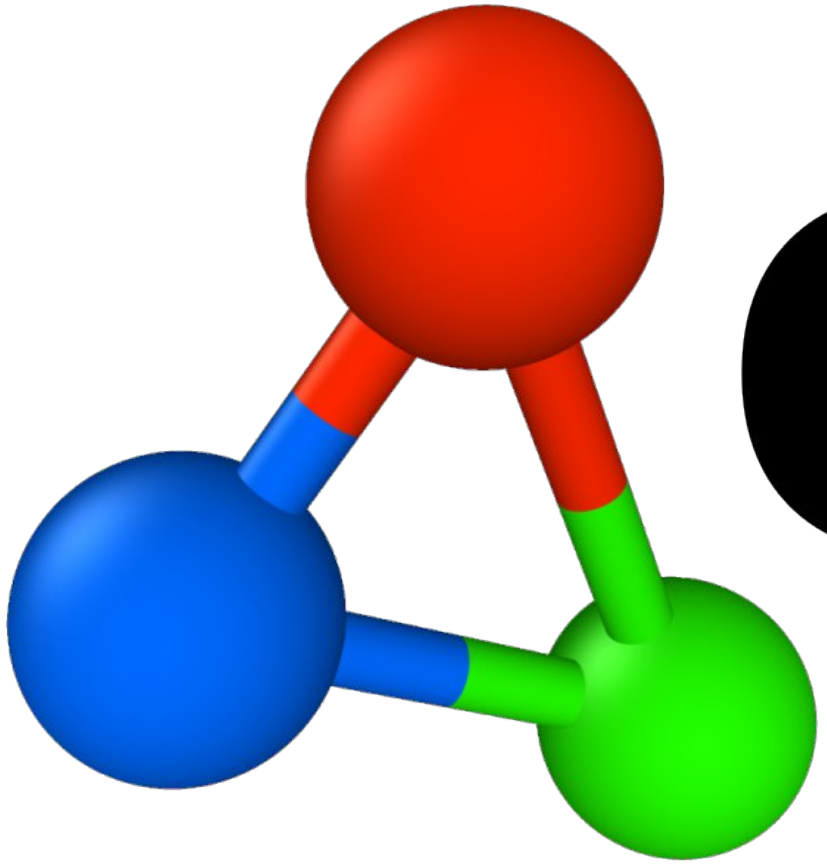


OVITO

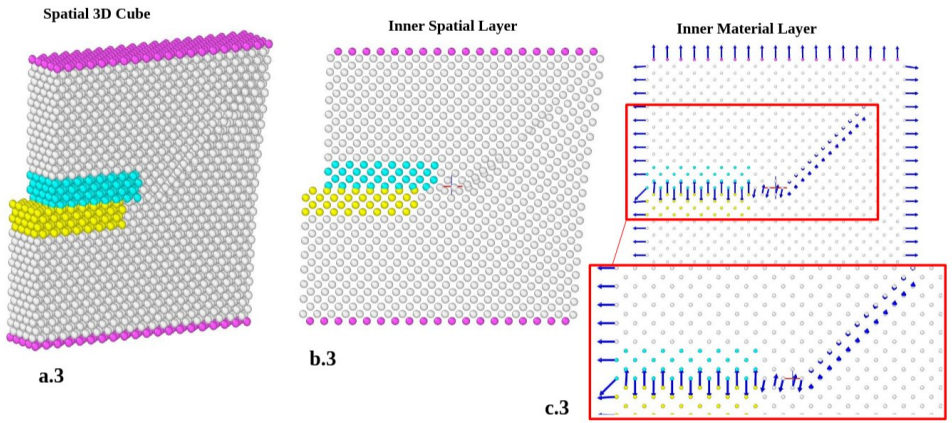
LAMMPS – MD Simulation → Dump file → Visualization by Ovito

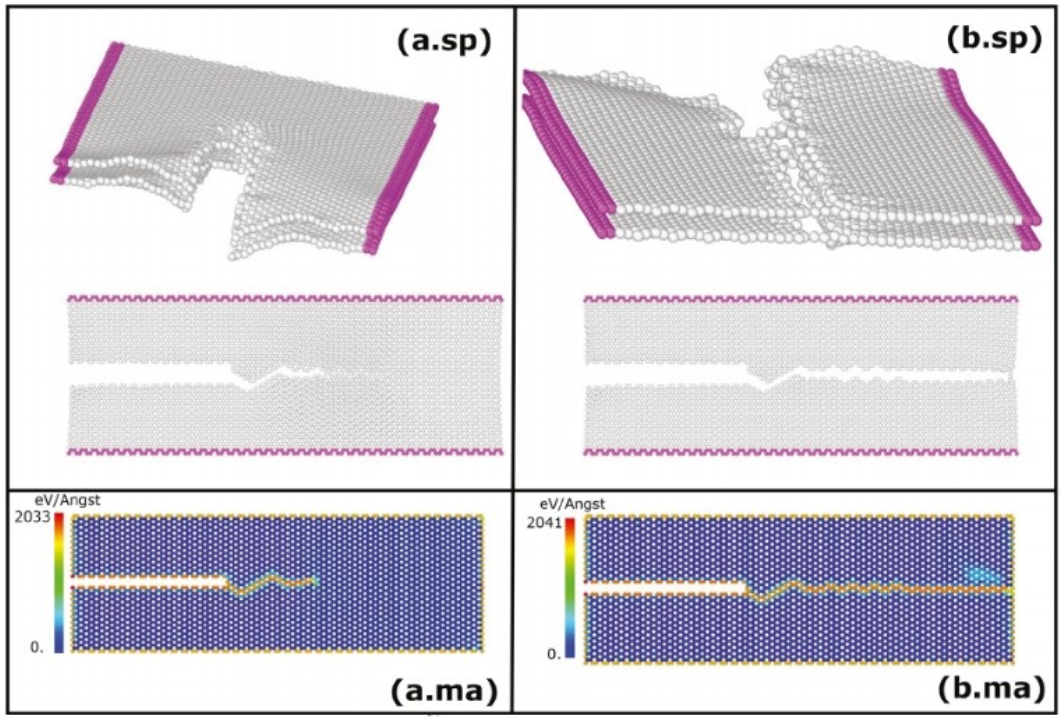
The Open Visualization Tool

https://www.ovito.org/

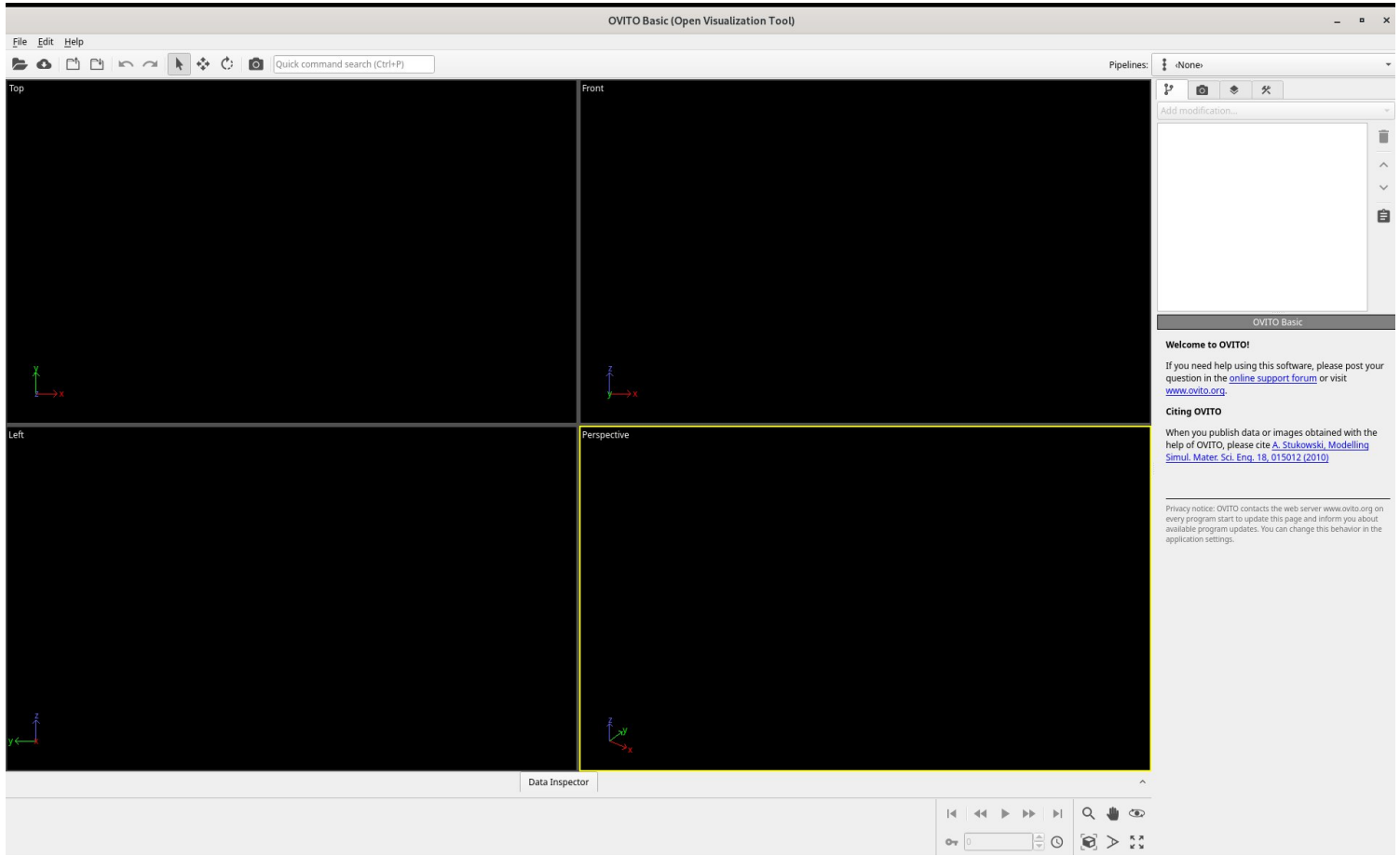
Main features

- 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.


Spatial 3D Cube
Inner Spatial Layer
Inner Material Layer
a.3
b.3
c.3


(a.sp)
(b.sp)
eV/Angst
2033
0.
eV/Angst
2041
0.
(a.ma)
(b.ma)

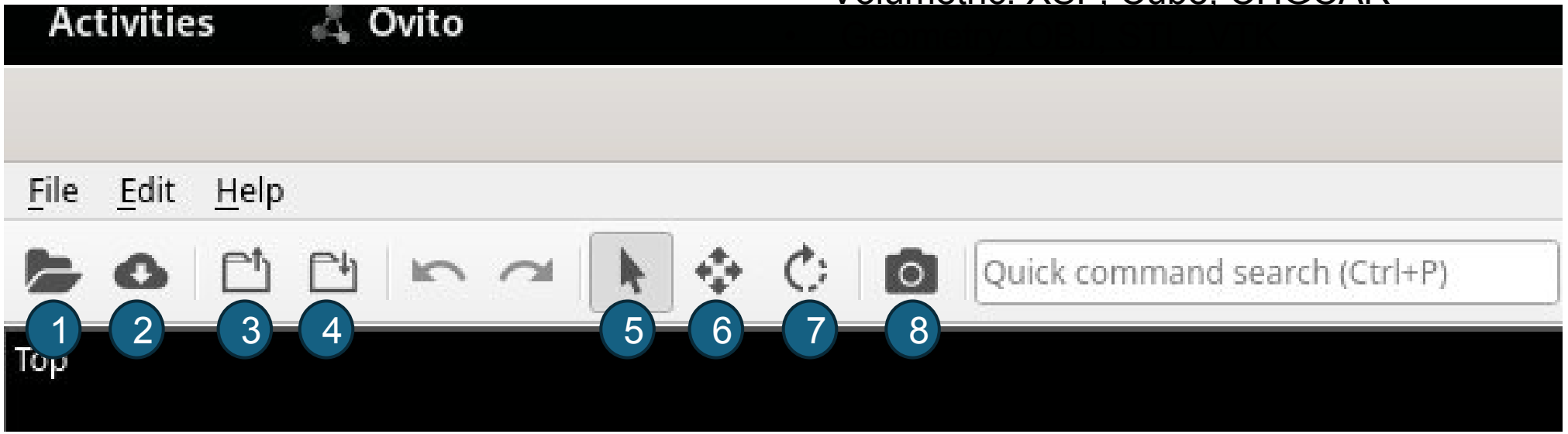
Introduction to GUI



Data Input/Output

Supported input file formats

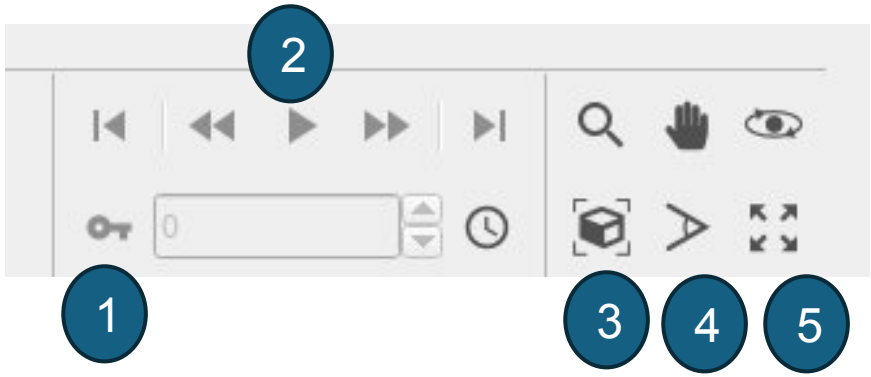
- XYZ (basic and extended variants)
- NetCDF (written with ‘dump netcdf’ command)
- CFG, GSD/HOOMD, IMD, PDB, GALAMOST, DL_POLY
- Ab initio codes: POSCAR, FHI-aims, QE, CASTE
- Volumetric: XSF, Cube, CHGCAR

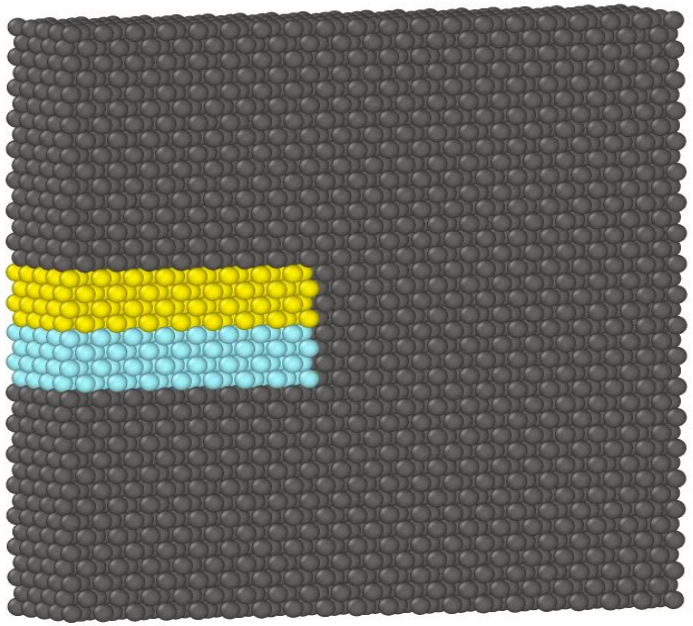


1. Load a file from local machine
2. Load a file from remote machine using OpenSSH
3. Save the current session
4. Load the saved session
5. Make mouse left-click button to Select
6. Make mouse left-click button to Move
7. Make mouse left-click buttoon to Rotate
8. Render active view-point

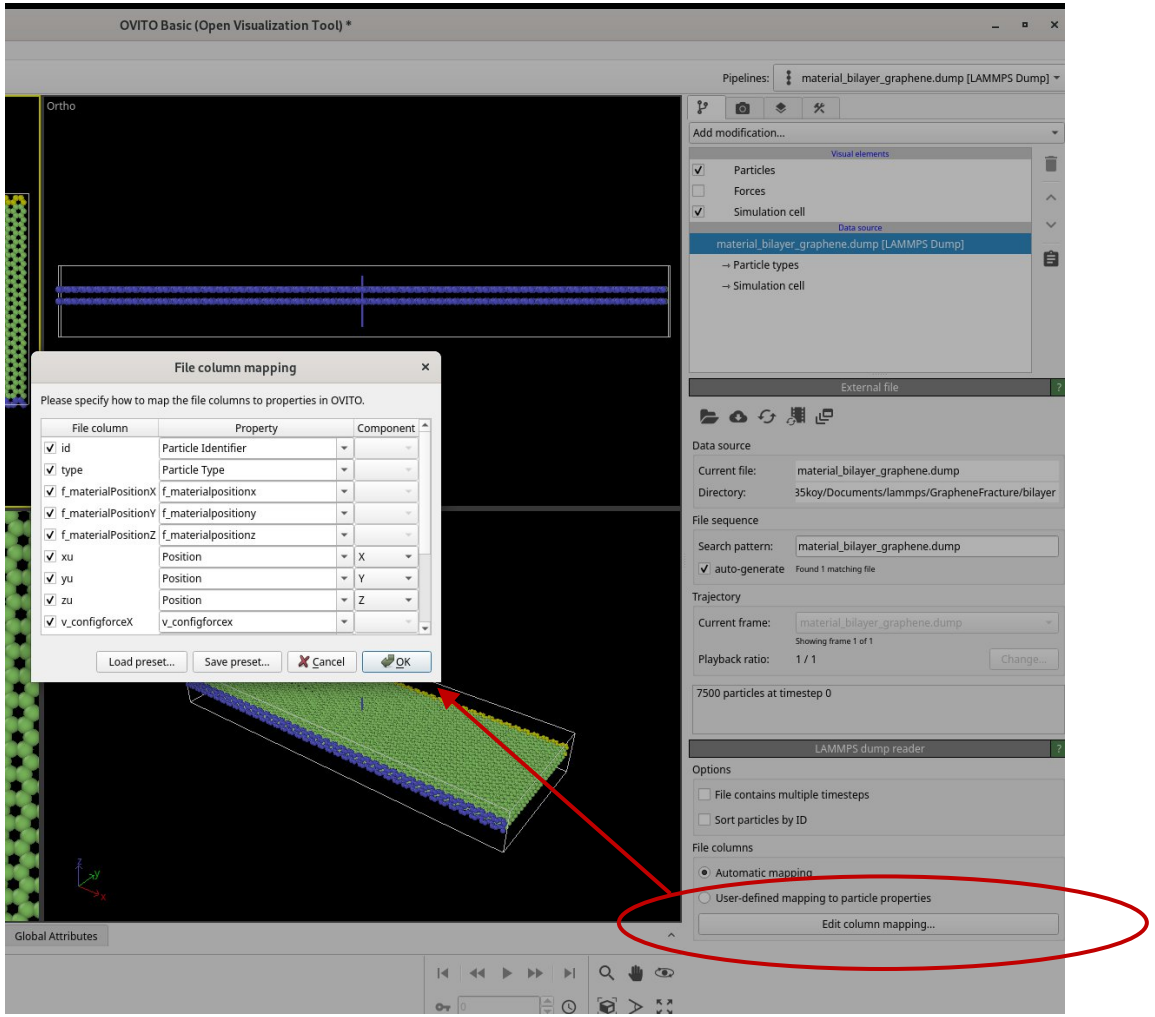
Movie and Zoom

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, ...

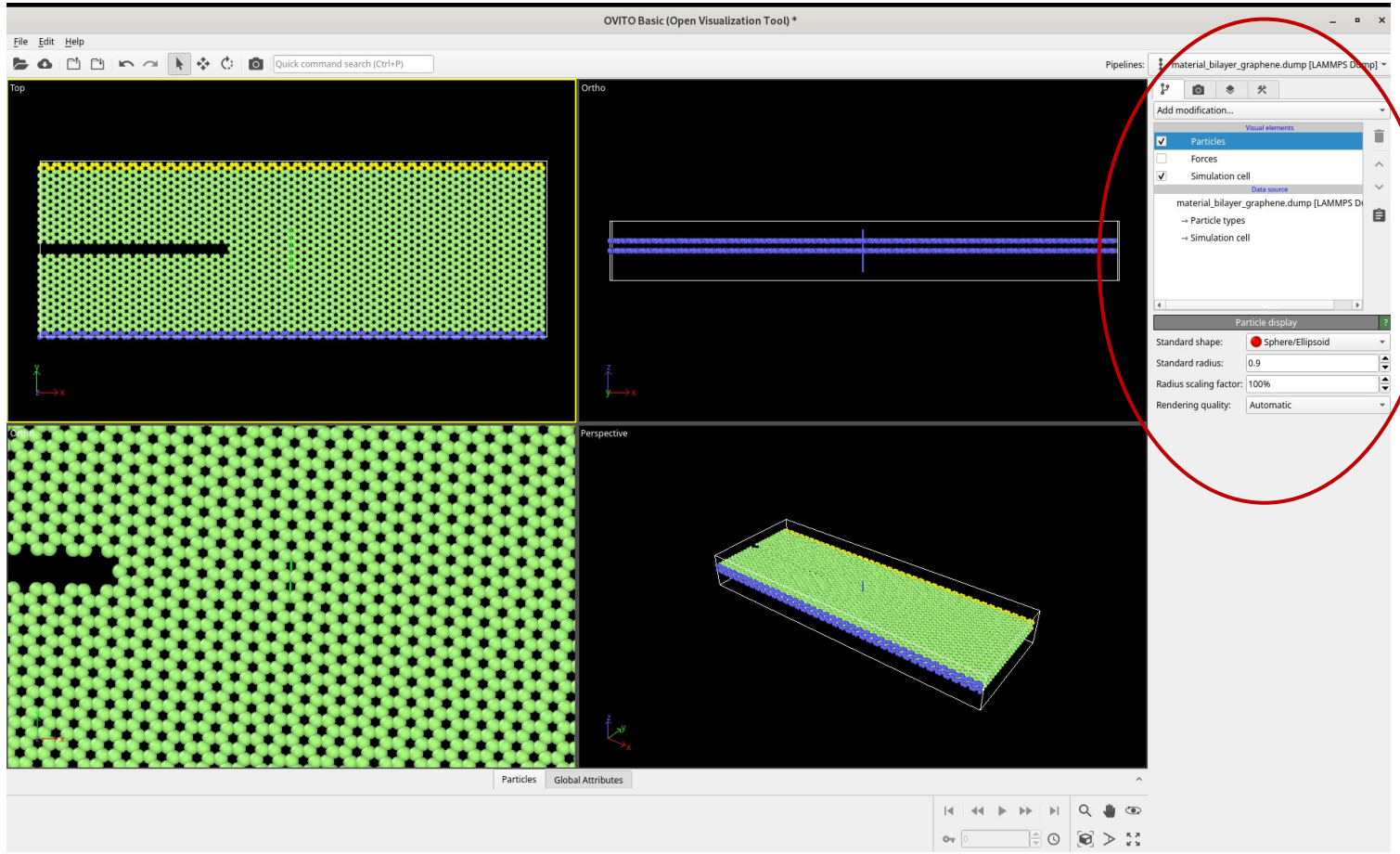
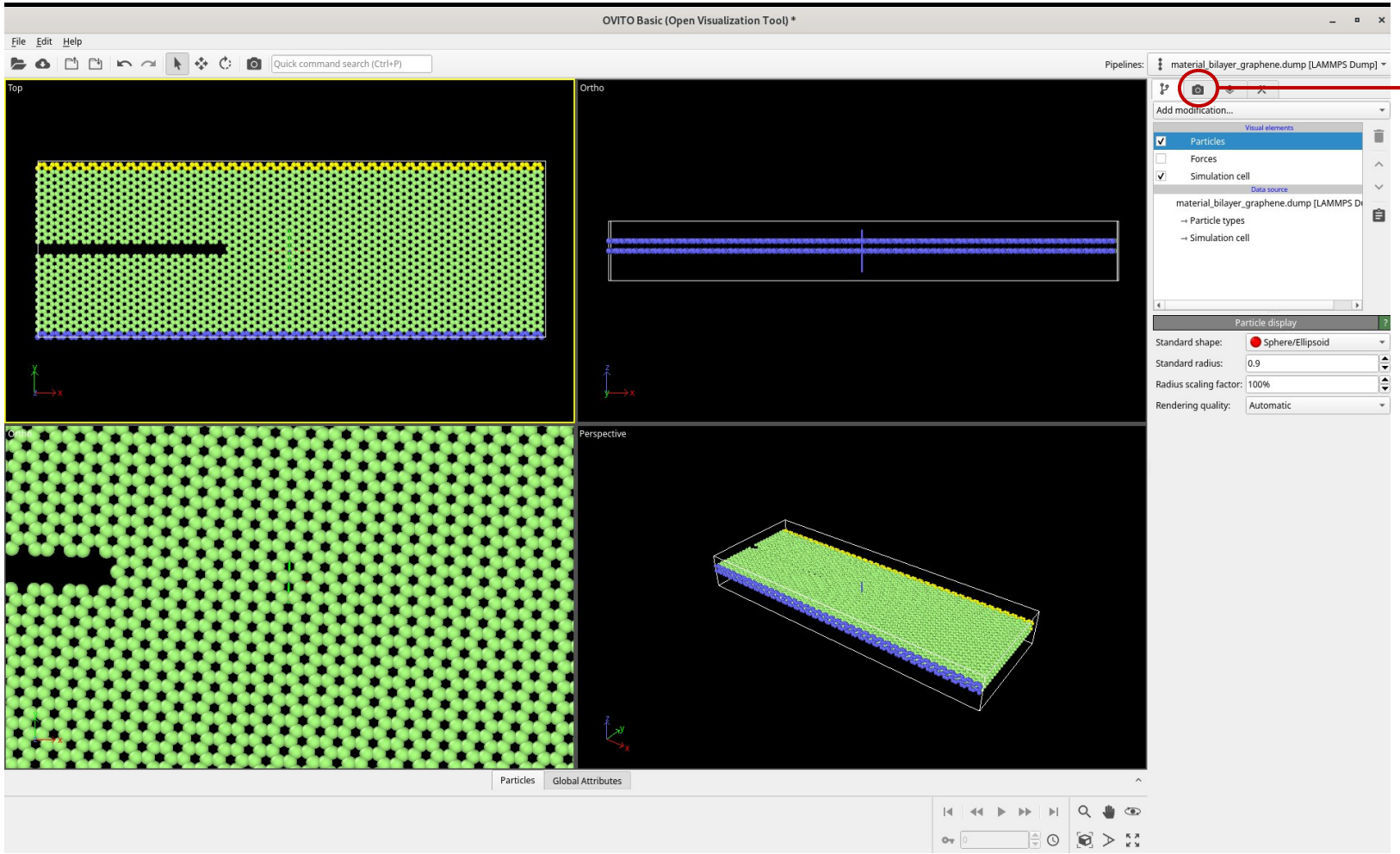
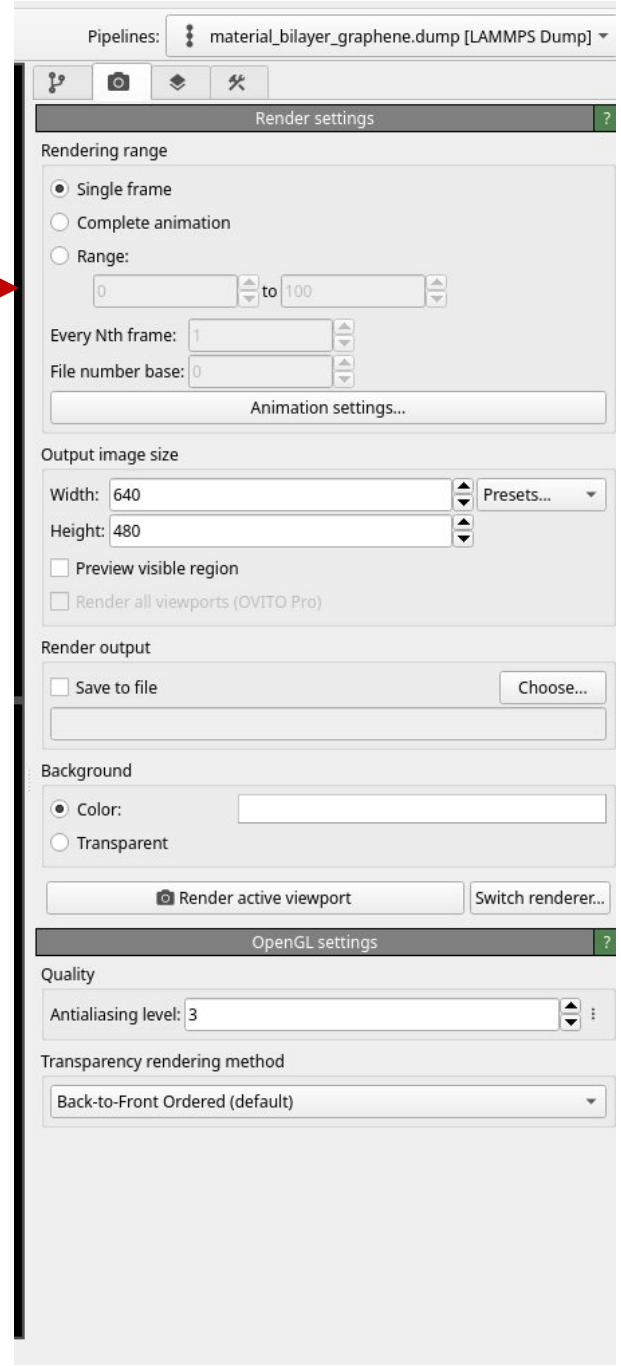
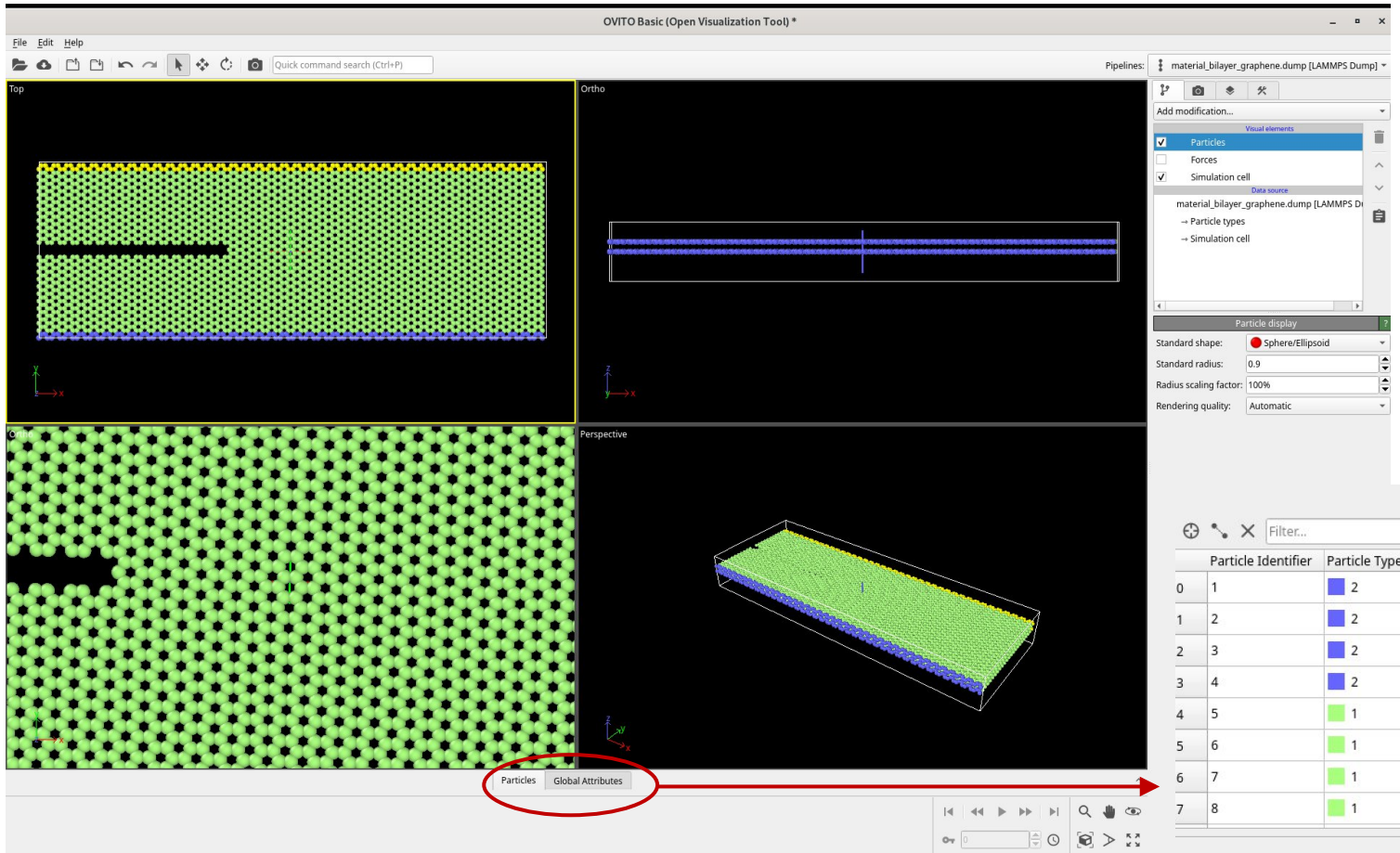


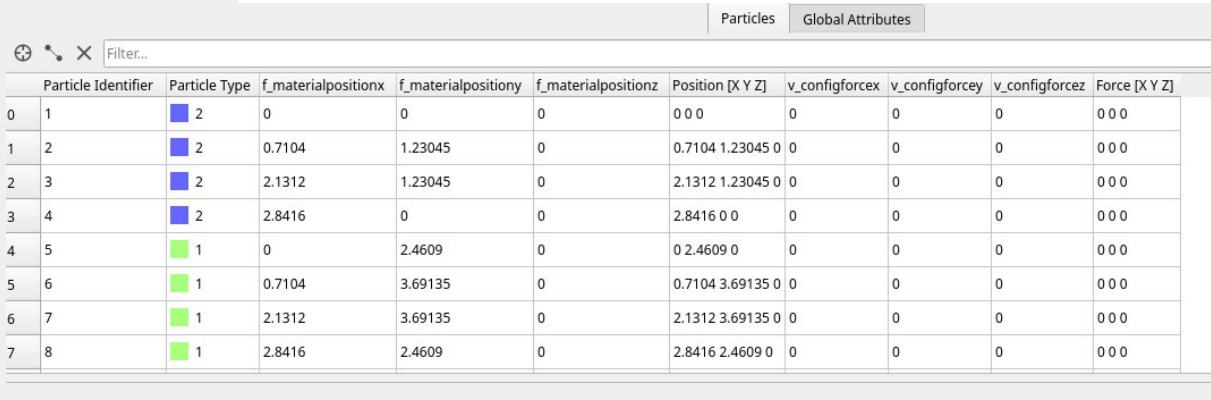
Image Export





Particles menu



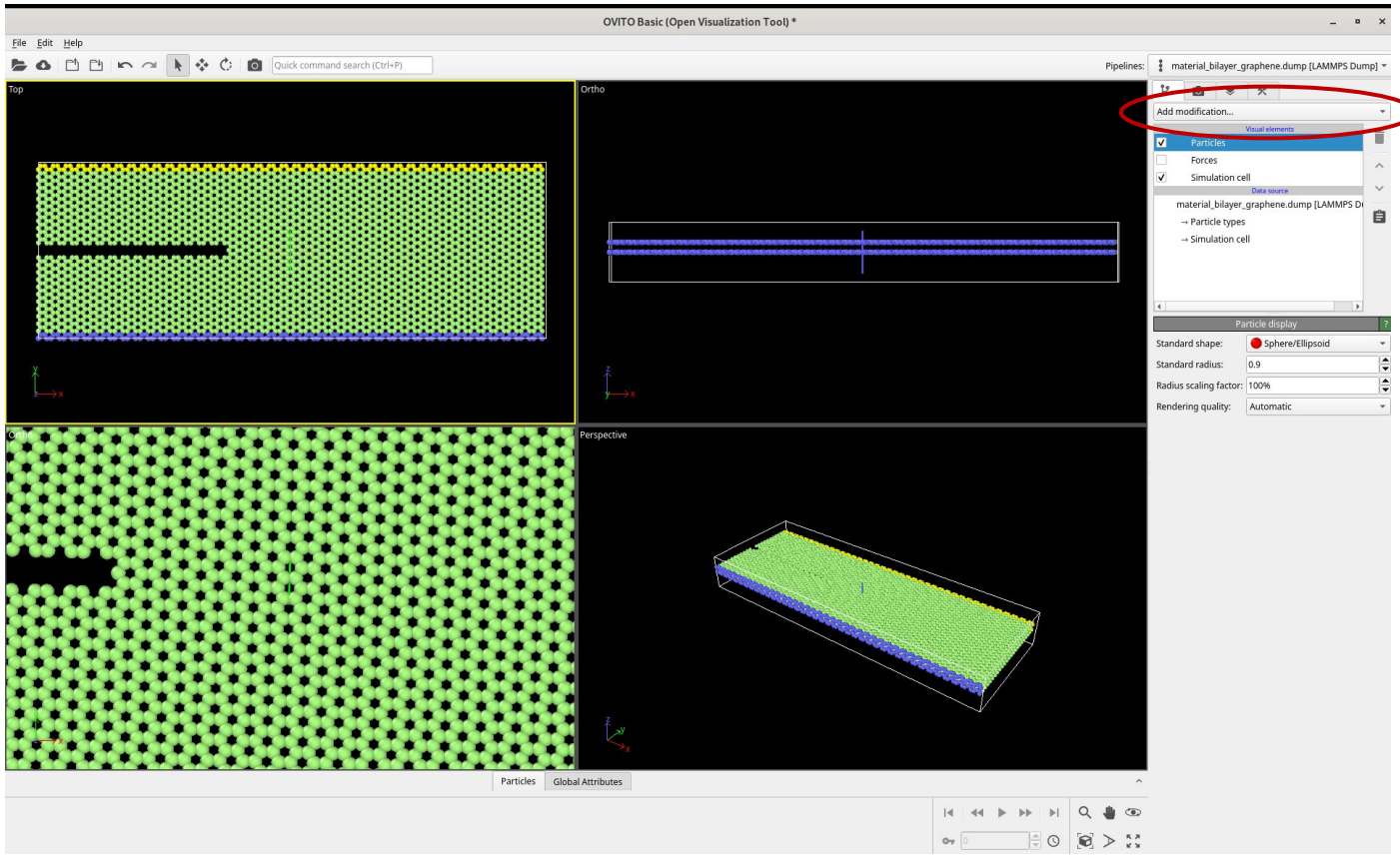


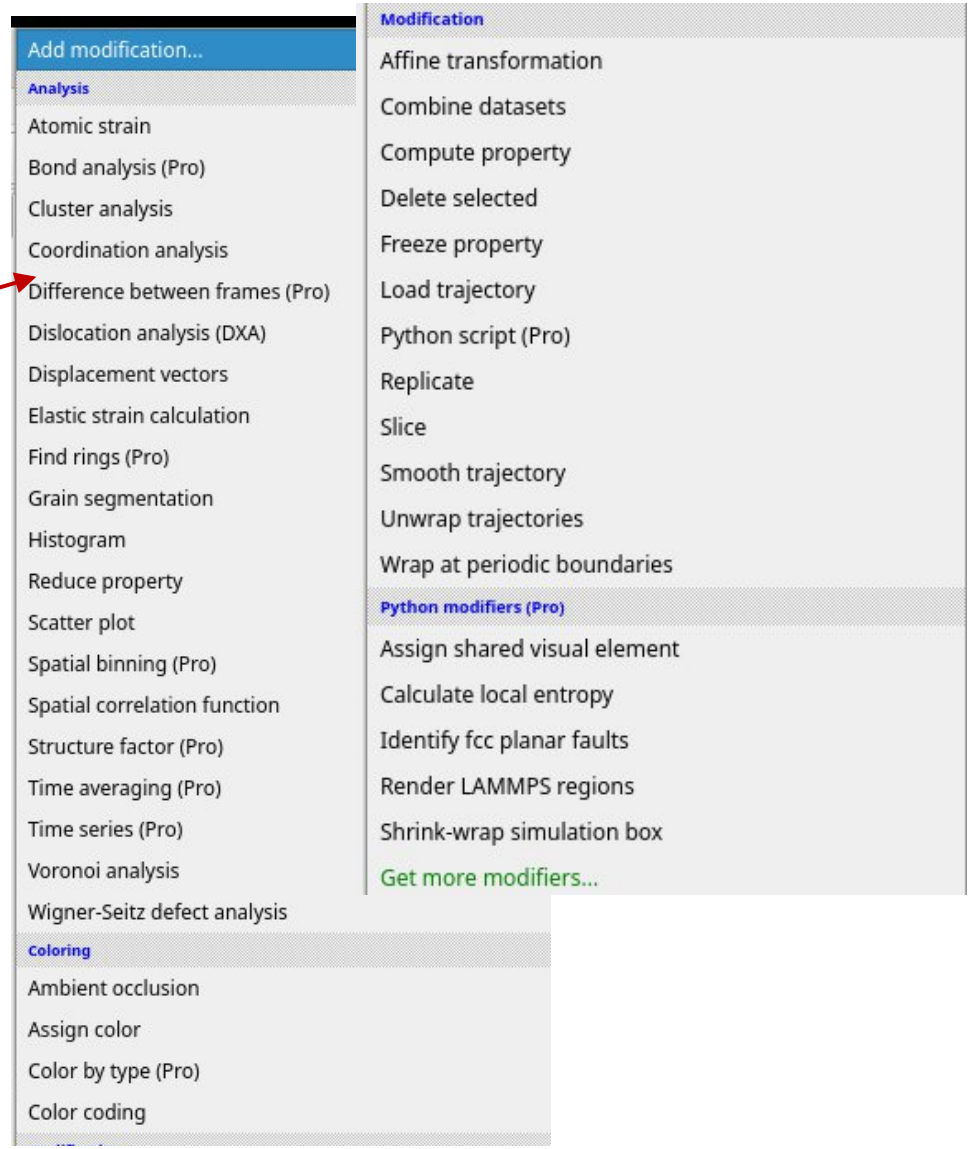
Particles | Global Attributes

Filter...

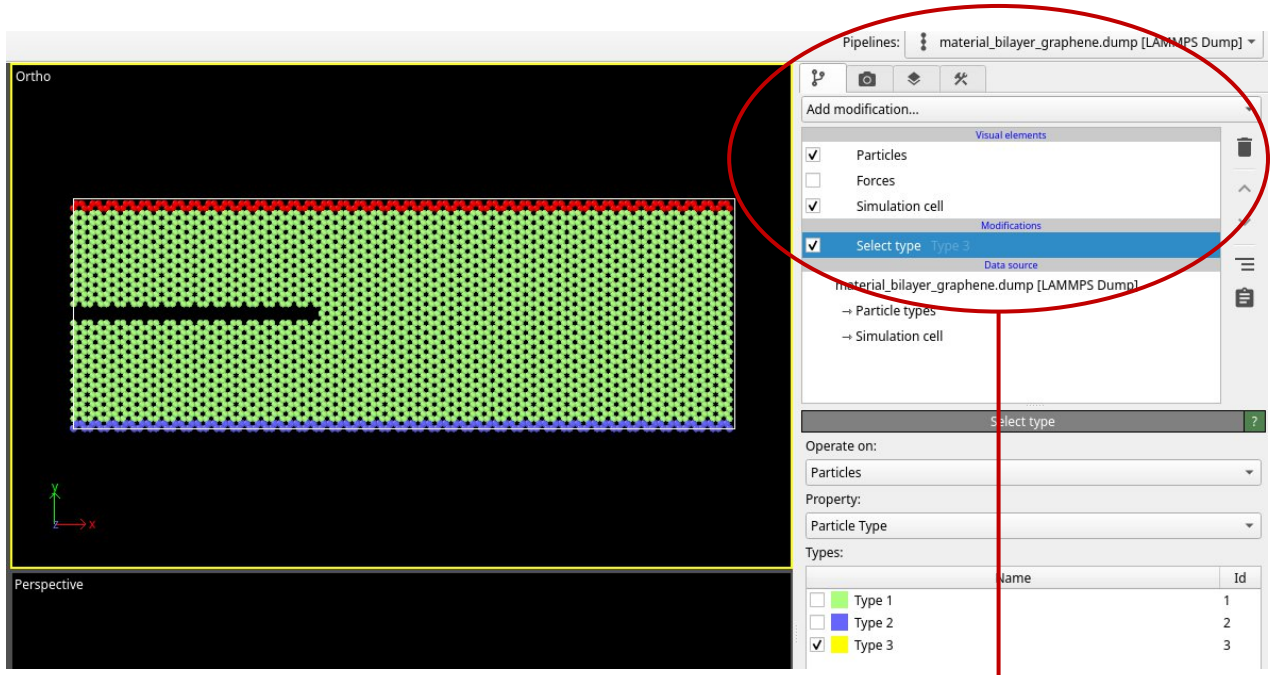
	Particle Identifier	Particle Type	f_materialpositionx	f_materialpositiony	f_materialpositionz	Position [X Y Z]	v_configforcex	v_configforcey	v_configforcez	Force [X Y Z]
0	1	2	0	0	0	0 0 0	0	0	0	0 0 0
1	2	2	0.7104	1.23045	0	0.7104 1.23045 0	0	0	0	0 0 0
2	3	2	2.1312	1.23045	0	2.1312 1.23045 0	0	0	0	0 0 0
3	4	2	2.8416	0	0	2.8416 0 0	0	0	0	0 0 0
4	5	1	0	2.4609	0	0 2.4609 0	0	0	0	0 0 0
5	6	1	0.7104	3.69135	0	0.7104 3.69135 0	0	0	0	0 0 0
6	7	1	2.1312	3.69135	0	2.1312 3.69135 0	0	0	0	0 0 0
7	8	1	2.8416	2.4609	0	2.8416 2.4609 0	0	0	0	0 0 0

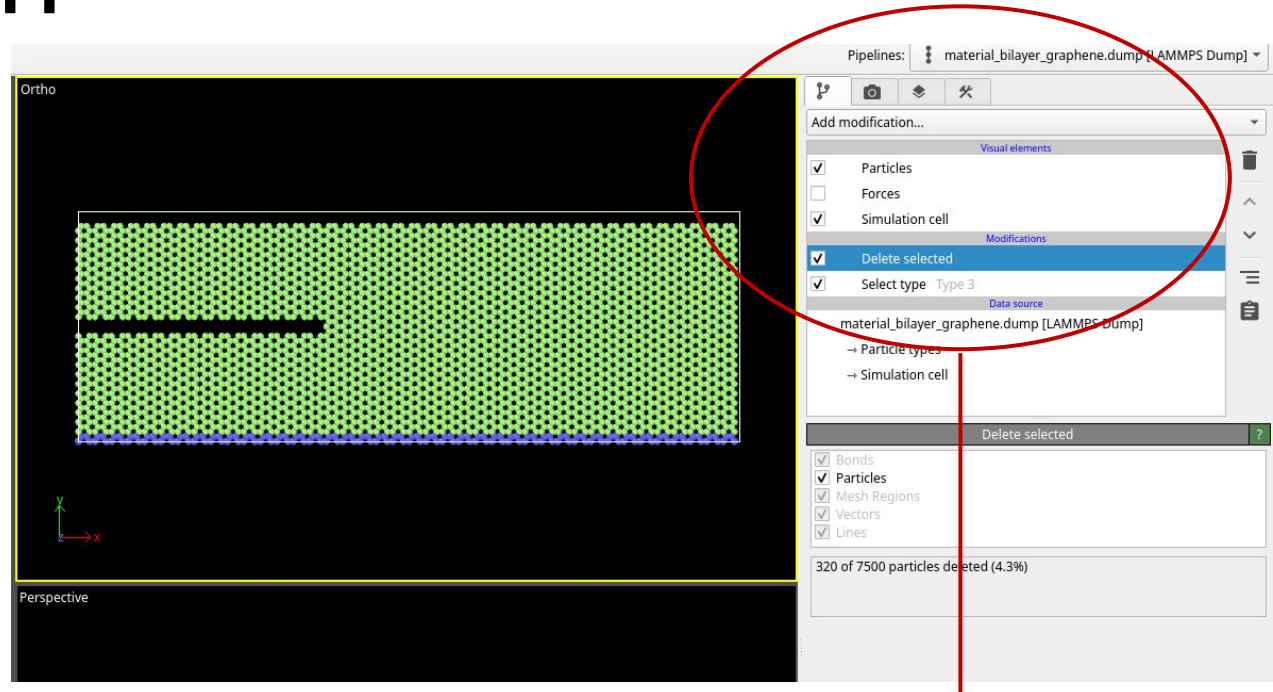
Modifier library – Post processing

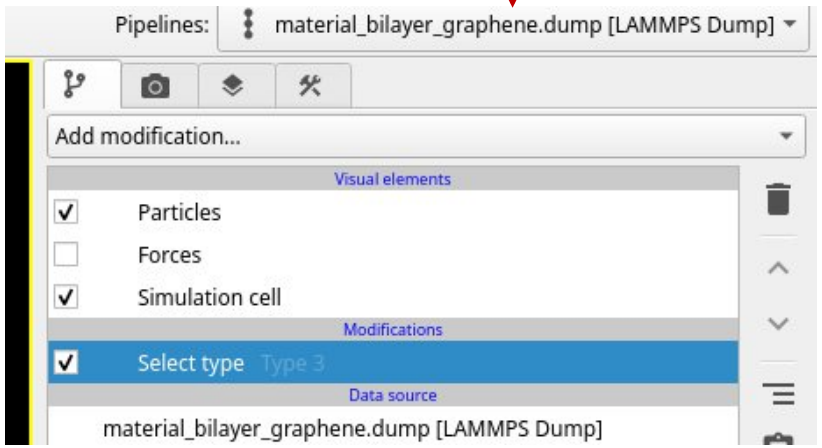


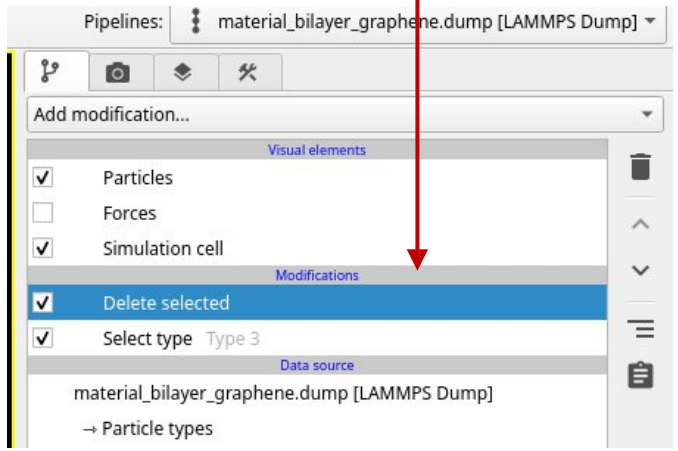


Selection and deletion

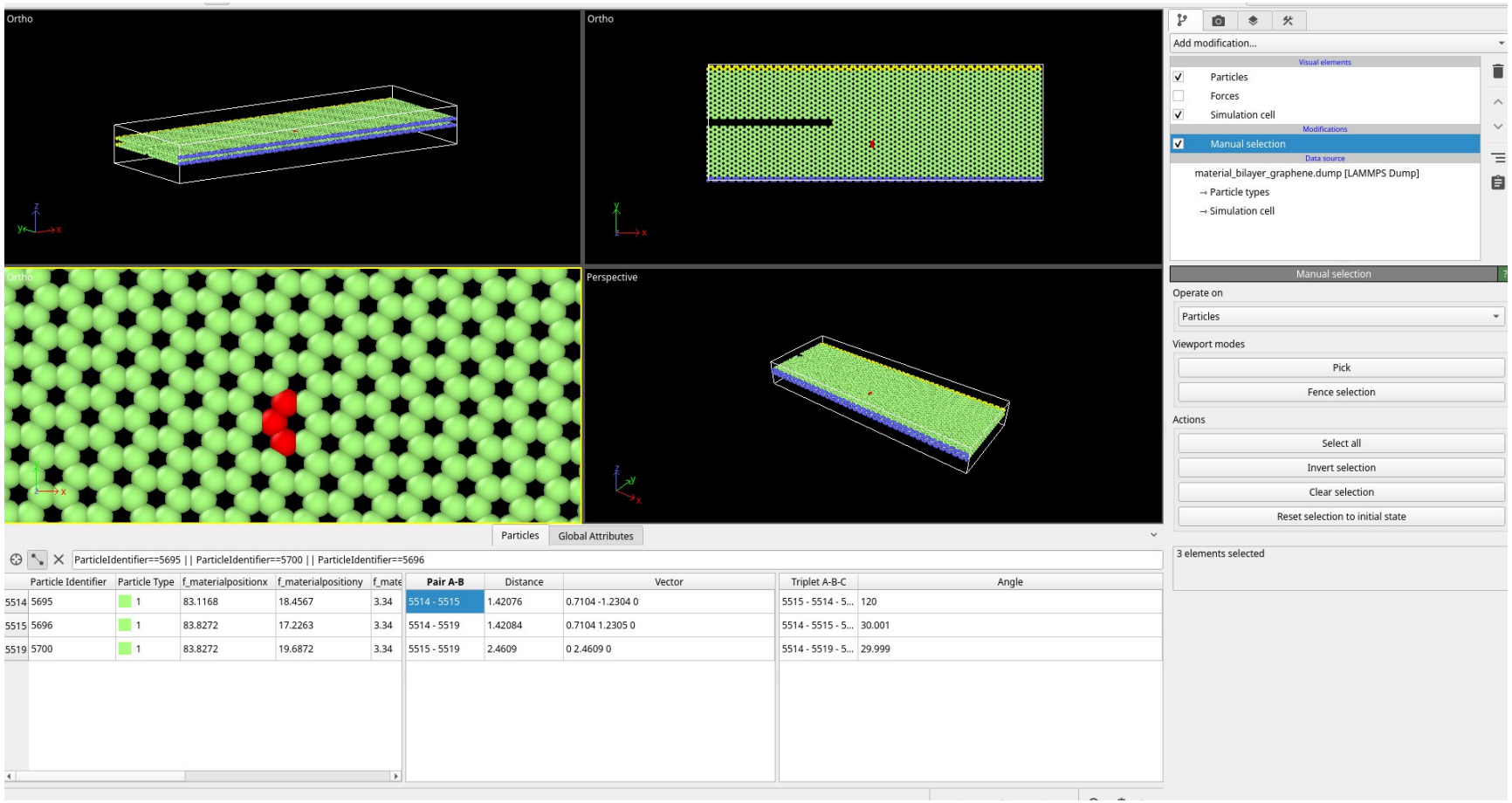




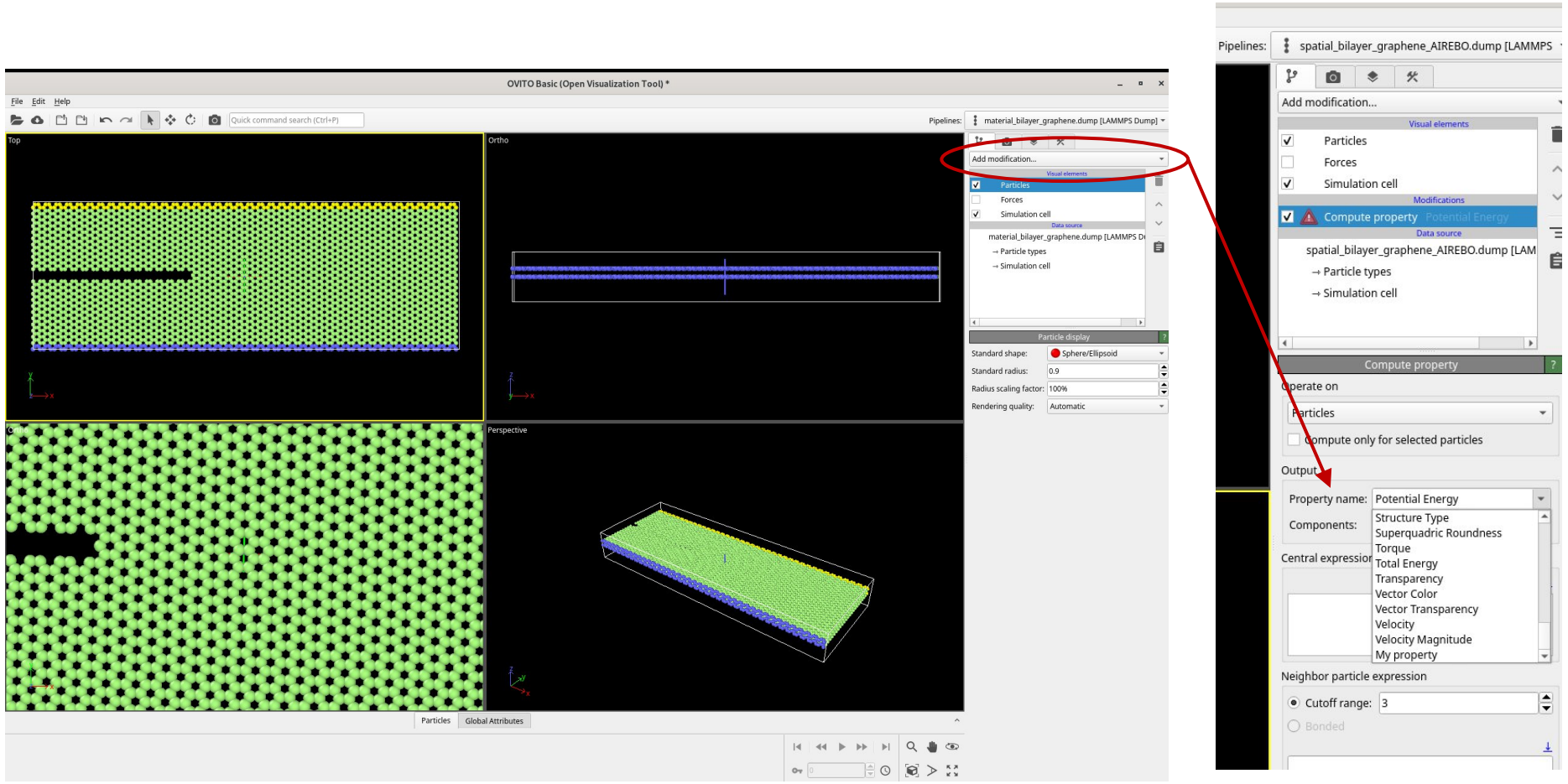




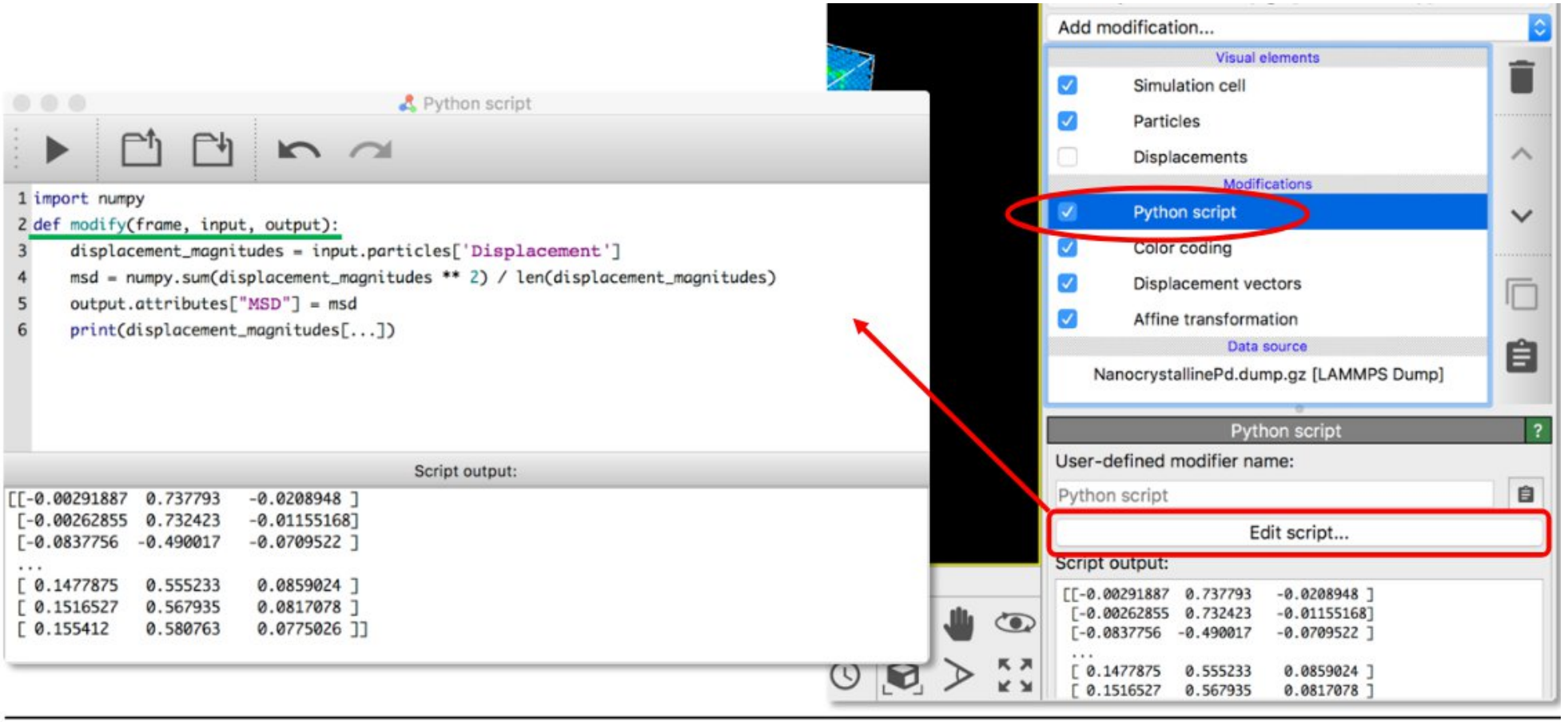
Manual selection – Topology information



Compute Property



Python Script



Calculation of atomistic frequency are done using python script.