

# OVITO

LAMMPS –  
MD  
Simulation



Dump file



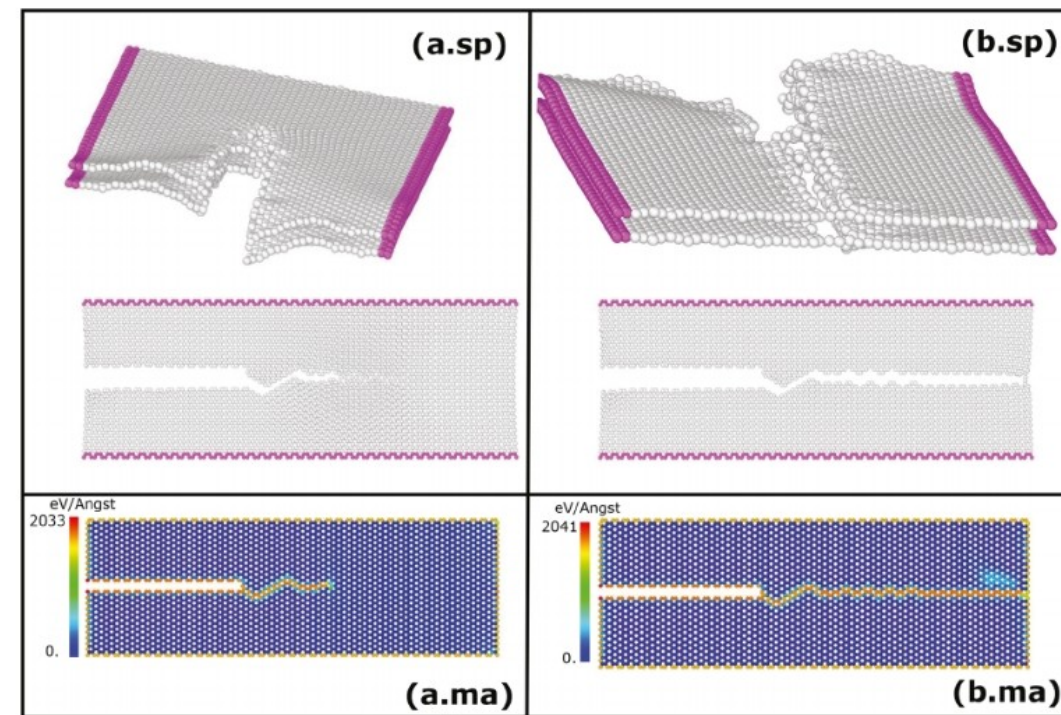
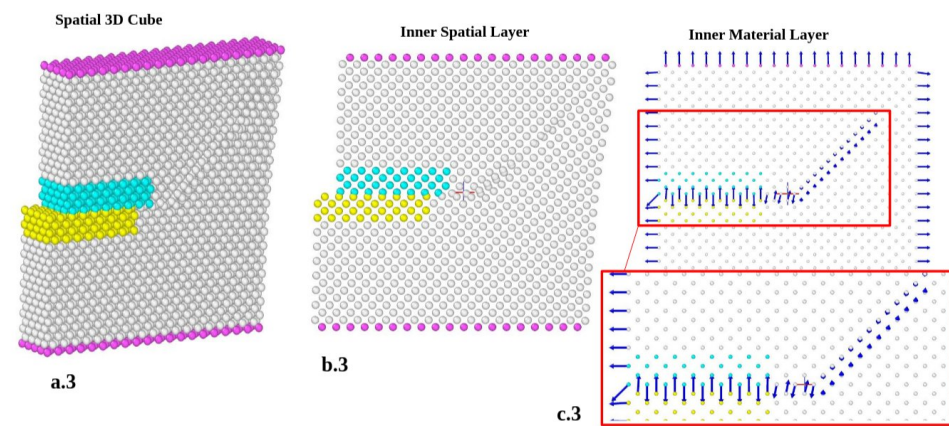
Visualization  
by Ovito

The Open Visualization Tool

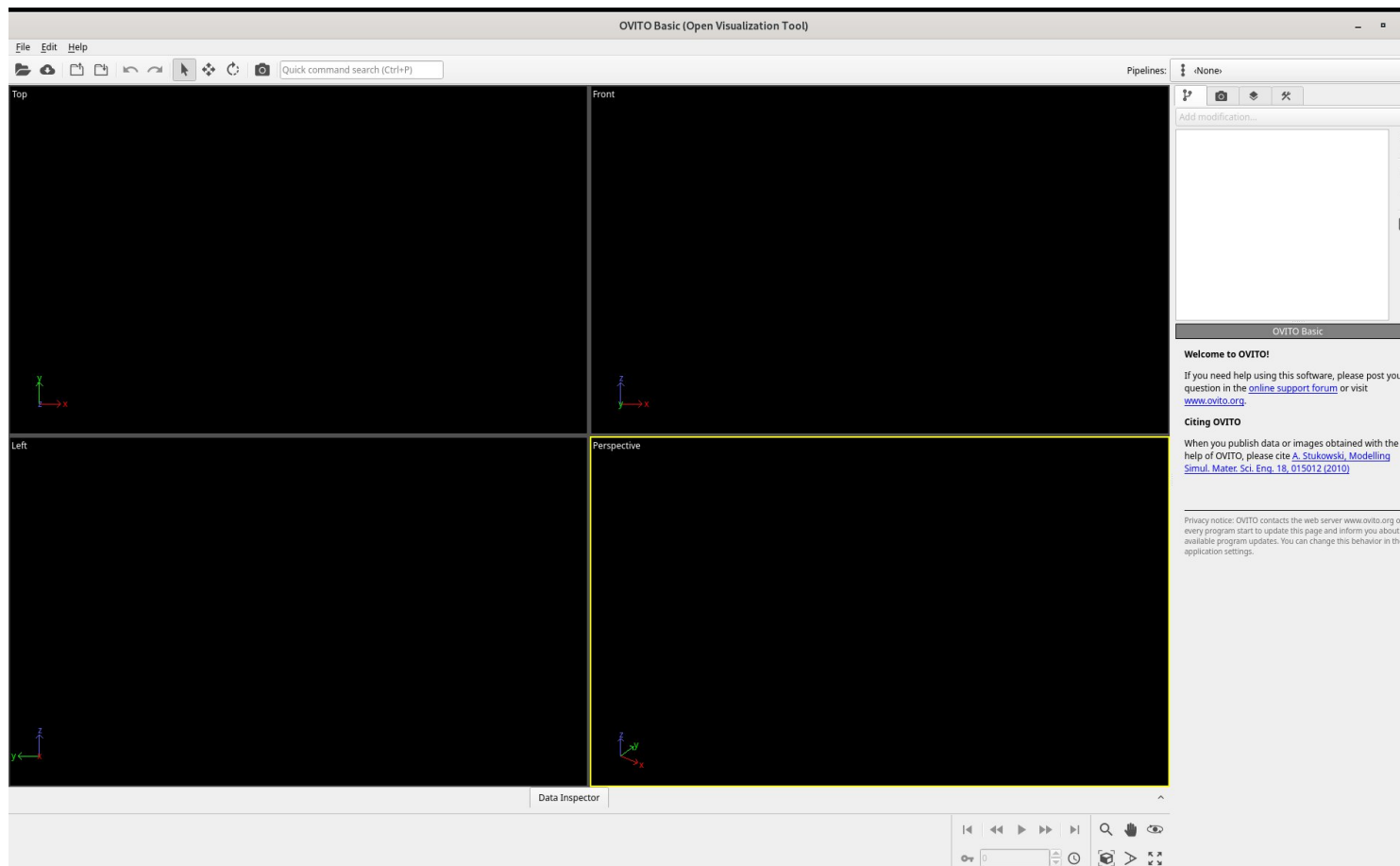
<https://www.ovito.org/>

# 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.



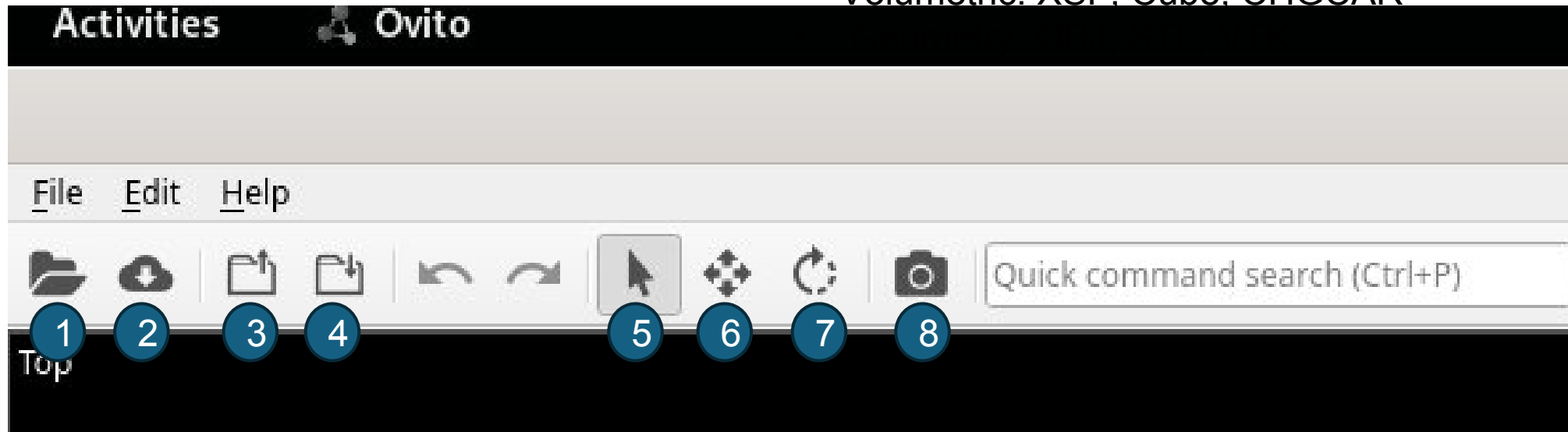
# Introduction to GUI



# 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

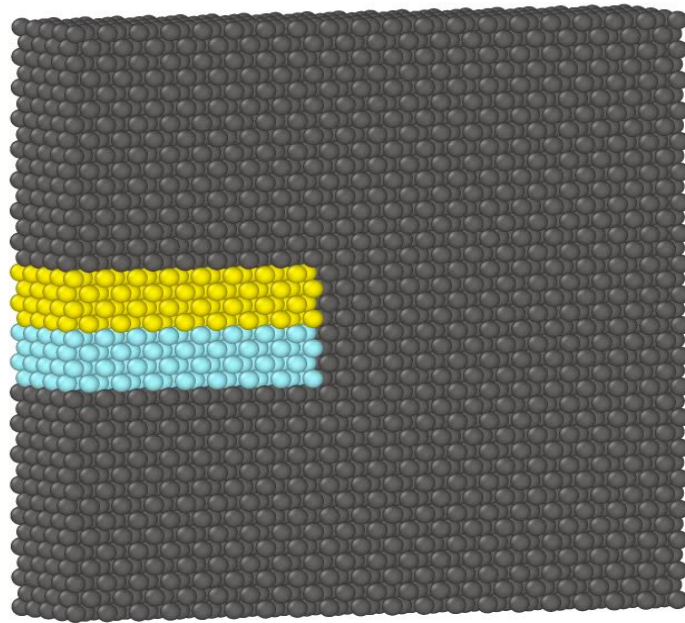


1. Load a file from local machine
2. Load a file from remote machine using OpenSSH
3. Save the current session
4. Load the saved session

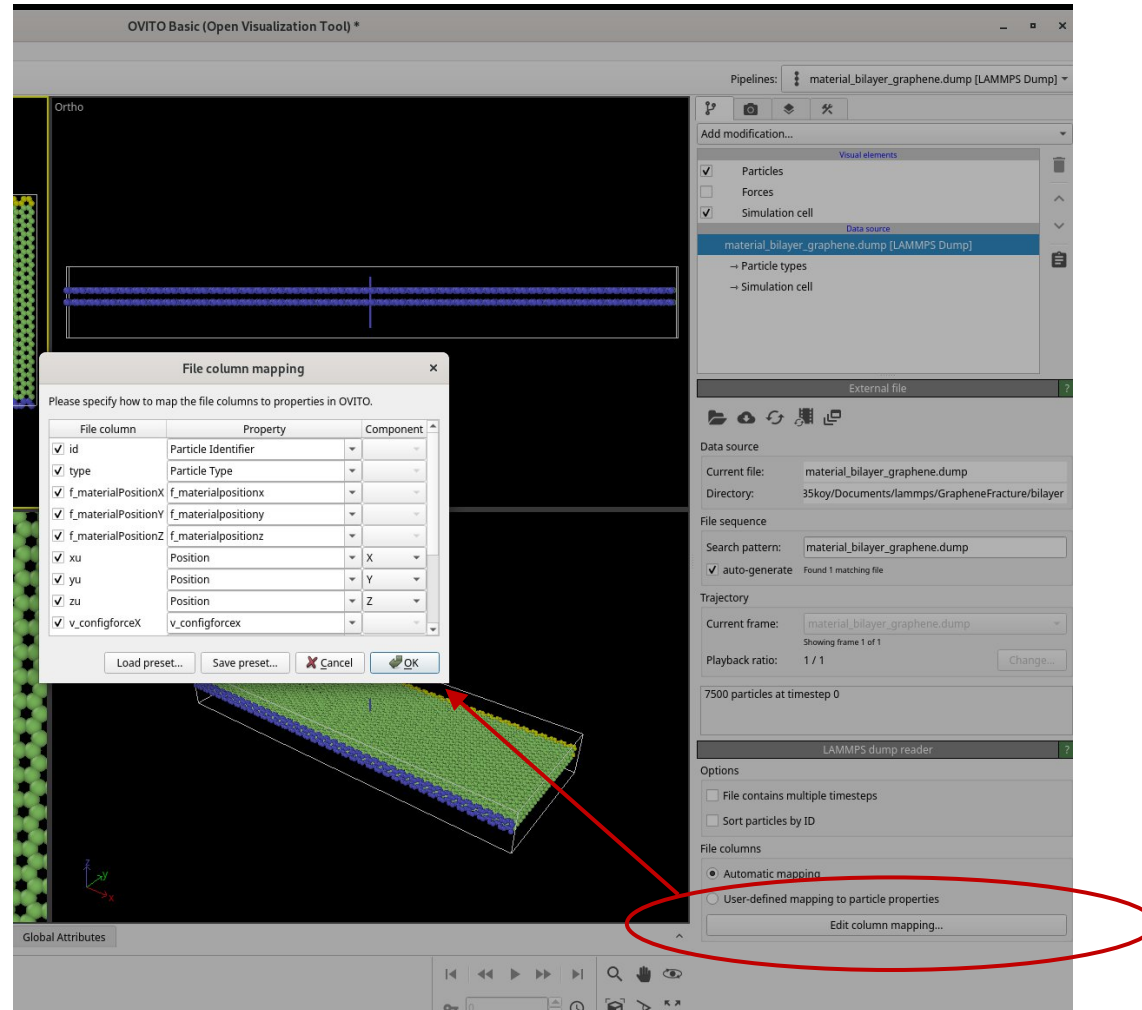
5. Make mouse left-click button to Select
6. Make mouse left-click button to Move
7. Make mouse left-click button to Rotate
8. Render active view-point

# 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

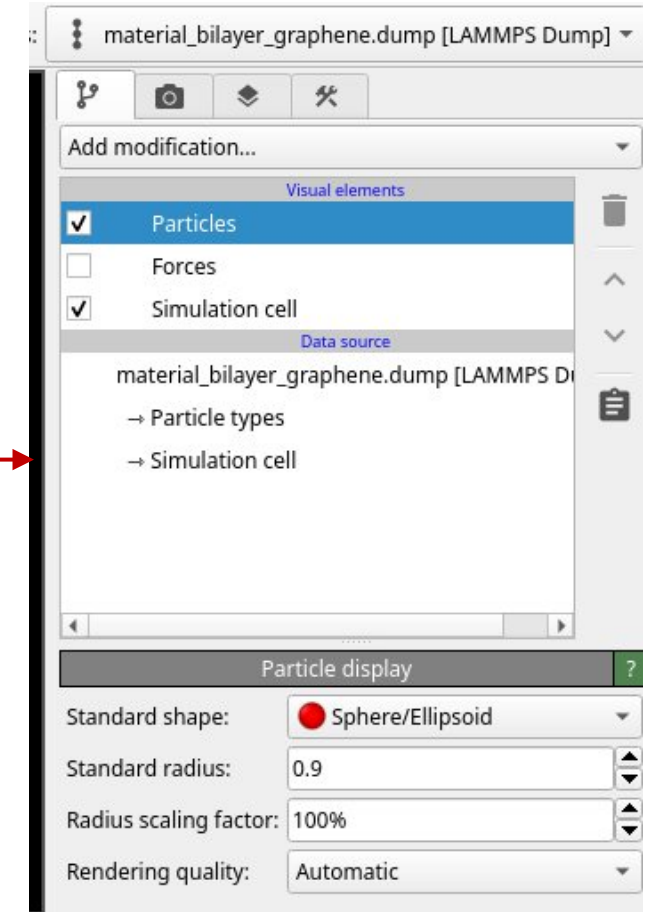
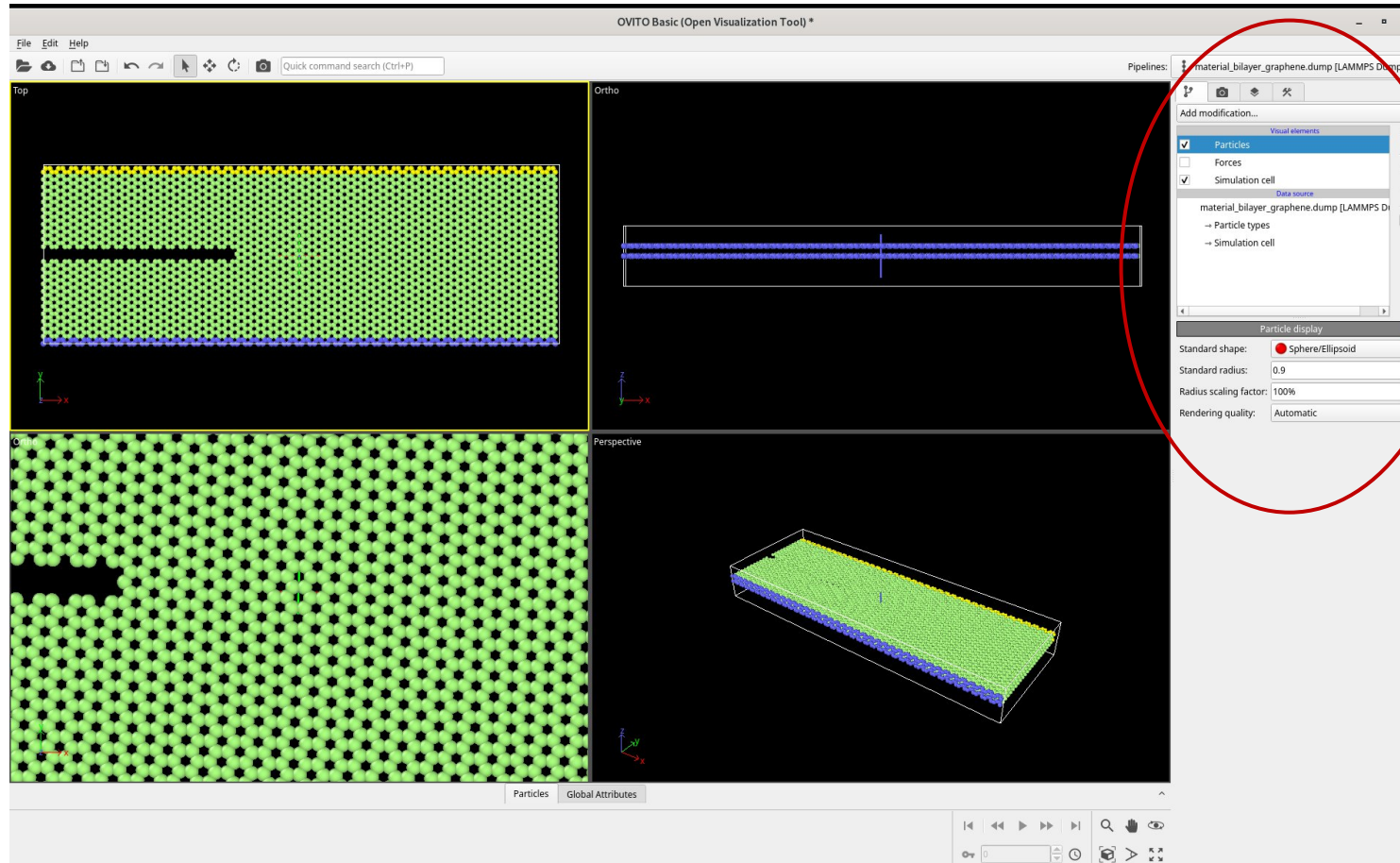




# Visualization elements

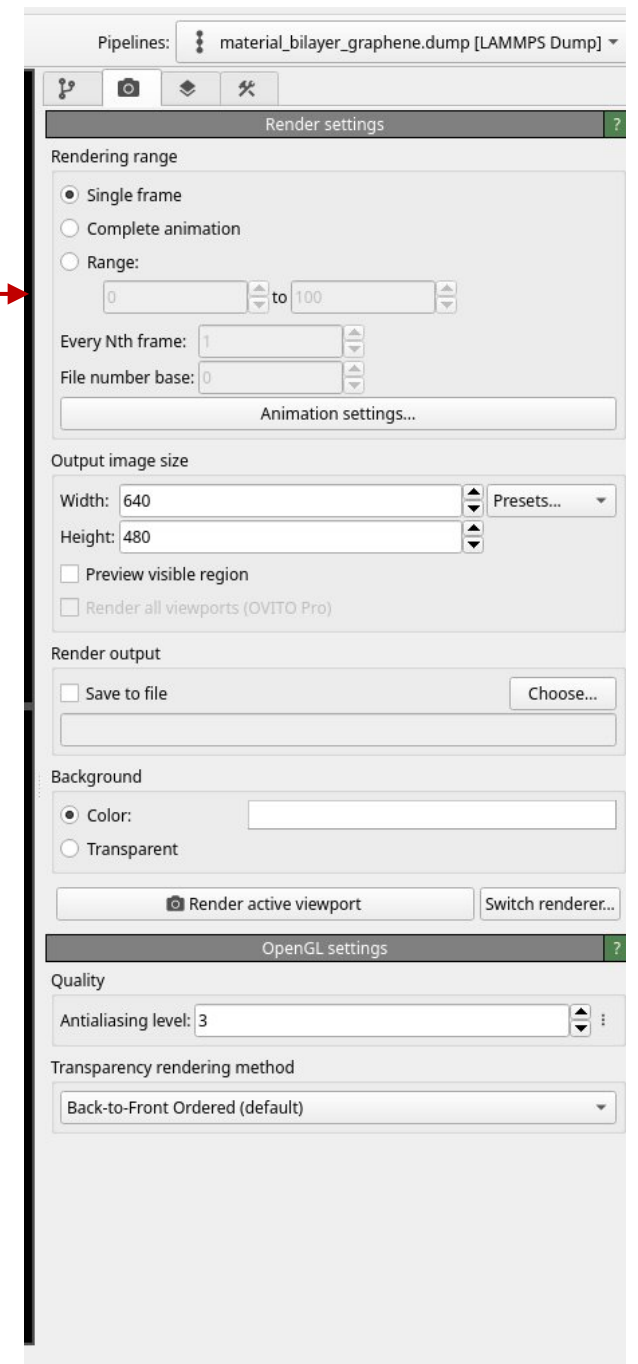
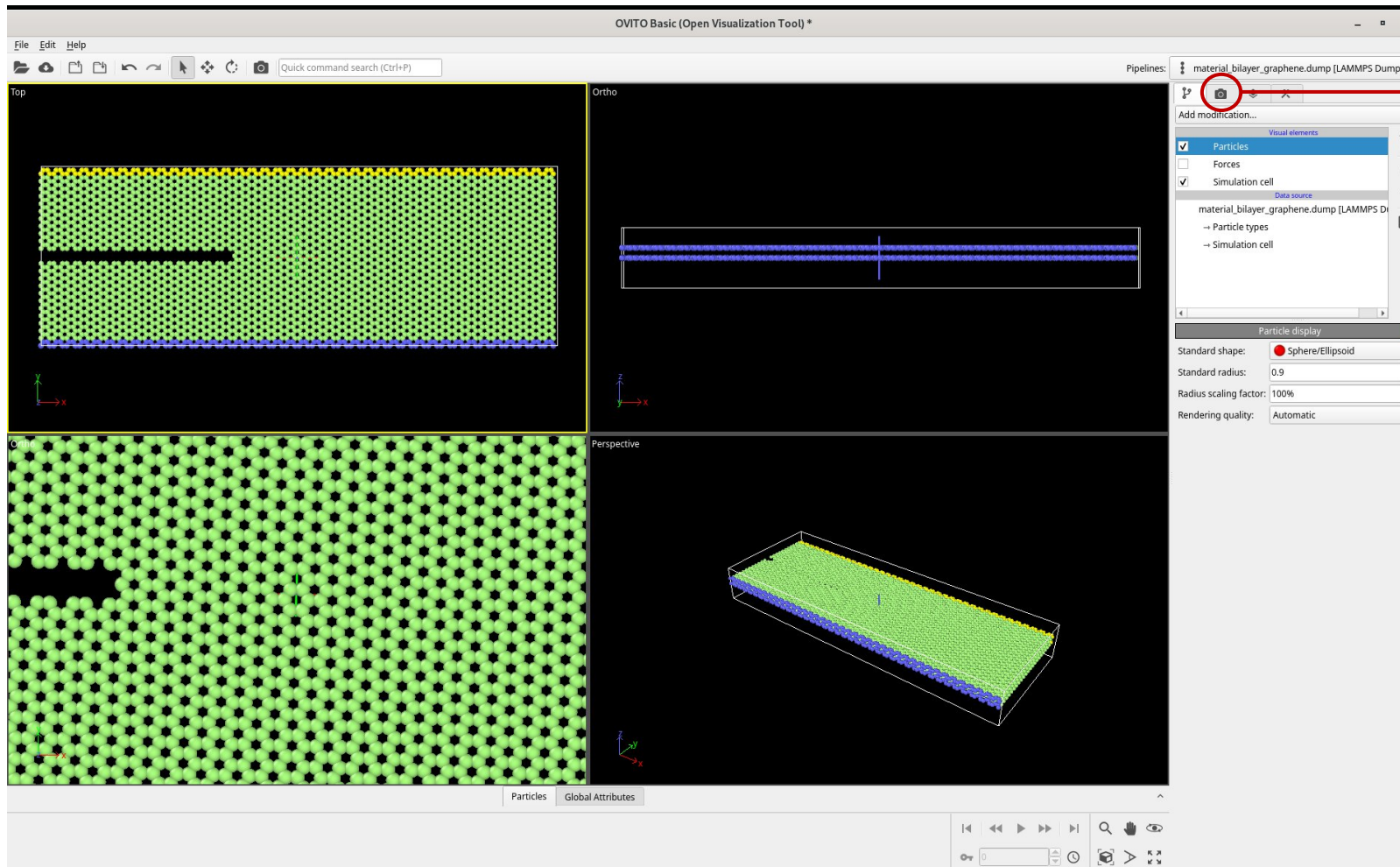
Visual elements are *graphical representations of data*.

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





# Image Export



# Particles menu

The screenshot shows the OVITO Basic (Open Visualization Tool) interface. The main 3D view displays a simulation of a material bilayer, with particles represented as green and blue spheres. The interface includes a menu bar (File, Edit, Help), a toolbar with various visualization tools, and a status bar at the bottom. A red circle highlights the 'Particles' button in the bottom toolbar, which is used to open the 'Particles' panel.

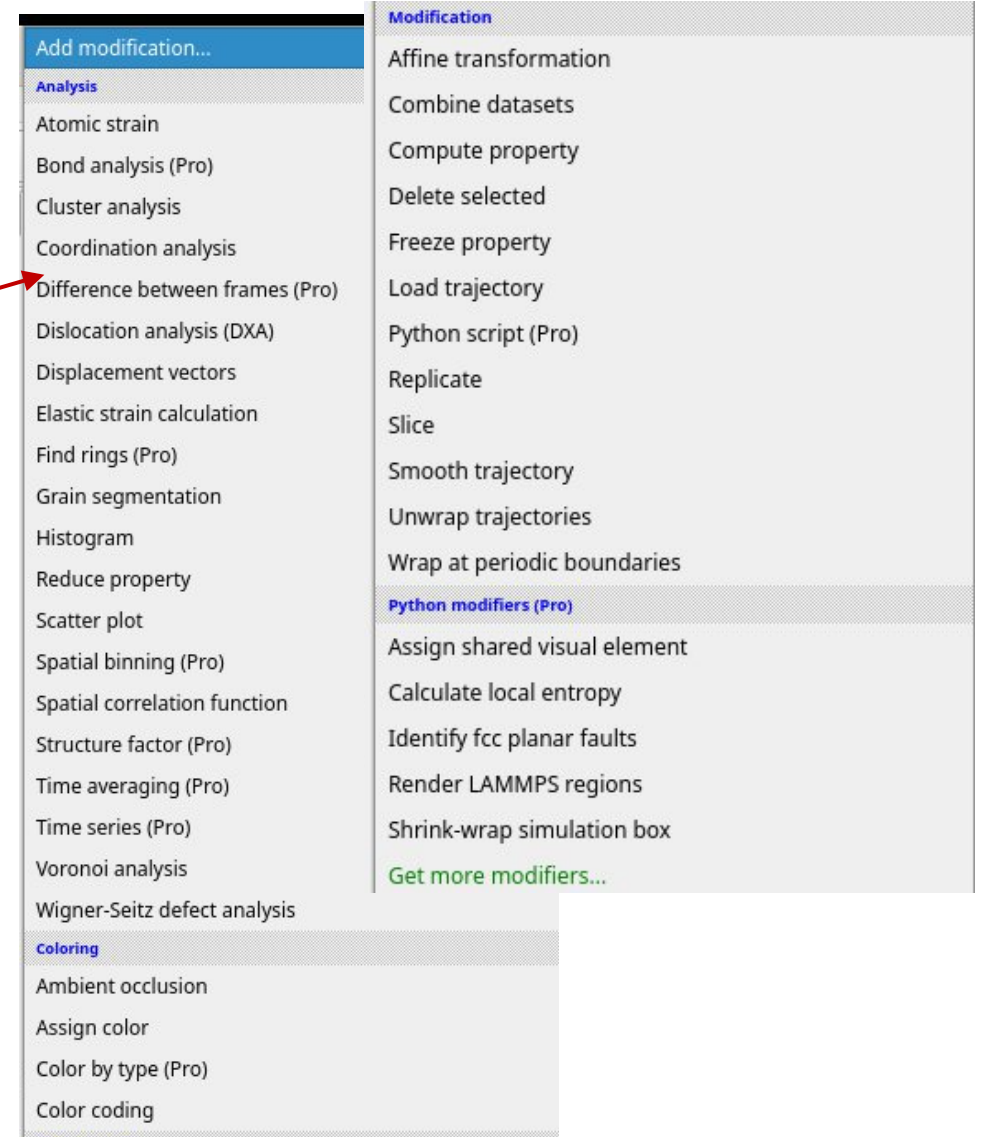
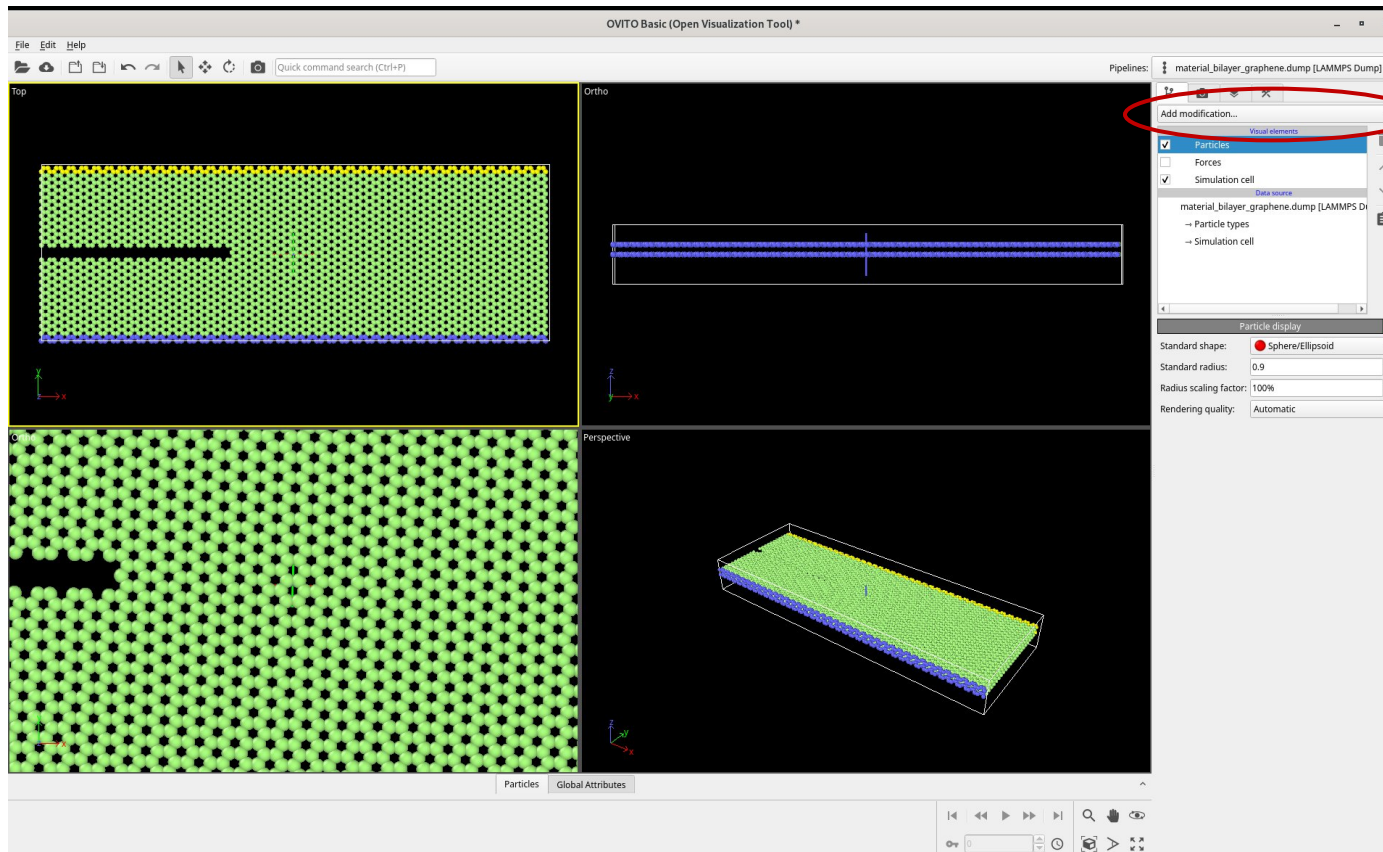
The 'Particles' panel on the right side of the interface shows the following settings:

- Visual elements:** Particles (checked), Forces (unchecked), Simulation cell (checked).
- Data source:** material\_bilayer\_graphene.dump [LAMMPS Dump]
- Particle display:** Standard shape: Sphere/Ellipsoid, Standard radius: 0.9, Radius scaling factor: 100%, Rendering quality: Automatic.

Below the 'Particles' panel, a table displays the simulation data for the selected particles. The table has columns for Particle Identifier, Particle Type, f\_materialpositionx, f\_materialpositiony, f\_materialpositionz, Position [X Y Z], v\_configforcex, v\_configforcey, v\_configforcez, and Force [X Y Z].

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
1	2	2	0.7104	1.23045	0.7104 1.23045 0	0	0	0	0 0 0
2	3	2	2.1312	1.23045	2.1312 1.23045 0	0	0	0	0 0 0
3	4	2	2.8416	0	2.8416 0 0	0	0	0	0 0 0
4	5	1	0	2.4609	0 2.4609 0	0	0	0	0 0 0
5	6	1	0.7104	3.69135	0.7104 3.69135 0	0	0	0	0 0 0
6	7	1	2.1312	3.69135	2.1312 3.69135 0	0	0	0	0 0 0
7	8	1	2.8416	2.4609	2.8416 2.4609 0	0	0	0	0 0 0

# Modifier library – Post processing





# Selection and deletion

The image illustrates the process of selecting and deleting particles in a simulation using a software interface. The interface includes a main view area with Ortho and Perspective views, a Pipelines panel, and a right-hand panel for modifications.

**Selection Process:**

- Pipelines:** material\_bilayer\_graphene.dump [LAMMPS Dump]
- Add modification...** dropdown menu.
- Visual elements:** Particles (checked), Forces (unchecked), Simulation cell (checked).
- Modifications:** Select type Type 3 (checked).
- Data source:** material\_bilayer\_graphene.dump [LAMMPS Dump]
- Operation on:** Particles
- Property:** Particle Type
- Types:** Type 1 (unchecked), Type 2 (unchecked), Type 3 (checked).

**Deletion Process:**

- Modifications:** Delete selected (checked), Select type Type 3 (checked).
- Data source:** material\_bilayer\_graphene.dump [LAMMPS Dump]
- Operation on:** Delete selected
- Confirmation:** 320 of 7500 particles deleted (4.3%)

# Manual selection – Topology information

The screenshot displays a molecular dynamics simulation interface with four viewports: Ortho (top-left), Ortho (top-right), Ortho (bottom-left), and Perspective (bottom-right). The Ortho (bottom-left) view shows a close-up of a hexagonal lattice of green spheres with three red spheres. The Perspective view shows a 3D rectangular simulation cell. A right-hand sidebar contains a 'Manual selection' panel with a list of modifications and actions. Below the viewports is a table showing topology information for selected particles.

**Manual selection panel:**

- Add modification...
- Visual elements:
  - ☒ Particles
  - ☐ Forces
  - ☒ Simulation cell
- Modifications:
  - ☒ Manual selection
- Data source:
  - material\_bilayer\_graphene.dump [LAMMPS Dump]
  - Particle types
  - Simulation cell

**Actions:**

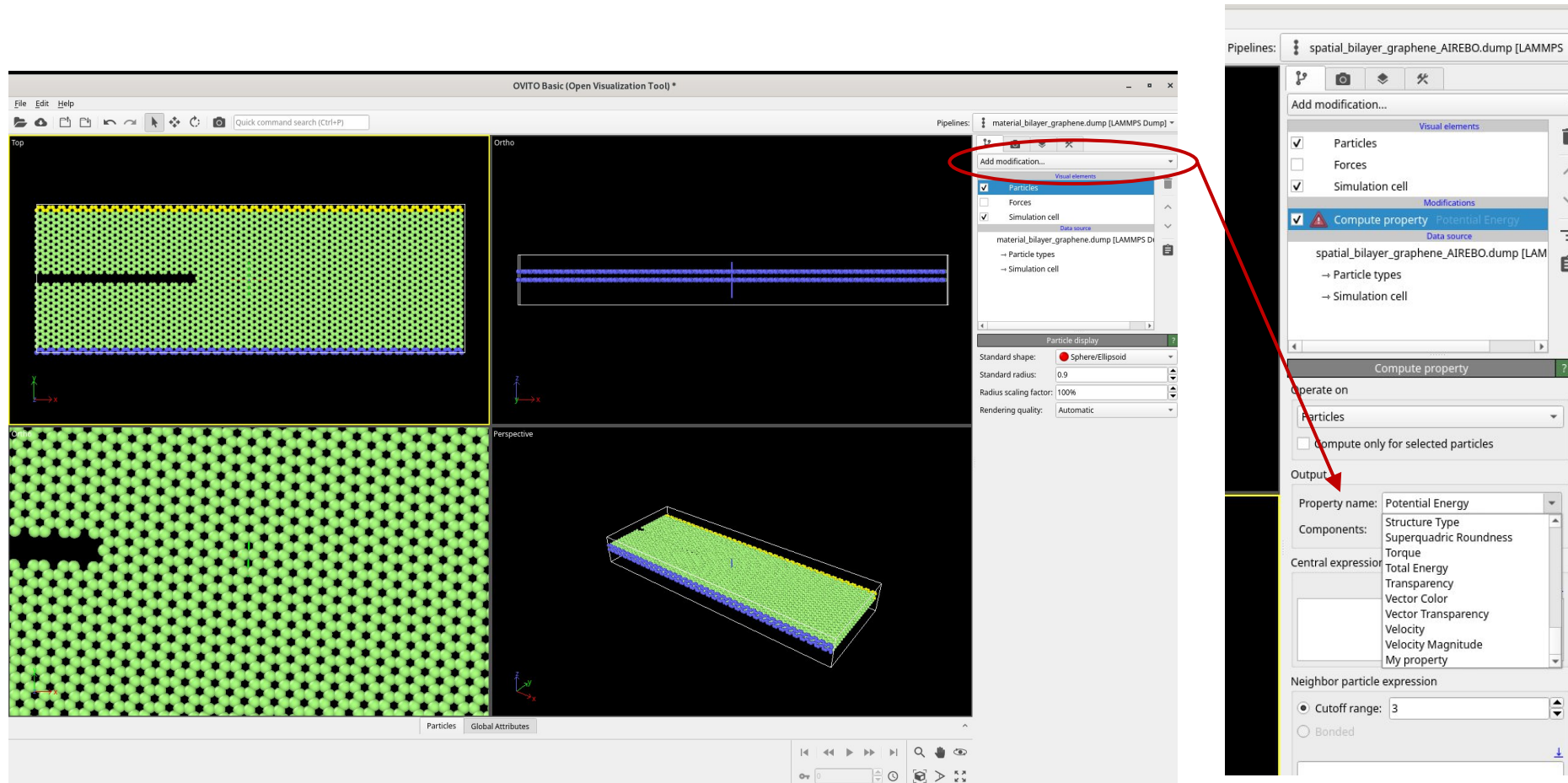
- Operate on: Particles
- Viewport modes: Pick, Fence selection
- Actions: Select all, Invert selection, Clear selection, Reset selection to initial state

**3 elements selected**

**Table:**

Particle Identifier	Particle Type	f_materialpositionx	f_materialpositiony	f_mate	Pair A-B	Distance	Vector	Triplet A-B-C	Angle
5514	5695	83.1168	18.4567	3.34	5514 - 5515	1.42076	0.7104 -1.2304 0	5515 - 5514 - 5...	120
5515	5696	83.8272	17.2263	3.34	5514 - 5519	1.42084	0.7104 1.2305 0	5514 - 5515 - 5...	30.001
5519	5700	83.8272	19.6872	3.34	5515 - 5519	2.4609	0 2.4609 0	5514 - 5519 - 5...	29.999

# Compute Property





# Python Script

The image shows a software interface with a Python script editor on the left and a modification menu on the right. The script editor contains the following code:

```
1 import numpy
2 def modify(frame, input, output):
3     displacement_magnitudes = input.particles['Displacement']
4     msd = numpy.sum(displacement_magnitudes ** 2) / len(displacement_magnitudes)
5     output.attributes["MSD"] = msd
6     print(displacement_magnitudes[...])
```

Below the script editor, the "Script output:" section displays a 3x3 grid of numerical values:

[-0.00291887	0.737793	-0.0208948 ]
[-0.00262855	0.732423	-0.01155168]
[-0.0837756	-0.490017	-0.0709522 ]
...		
[ 0.1477875	0.555233	0.0859024 ]
[ 0.1516527	0.567935	0.0817078 ]
[ 0.155412	0.580763	0.0775026 ]]

The modification menu on the right, titled "Add modification...", lists several options under different categories:

- Visual elements:**
  - ☒ Simulation cell
  - ☒ Particles
  - ☐ Displacements
- Modifications:**
  - ☒ Python script (highlighted with a red circle)
  - ☒ Color coding
  - ☒ Displacement vectors
  - ☒ Affine transformation
- Data source:**
  - NanocrystallinePd.dump.gz [LAMMPS Dump]

Below the menu, the "Python script" section shows a "User-defined modifier name:" field with the value "Python script" and an "Edit script..." button (highlighted with a red rectangle). The "Script output:" section in this panel displays the same 3x3 grid of numerical values as the main script editor.

Calculation of atomistic frequency are done using python script.

