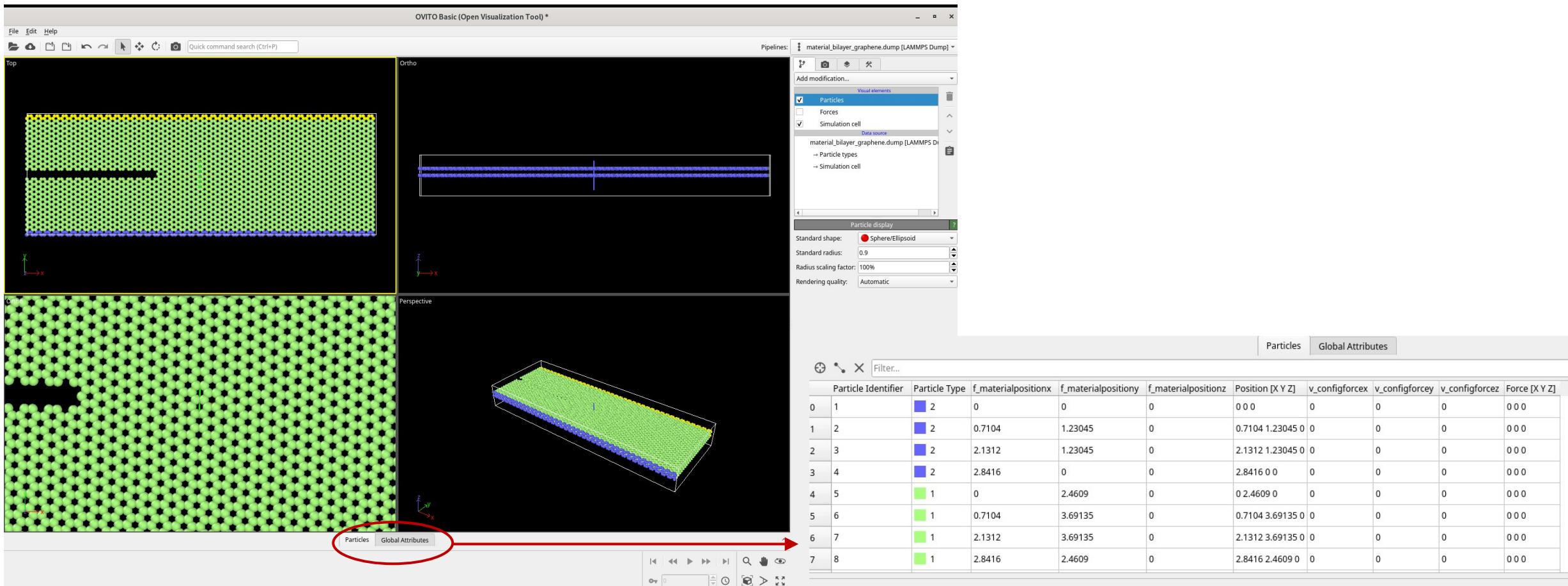
Antialiasing level: 3

Transparency rendering method

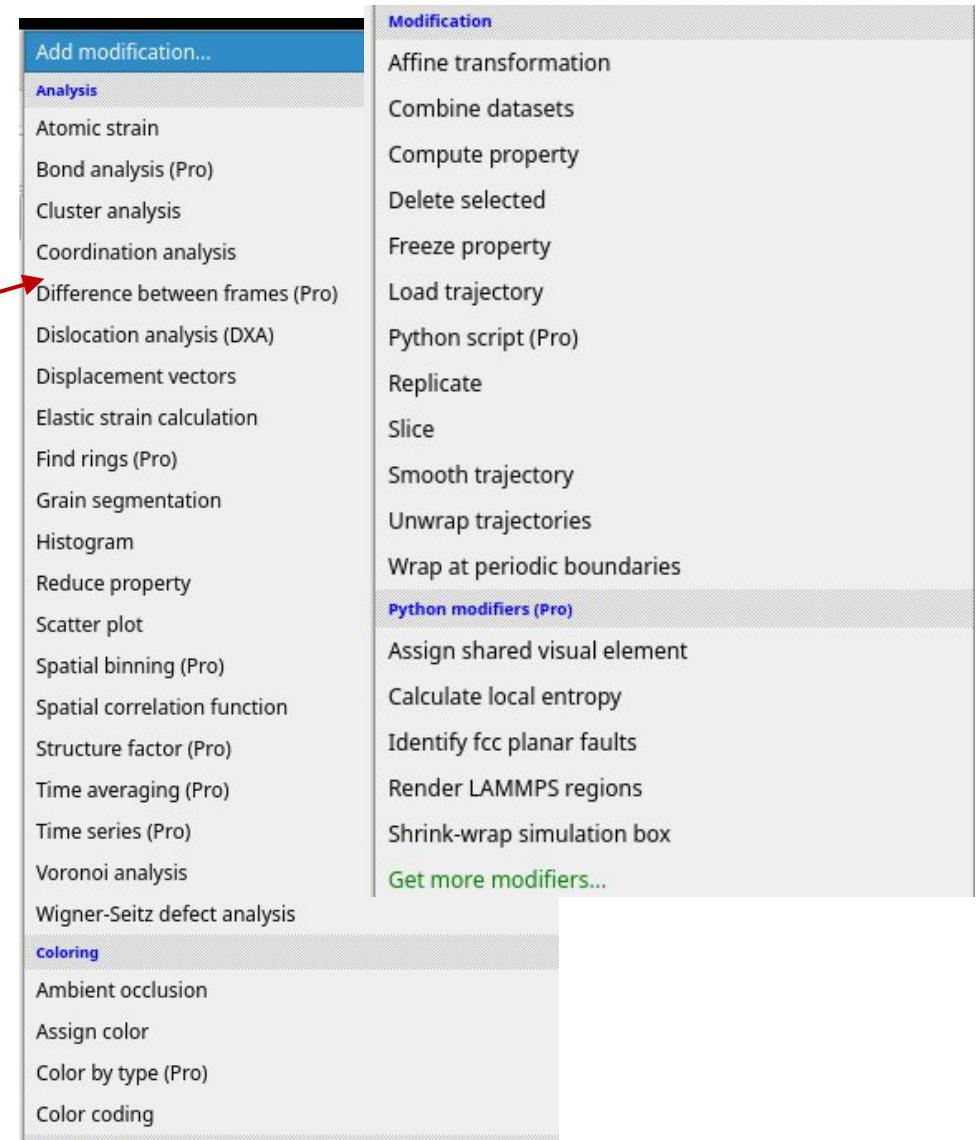
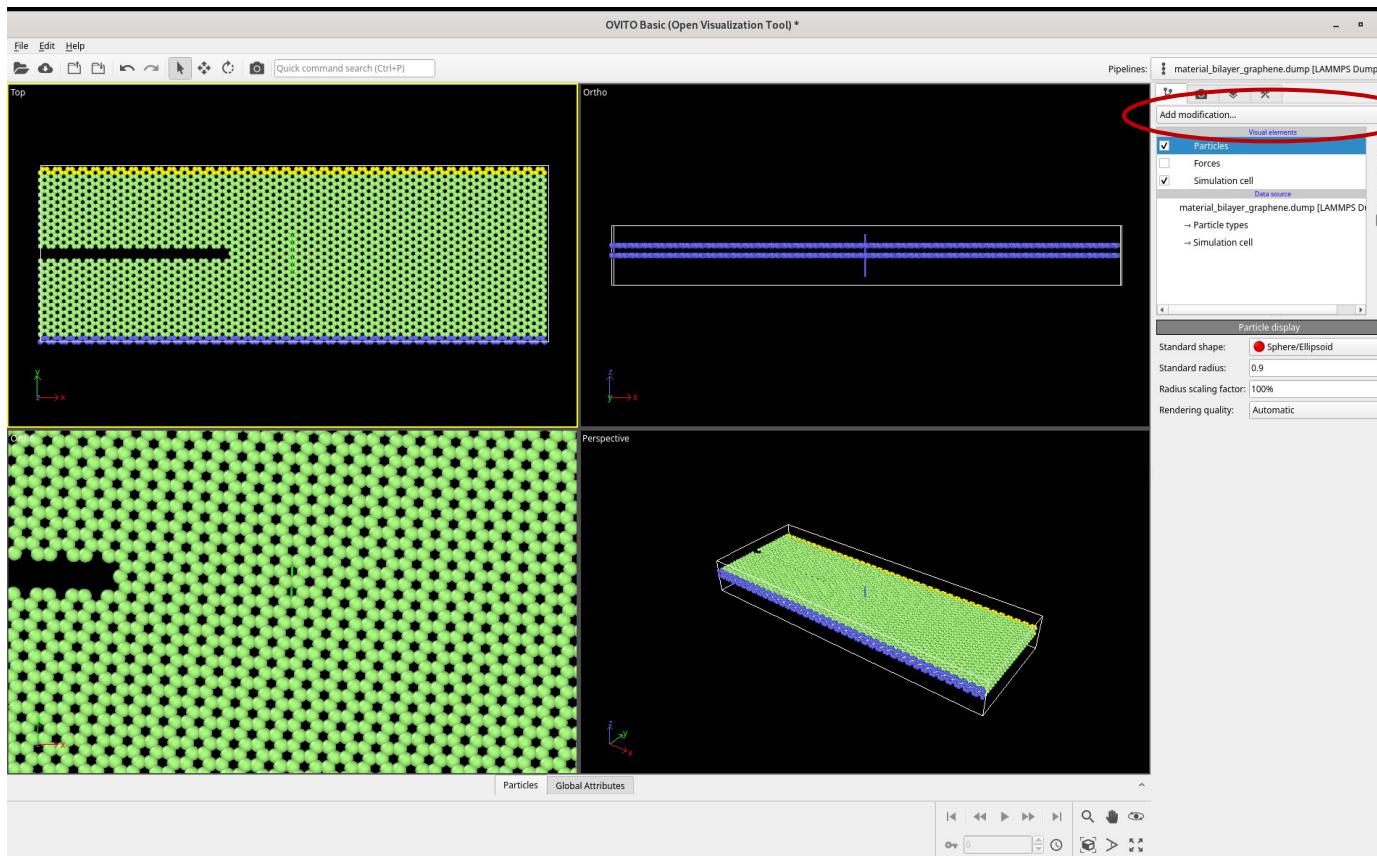
Back-to-Front Ordered (default)

A screenshot of the OVITO Basic visualization tool. The main window displays a simulation of a bilayer graphene structure. The Ortho and Top viewports show the top and side cross-sections of the bilayer, respectively, with particles represented as green spheres. The Perspective viewport shows the 3D structure of the bilayer. The Pipeline panel on the right lists the data source 'material_bilayer_graphene.dump [LAMMPS Dump]' and visual elements like 'Particles' and 'Simulation cell'. The Render settings panel on the far right contains options for rendering a single frame, complete animation, or a range of frames (0 to 100). It also includes settings for output image size (Width: 640, Height: 480), background color, and transparency rendering method. A red arrow highlights the camera icon in both the Pipeline panel and the Render settings panel.

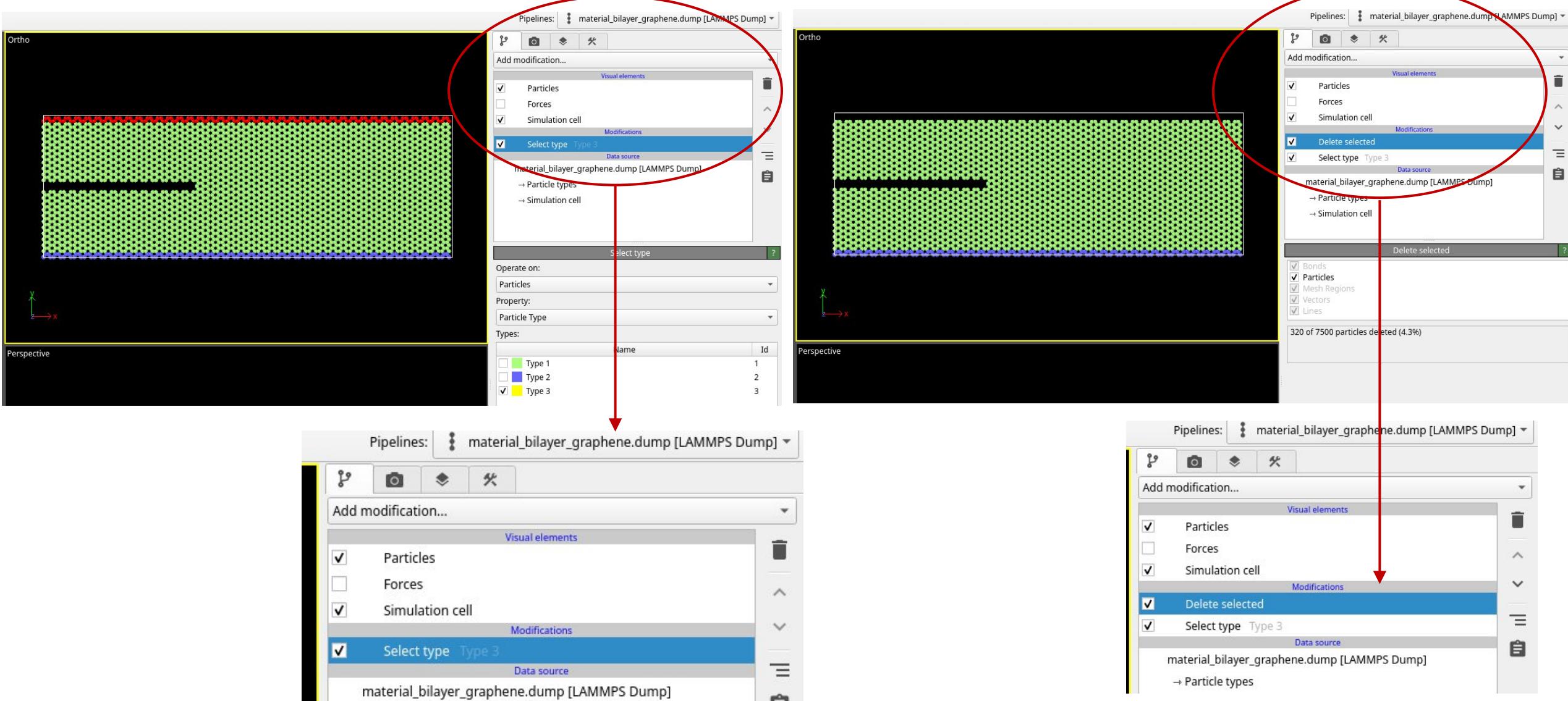
Particles menu



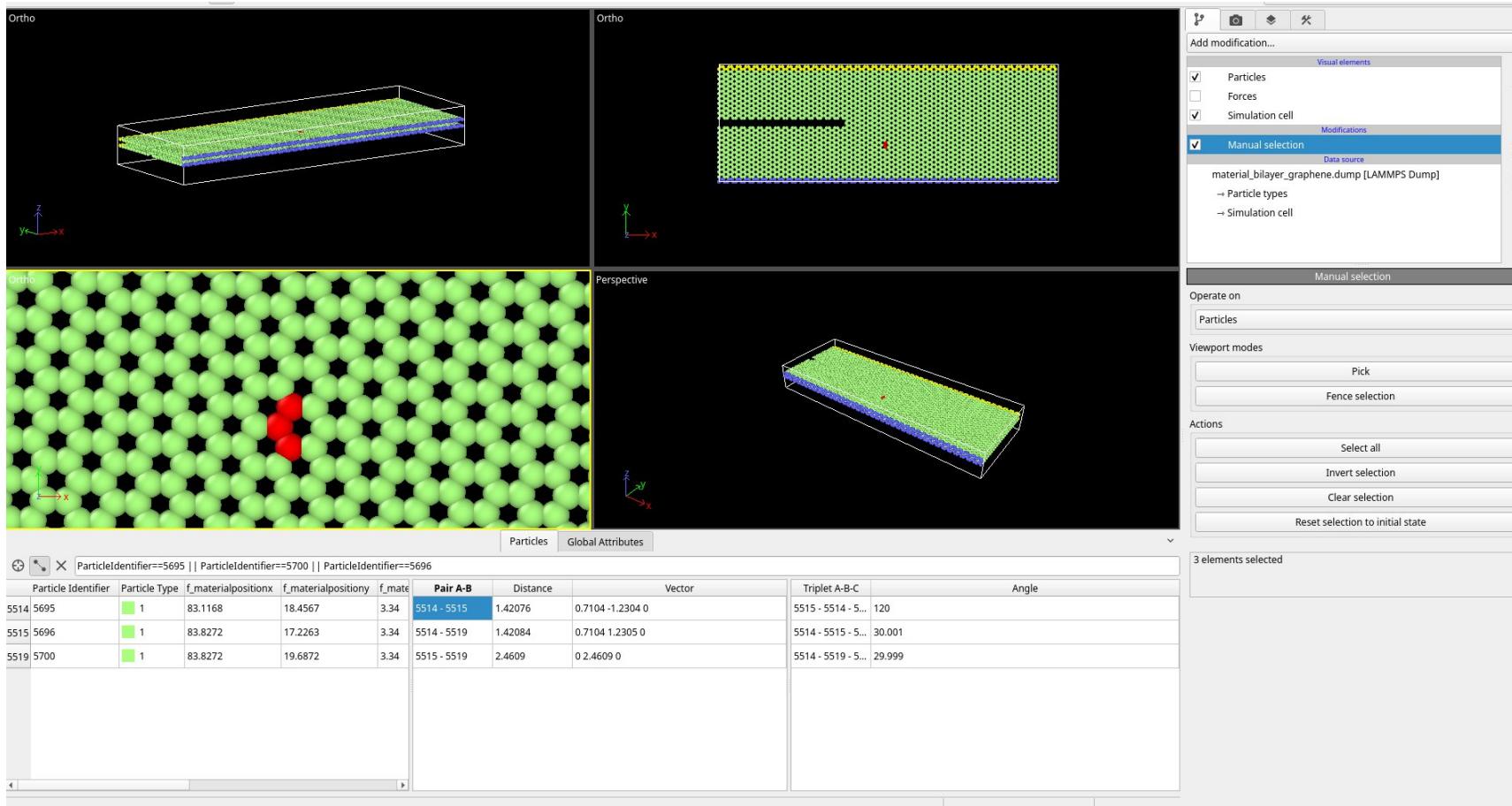
Modifier library – Post processing



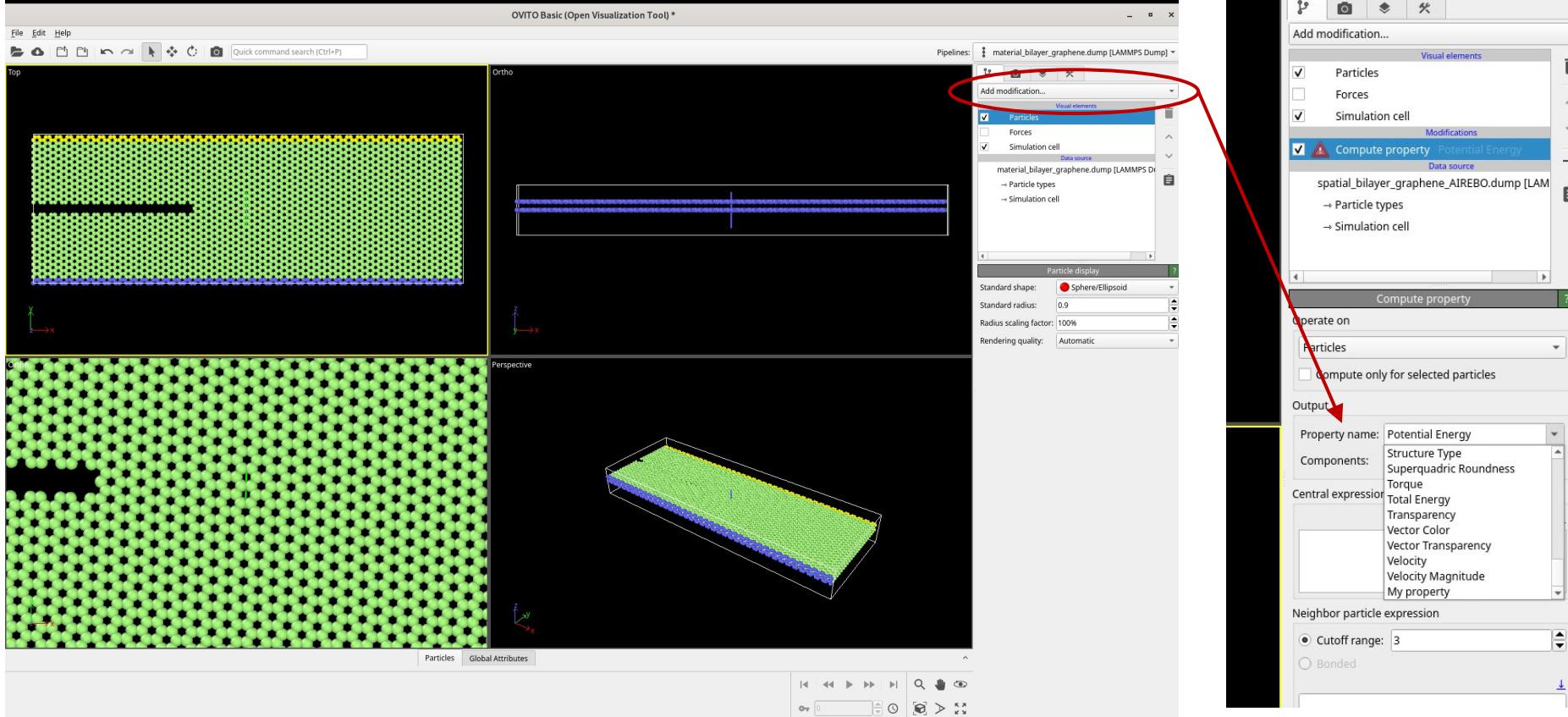
Selection and deletion



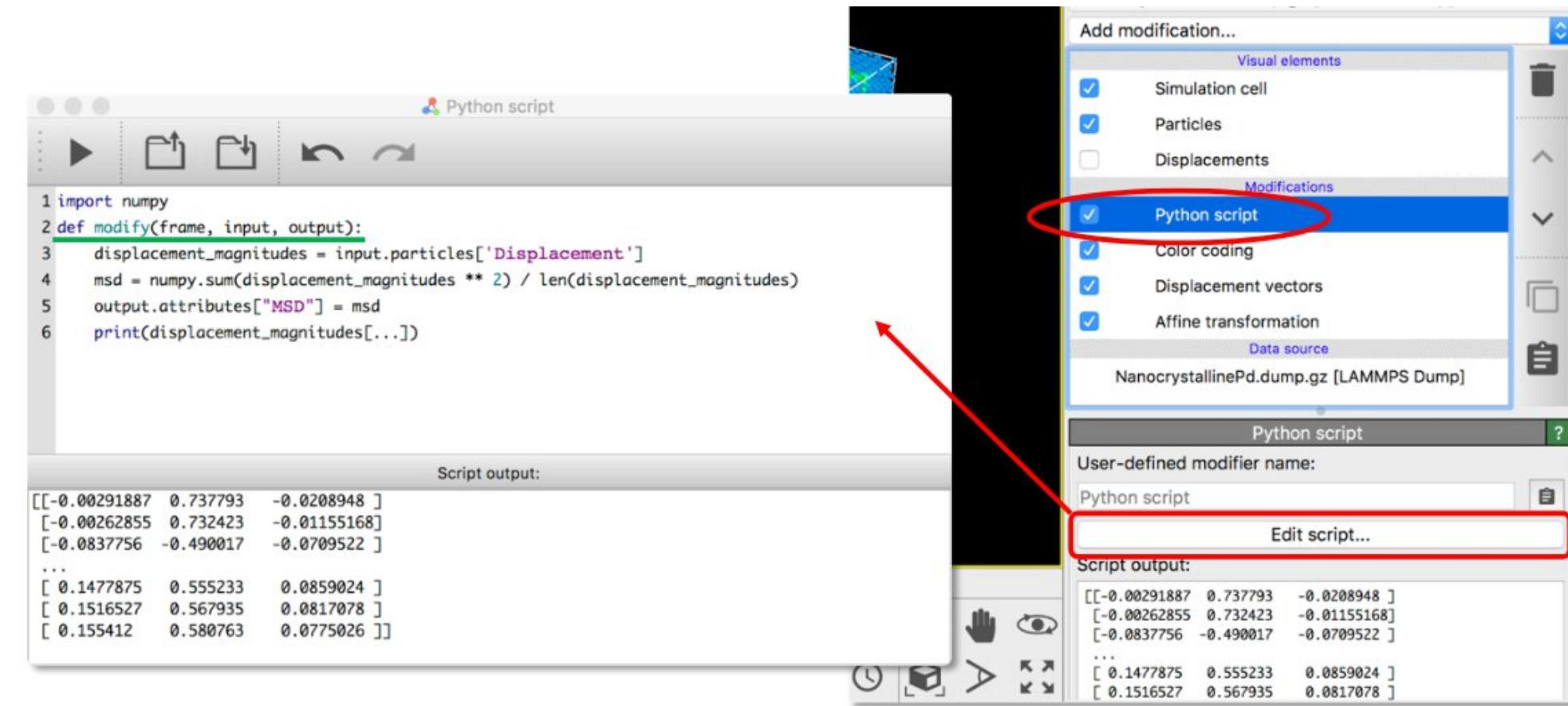
Manual selection – Topology information



Compute Property



Python Script



Calculation of atomistic frequency are done using python script.

