

MANUAL FOR THE "Y_NANO" COMPUTER PROGRAM

1. Introduction

Y_NANO is a Molecular Dynamics (MD) code developed for larger time and space scale molecular level calculations. It is especially focused on the field of nanotechnology. In the version accompanying the book “Computational Mechanics of Discontinua”, a simple cubic solid wall boundary is employed for the simulation of micro/nano Argon gas systems. The contact search is done by using an implementation of the MR-Linear contact detection algorithm.

1.1. Installation

The source code for YNANO can be compiled either under Windows or under Linux. The user will have to unpack the zip file that contains the following directories:

- Source: containing all of the source files (compressed in Y_NANO.zip).
- Tutorial: containing the manual, i.e. this file, together with all of the examples.

In order to run the code the syntax to be used is the following: YNANO <Input Filename>

2. Input and Output Files

Currently three input files are required to run a particular project with the Y_NANO code:

1. YNANO setup file: to change the main modelling parameters. A description of the contents of this file is shown in Table 1.
2. SEQ file: to control the total calculation time, i.e. number of time steps, the time step size and the output frequency, see Figure 1. A sequential order number, (0, 1, 2, 3, 4, ..., etc.) is given to distinguish the different steps of the calculation, with a sequential range of time steps followed, e.g. 0 to 10000; and a number "-1" given could end the whole simulation process. The frequency of writing output files is given behind these ranges, e.g. 200, followed by the duration of one single time step, e.g. 0.005. Different calculation steps divided by different sequential order number can have different output frequency or even different length of a time step. Spaces should be placed in-between to distinguish different definitions from each other.
3. ATO file: to define which atoms are to be “followed” during the simulation, see Figure 2. A maximum of 500 atoms can be tracked at one time with the ATO file. The total number of atoms tracked is first and foremost given at the top of the file, e.g. 8. The IDs of atoms followed are then listed one by one with each in a different line. The first ID is taken as the first atom to be followed, and corresponds to the first following atom output which is denoted by a "0000" sequential number in the output file name, while the second ID corresponds to the second one, i.e. having a 0001 sequential number, and so on. In Y_NANO programme, atoms' ID is ranged from 0 to n_{atoms} -1, where n_{atoms} represents the total number of atoms in the whole system.

The length and the time units for Y_NANO are 10^{-10} m and 10^{-12} s respectively.

Table 1. General description of the YNANO setup input file

IOUTI	Start from the outputs of a previous calculation. Set as 0.
ISFIRST	To start a fresh project, always give a number 2.
IFQUADRATIC	Selection of contact search algorithm: 0 = MR linear contact search algorithm 1 = quadratic search (for debugging purposes)

BNDMODEL	Selection of boundary wall potentials. 0 = BND3-9 1 = BNDWCA
ARARMODEL	Selection for argon-argon interaction potentials 0 = Lennard-Joes 12-6 1 = BUF14-7
NPRNTFREQ	Output frequency.
A	Lattice constant for the <i>fcc</i> Argon crystal.
DSELECTRAD	Parameters for RDF (radial distribution function) calculation.
DMAXRADIST	
DMINRADIST	
DTEMP	Initial temperature at the atom raster.
DWALLTEMP	Wall temperature (not in use!).
CUBCC1X	Dimensions to define the cubic boundary.
CUBCC1Y	
CUBCC1Z	
CUBCC2X	
CUBCC2Y	
CUBCC2Z	
CUBDIST	Distance between Argon atoms in the cube (in the cases of gas argon).
NX	Number of argon <i>fcc</i> cells in <i>x</i> , <i>y</i> , <i>z</i> directions, respectively.
NY	
NZ	
NFREQFOLLOW	Printing frequency for the trajectory of the “followed” atoms.
NSETSTOFOLLOW	How many sets of points in the trajectory. Each set contains 500 points.

Sequence Index	Starting Time Step	Ending Time Step	Output Frequency	Time Step Size
0	0	10000	200	0.025
1	10000	30000	200	0.025
2	30000	50000	200	0.025
:	:	:	:	:
n	100000	150000	200	0.025
-1				

End of Simulation Flag

Figure 1. General example of a SEQ file.

8	Number of Atoms to be “Followed”
26	
48	
56	
87	
98	
156	
246	
300	

IDs of the atoms to be “followed”

Figure 2. General example of a ATO file.

2.1. Output Files

YNANO produces two main types of output files:

- “.xyz” files that contain the tracking information for each one of the atoms specified in the “.ATO” file
- “.vtk” files that contain a snapshot of the system at the desired stages during the simulation.

2.1.1. XYZ Outputs

Coordinate and velocity records are stored in these files. A sequential number ranging from 0000 to 9999 is inserted in the filename to distinguish each one of the atoms being tracked (which were defined in the ATO file). The tracking information is saved every NFREQFOLLOW time steps.

2.1.2. VTK Outputs

The snapshot results obtained with YNANO can be processed with a number of post-processing tools, such as: Visit, Paraview, LS-Dyna, etc. In this tutorial, the basic steps to process YNANO outputs with Visit are explained.

3. Post-Processing with Visit

After running the YNANO application a number of VTK files are generated. The naming convention for the VTK files is as follows: consider that the name of the main input file (.ynano) is highT.ynano, then the names of the output files will be:

- For the atoms: highT0000.vtk, highT0001.vtk, highT0002.vtk, etc.
- For the container: highTContainer.vtk.

The first file to be opened should be the one corresponding to the container, see Figure 3. In order to plot the mesh of the container a new plot must be added, see Figure 4. After the plot is added the “Draw” button must be pressed in order to render the plot on the screen, see Figure 5.

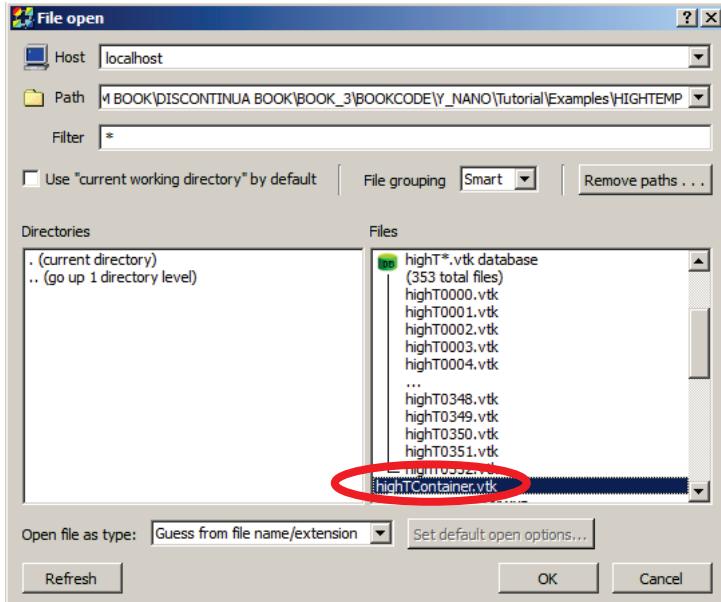


Figure 3. Open mesh file for container.

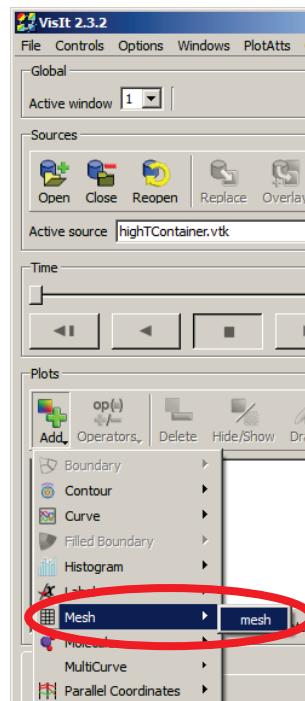


Figure 4. Generating a plot for the container mesh.

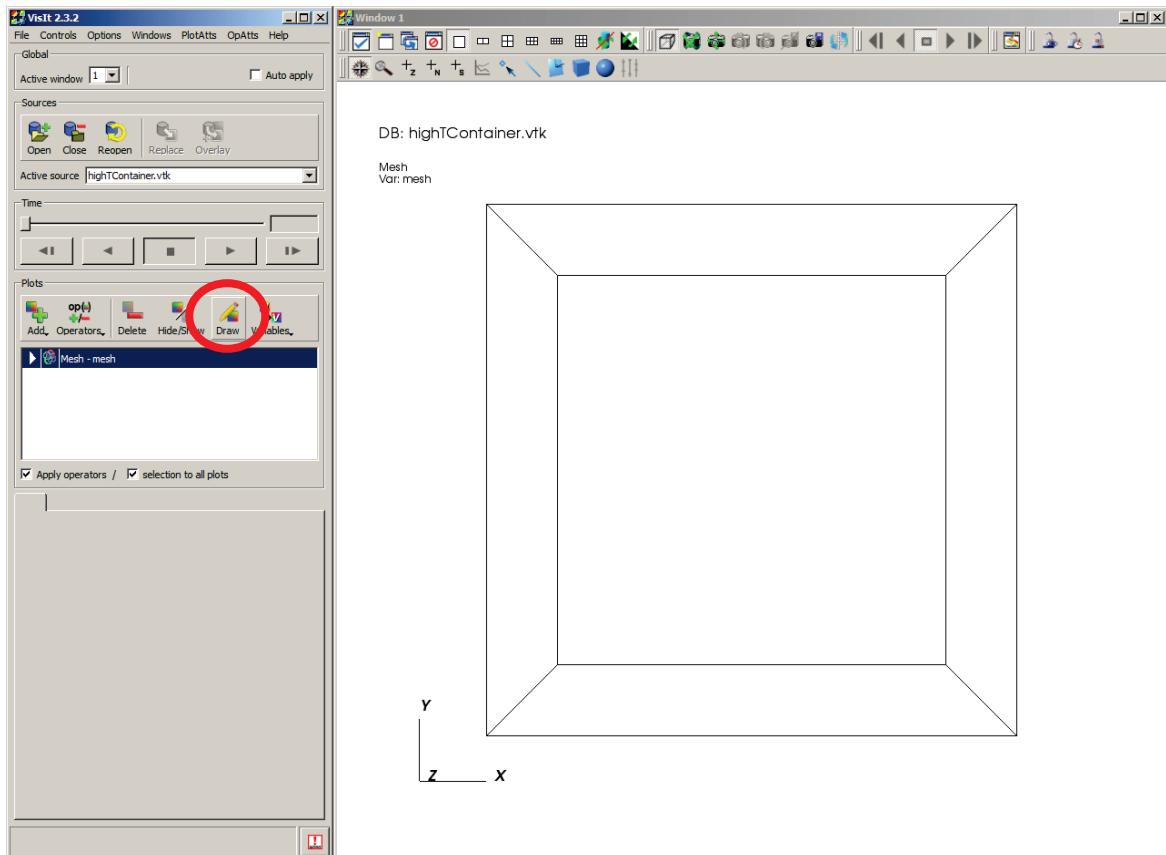


Figure 5. Plotting the container mesh.

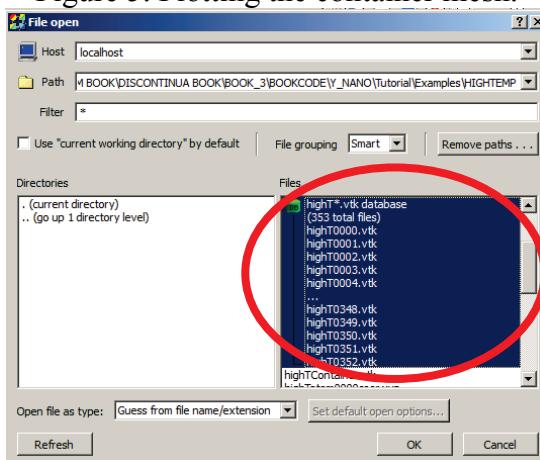


Figure 6. Opening the frame files for animation.

The next files to open are the snapshots files for the atoms, see Figure 6. The process is similar to the one explained for the container file. The main difference is that instead of adding a “mesh” plot we’ll be adding a “molecule” plot, as shown in Figure 7. Within the molecule plot, the Velocity_Magnitude option can be selected. Once the plot has been added, and the draw button has been pressed, the raster of atoms will appear on the rendering window, as shown in Figure 8.

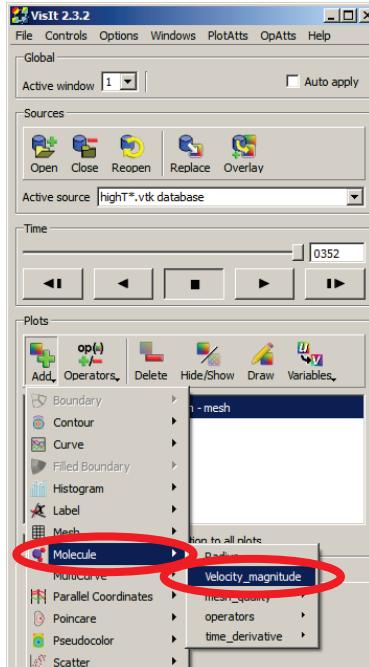


Figure 7. Generating a plot for the frames.

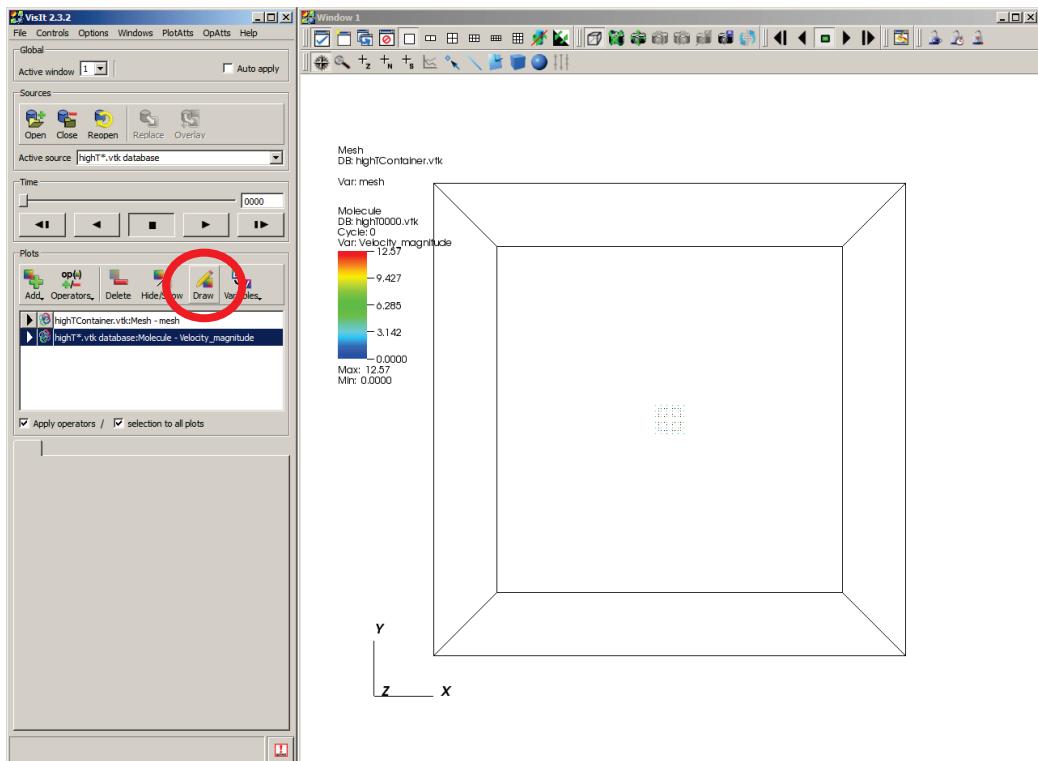


Figure 8. Generating a plot for the frames.

At this point, the size of the atoms is not the correct one. To solve this issue, we'll have to specify how big the atoms are. This information is contained also in the VTK files, but Visit needs to be informed about it. This is done by going to the PlotAtts (Plot Attributes) menu and selecting the Molecule option, as shown in Figure 9. A dialog box will appear where there are a number of options to set up how to plot the molecules or atoms, what level of quality to use when plotting the

molecules, what value to use for the radius, etc. In the case of YNANO the atomic radius is included in the vtk file for the Argon atoms. Because of this, in the “Radius based on” option the sub-option “scalar variable” should be selected, as shown in Figure 10. In the “Variable for atom radius” menu the “Scalars -> Radius” option should be selected and then the Apply button should be clicked. At this point the atoms are plotted with their nominal size. Visit also offers the option of scaling the radius of the atoms as desired. This is achieved through the “Atom radius scale factor” as shown in Figure 11.

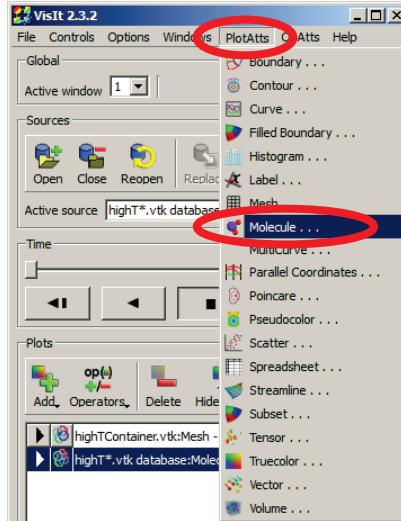


Figure 9. Adjusting plotting properties for atoms.

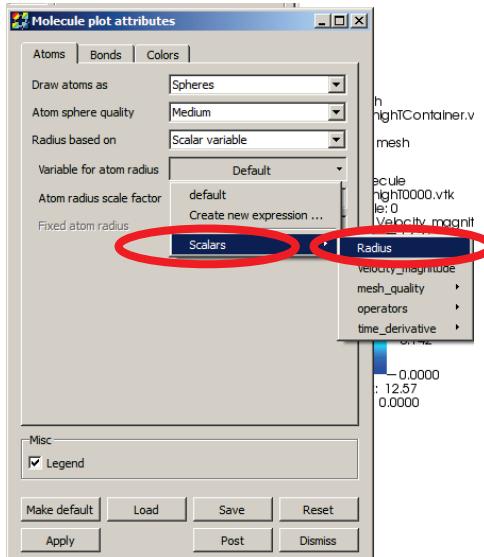


Figure 10. Setting the size of the atoms for plotting purposes.

There is a possibility of animating the sequence of VTK files in order to get an idea of the dynamics of the process. This can be done by playing with the animation controls available in Visit (Figure 12):

- Play Forward.
- Play Backward
- Stop
- Go to First Frame

- Go to Last Frame

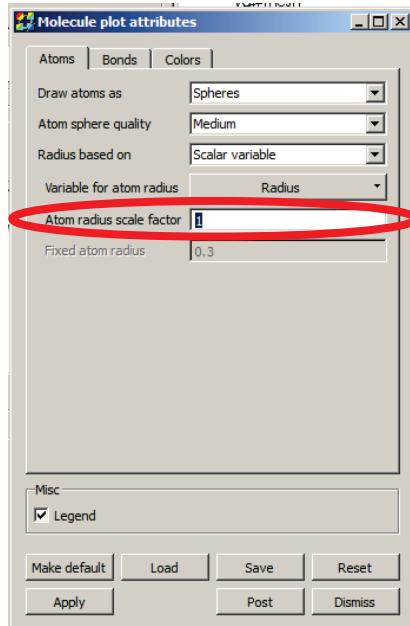


Figure 11. Scaling the atomic radius at will.

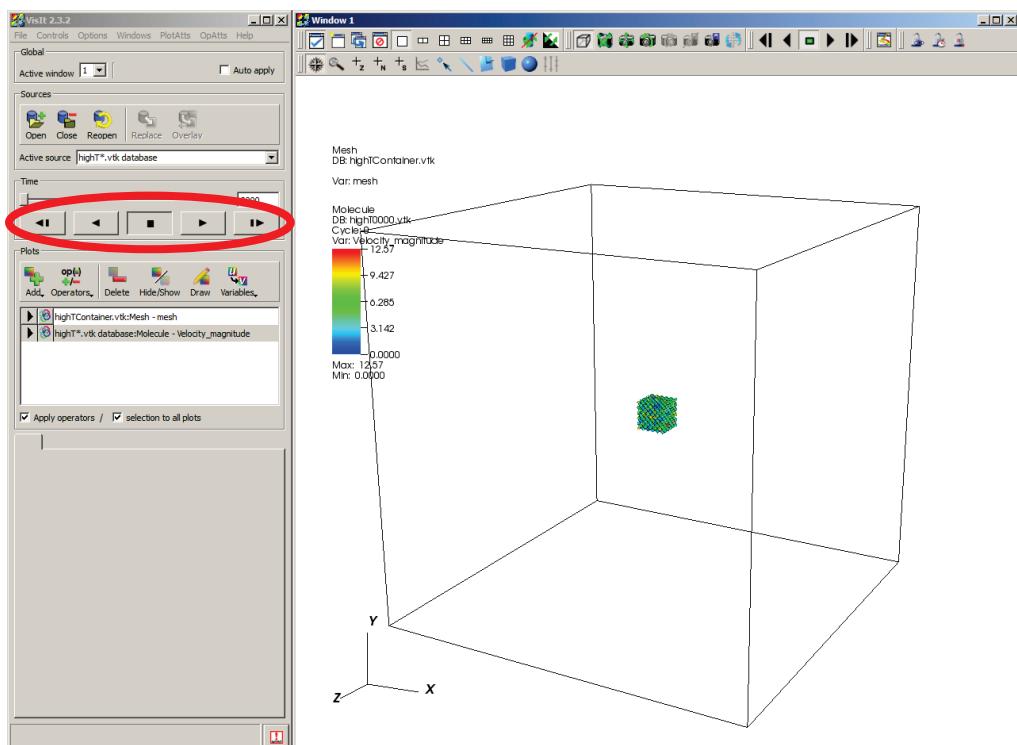


Figure 12. Animation control buttons.

An example of one instance of the animation of the highT test case is shown in Figure 13.

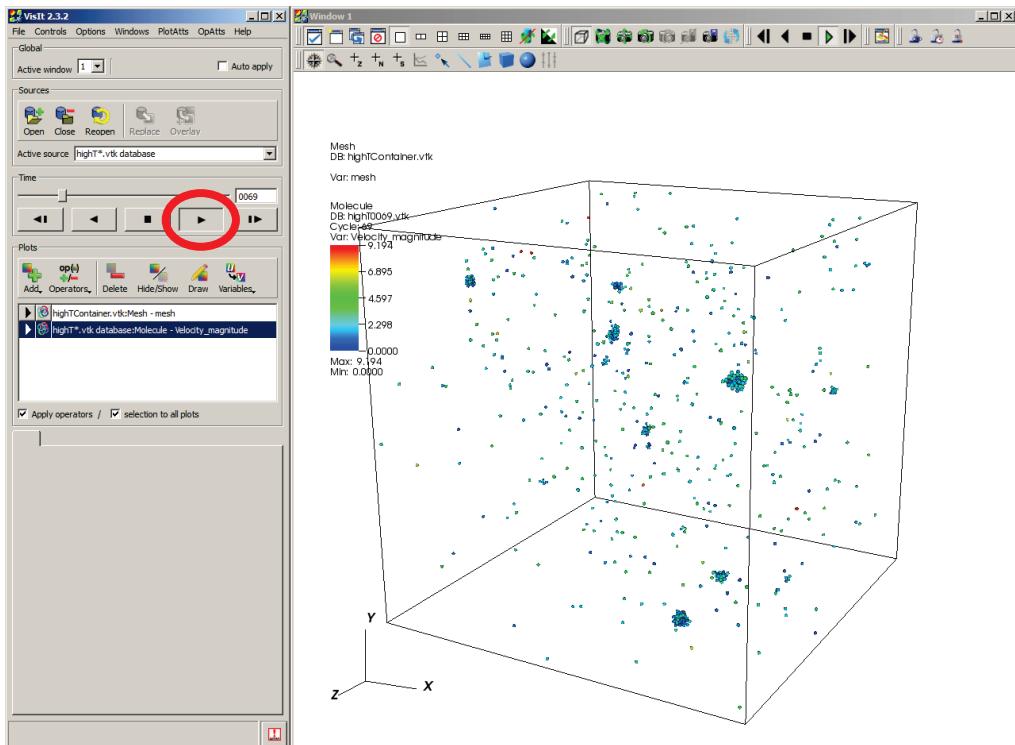


Figure 13. Animating the sequence of frames.

The tracked atoms' trajectories can also be superimposed to the dynamic animation of the system. First the files for the tracked atoms must be opened, as shown in Figure 14.

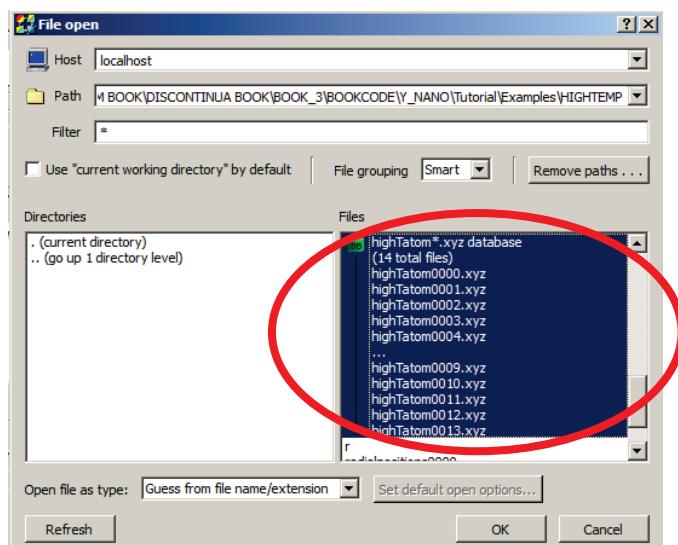


Figure 14. Opening the file for tracked atoms.

To plot the trajectories a Pseudocolor type of plot must be added, as shown in Figure 15. The legends var0, var1, var2 and var3 correspond to v_x , v_y , v_z and $|v|$ respectively.

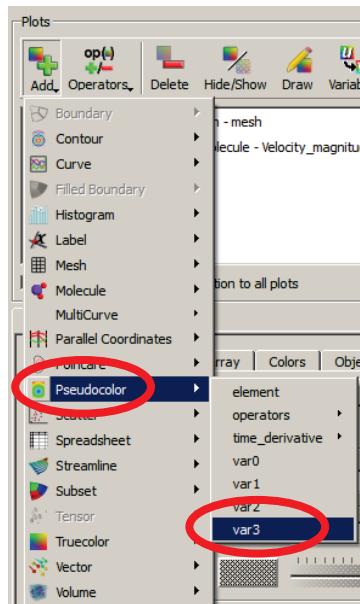


Figure 15. Adding a Pseudocolor plot.

When the draw button is clicked the graph of the trajectory for the first atom appears in the rendering window, as shown in Figure 16.

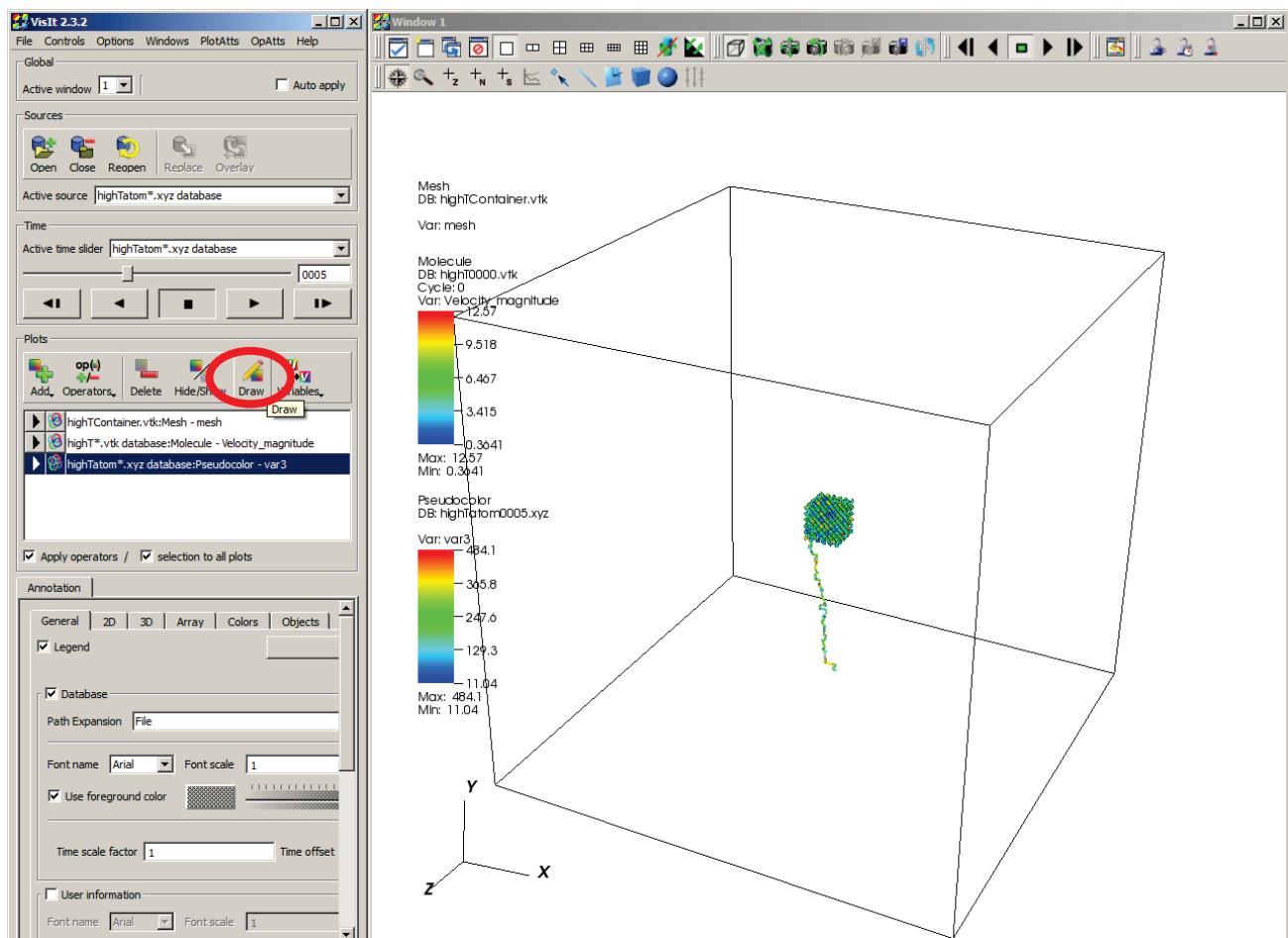


Figure 16. Plotting the trajectory of one of the tracked atoms.

The trajectory of other atoms can be retrieved by acting on the animation control buttons (Figure 12), see Figure 17.

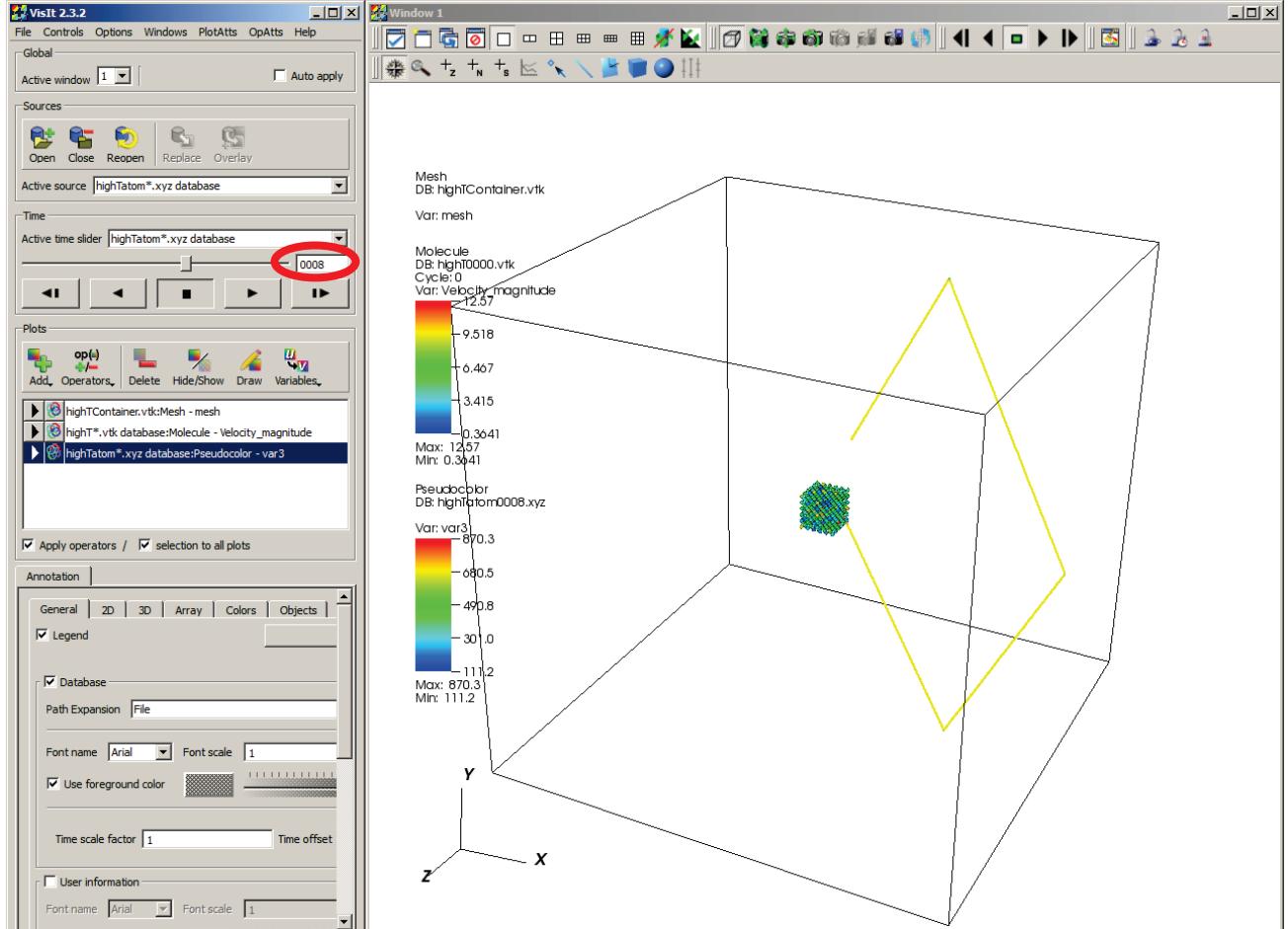


Figure 17. Plotting the trajectory of another of the tracked atoms.

The animation of the sequence of VTK files can be saved by using the “Save Movie” option within the File menu, as shown in Figure 18.

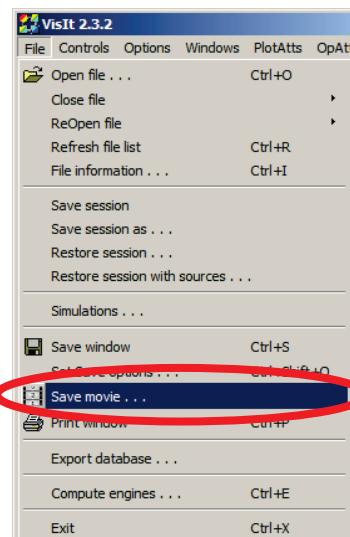


Figure 18. Saving the animation of the sequence of VTK files.

4. EXAMPLES

4.1. Argon Crystal of High Temperature

A total of 666 atoms are set up in an initial Argon crystal with a face centered (*fcc*) lattice structure and placed at the centre of a cubical rigid container. The size of the cubical container is 40 nm. The Argon-Argon interaction is described by the BUF14-7 potential and the interaction between the Argon atoms and the walls of the container is described by the WCA potential. Initially the temperature of Argon crystal is set to 500K. During the simulation the system is left to relax. Since the initial temperature is much higher than the crystal temperature the crystal melts suddenly.

4.1.1. Input

The example can be run as described in Section 1.1. In the SEQ file, the size of each time step is set to $0.025ps$ and a total of 240,000 steps are divided into 9 different series, with order numbers 0 through 8 beforehand. The output frequency for all of these time series is the same: 200. The number "-1" in the SEQ file defines where the simulation will stop. In this example the simulation will stop at 120,000 time steps. In the ATO file 14 atoms are specified to be tracked: Argon atoms with IDs 0, 20, 380, 400, 560, 462, 398, 100, 10, 390, 661, 299, 421 and 111.

4.1.2. Results

The snapshots of argon at different time step with Visit are illustrated in Figure 19 and Figure 20, respectively.

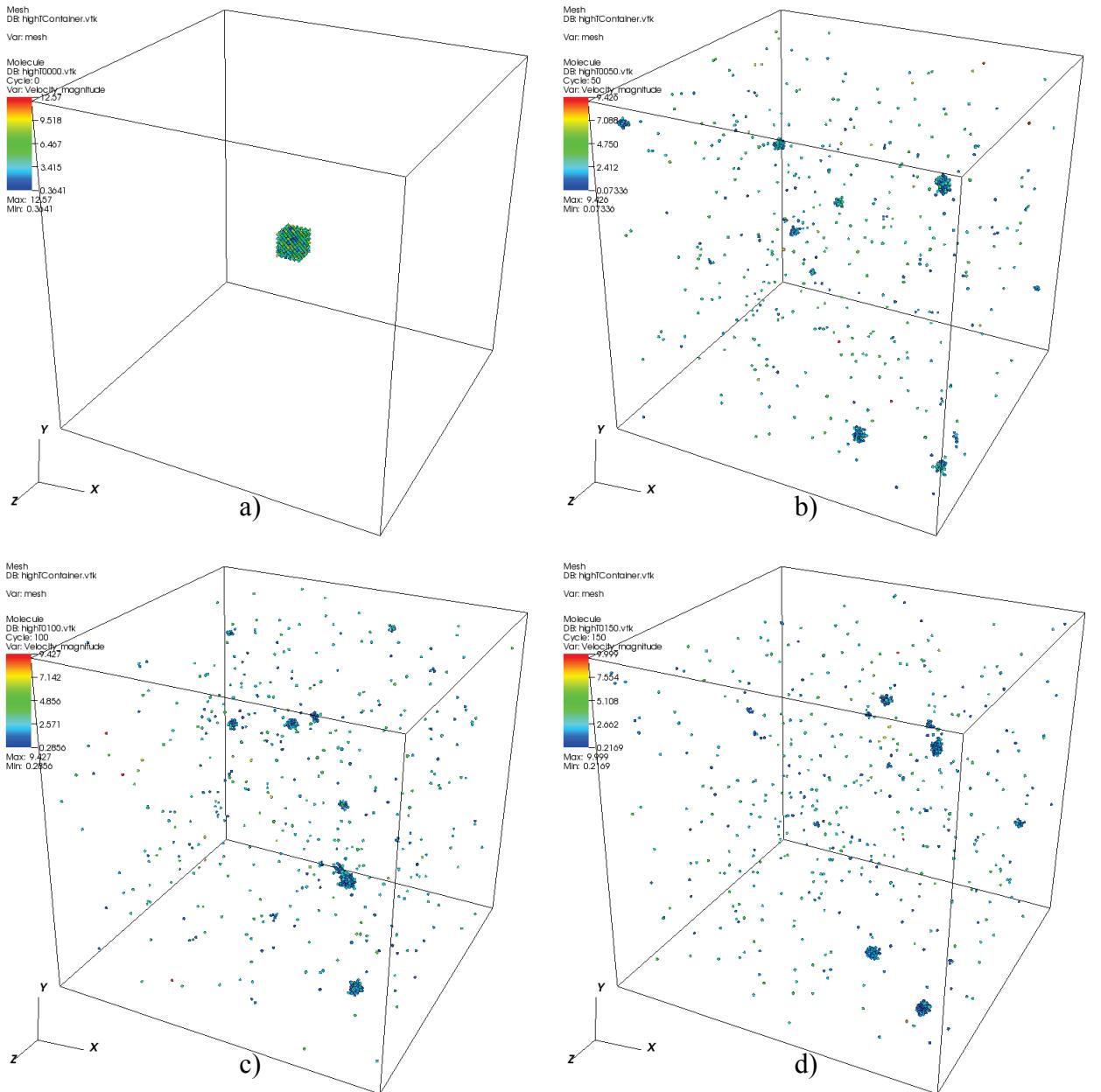


Figure 19. Snapshots of the system of Argon atoms. a) $time=0$ ps; b) $time=250$ ps; c) $time=500$ ps; d) $time=750$ ps.

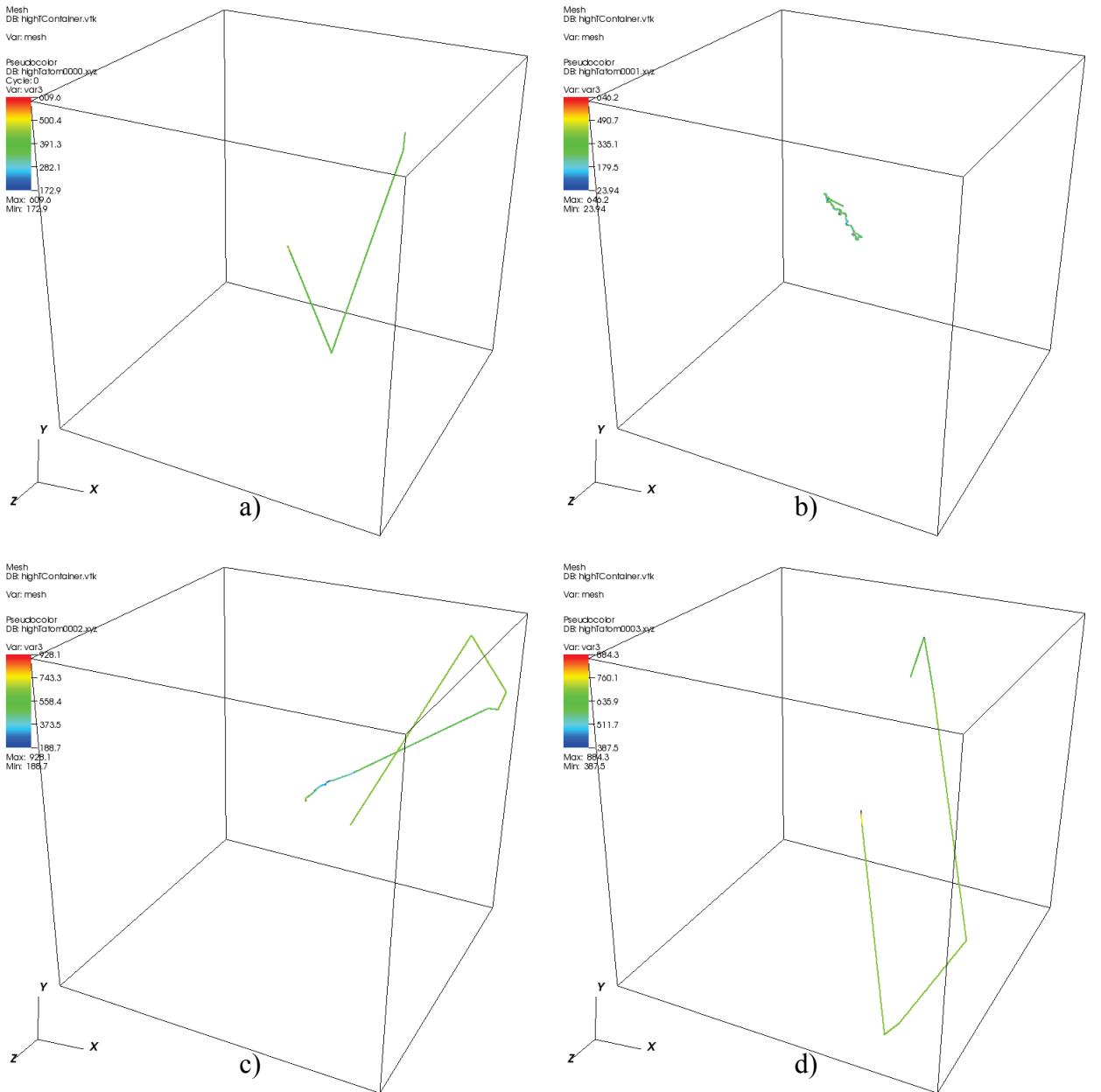


Figure 20. Trajectory of Argon atoms. a) Atom 0; b) Atom 20; c) Atom 380; d) Atom 400.

4.2. Follow Atoms of A Single Crystal

In this example 14 atoms are included in the initial crystal argon with *fcc* lattice structure and placed at the centre of the boundary cube. The cube size is 4nm in all three dimensions. Argon-Argon interaction is using LJ 12-6 and boundary potential WCA. The temperature of Argon is set 140 K at zero time step. All of the 14 atoms' trajectories are followed with the ATO input file.

4.2.1. Input

In the SEQ file, the length of each time step is 0.025 ps and a total of 240,000 steps are divided into 9 different series, with order numbers 0 through 8 beforehand. The output frequency during all of these time series are the same, saying 200. The IDs of all of the 14 atoms are orderly placed in the

ATO file, saying 0, 1, ..., 13. A total of 240,000 time steps are calculated. Following atom frequency is 5 and 20 sets of points (10,000 points in total) are recorded, which are given in the setup file.

4.2.2. Result

The coordinate and velocity trajectory of atom number 5 are illustrated in Figure 21 and Figure 22, respectively.

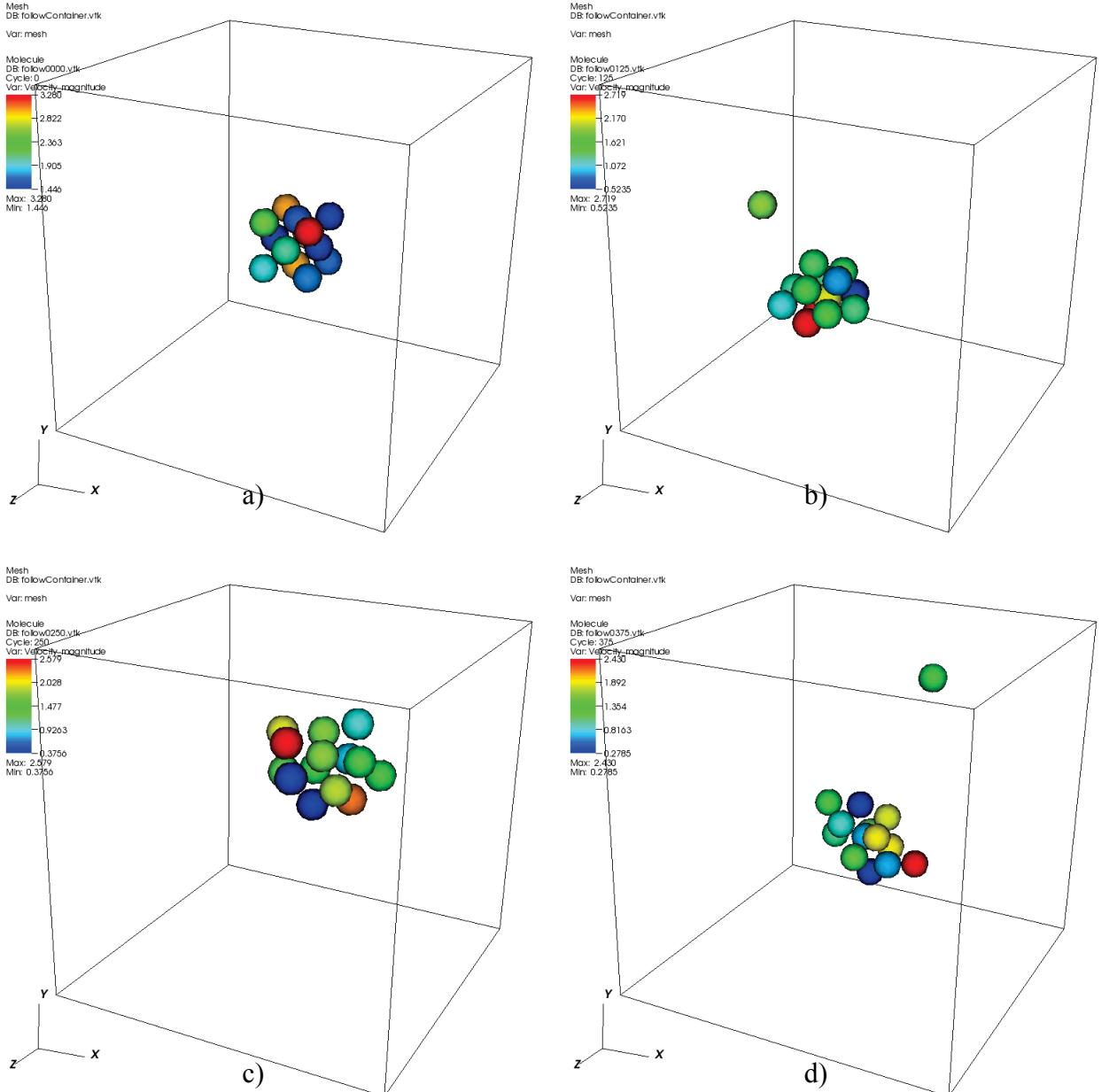


Figure 21. Snapshots of the system of Argon atoms. a) $time=0$ ns; b) $time=0.625$ ns; c) $time=1.250$ ns; d) $time=1.875$ ns.

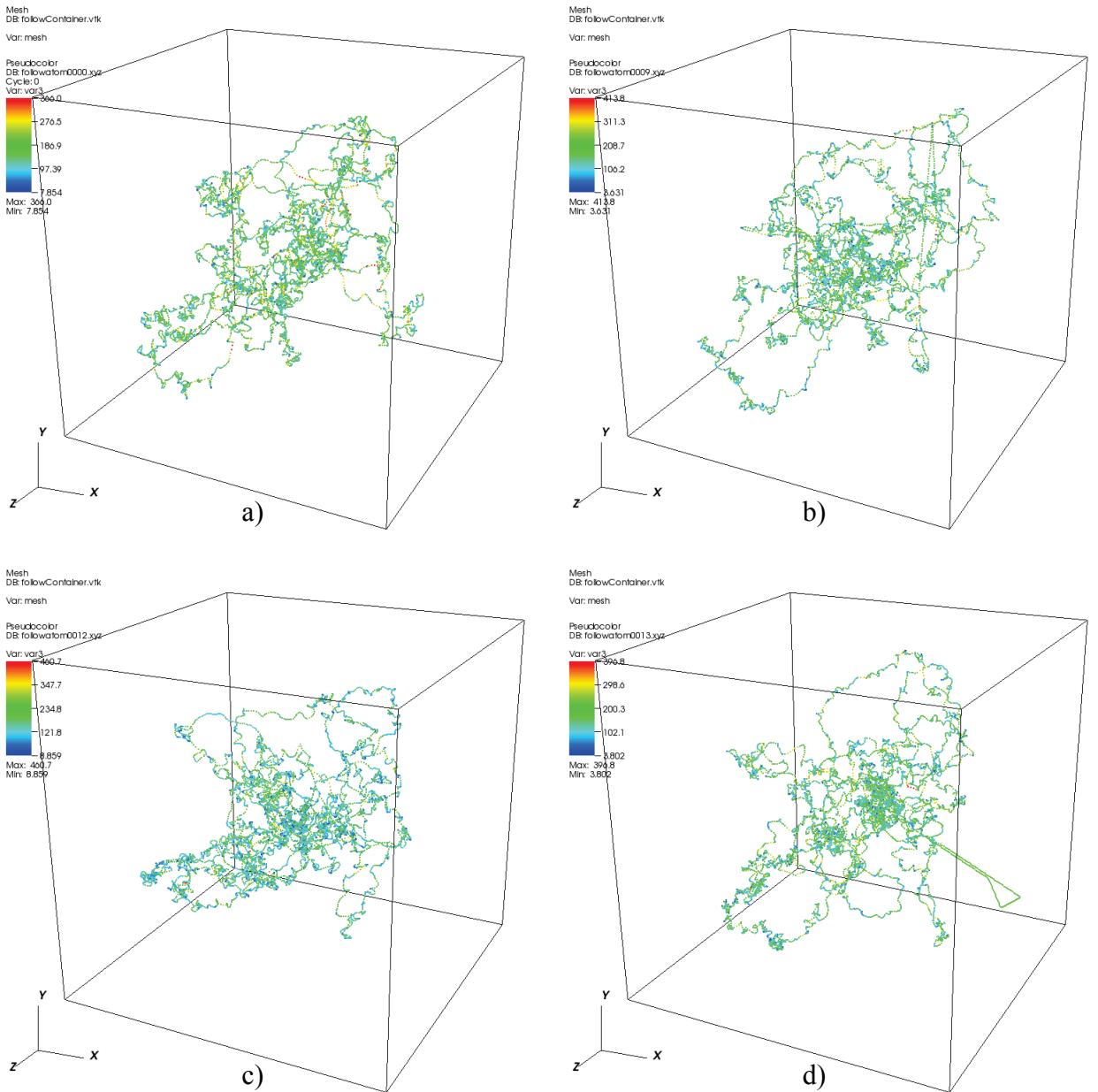


Figure 22. Trajectory of Argon atoms. a) Atom 0; b) Atom 9; c) Atom 12; d) Atom 13.

4.3. Crystal Layer

An Argon crystal comprising of 2723 atoms is initially positioned at the centre of a rigid cubical container. The size of the container is set to 1.8 nm in height and 14.4 nm in length and width. In agreement with the ratio of length to height (8:1) of the container, the crystal argon is 4.464 nm in length and height and 0.558 nm in thickness, forming shape of a "layer", as shown in Figure 23-a. The temperature of the crystal is set to 145K.

4.3.1. Input

In the SEQ file, the size of each time step is set to 0.025 ps and a total of 240,000 steps are divided into 9 different series, with order numbers 0 through 8. The number "-1" defines where the simulation will stop, e.g. in this example it was set at the time step 150,000. The output frequency

for all the time series is set to 100, i.e. every 2.5 ps. In the ATO file, 15 atoms are set to be tracked with a following frequency of 10, i.e. every 10 time steps.

4.3.2. Result

Results for this test case are shown in Figure 23 and Figure 24.

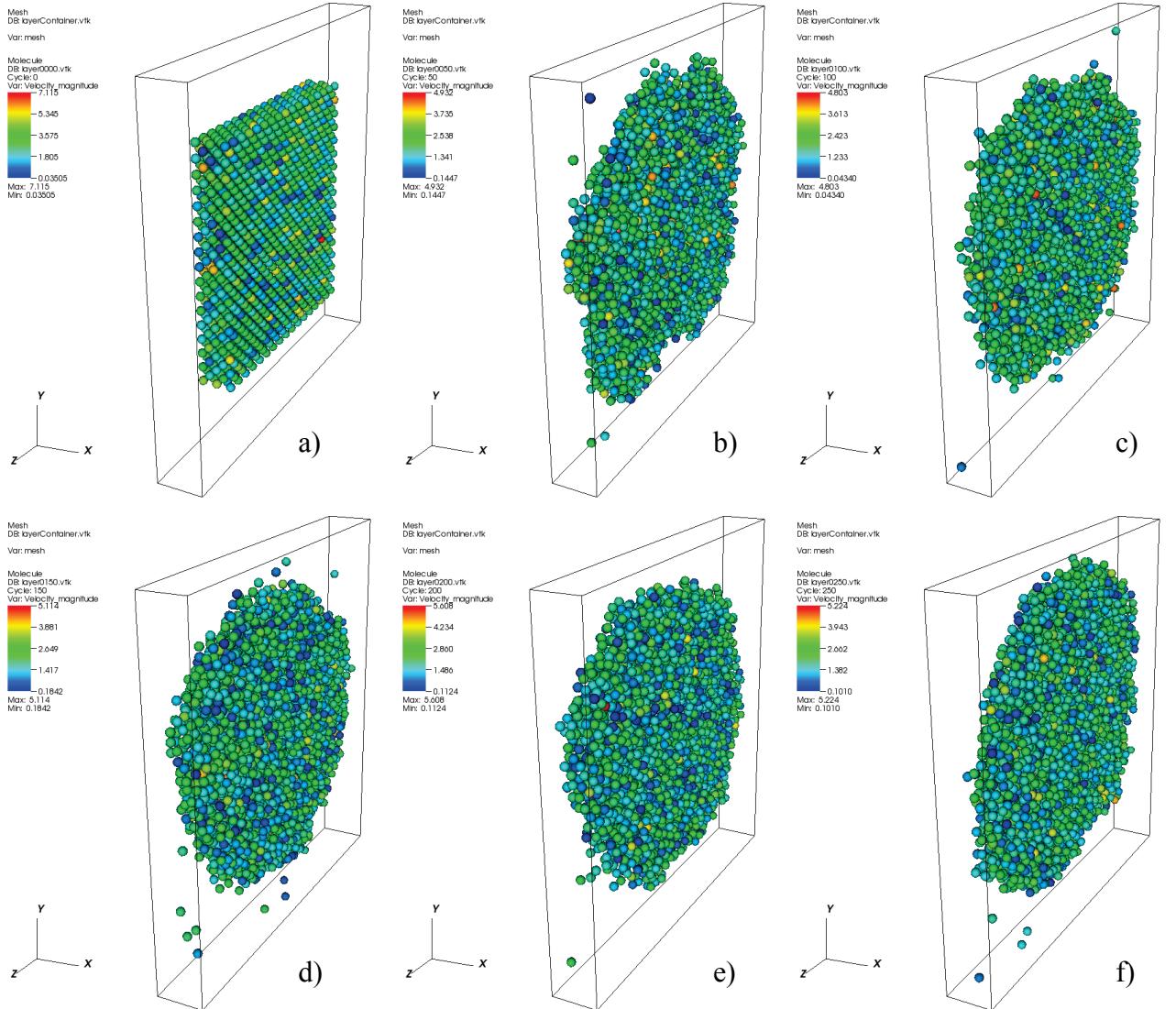


Figure 23. Sequence of a layer of atoms inside a rigid cubical container. a) $time=0$ ps; b) $time=250$ ps; c) $time=500$ ps; d) $time=750$ ps; e) $time=1000$ ps; f) $time=1250$ ps.

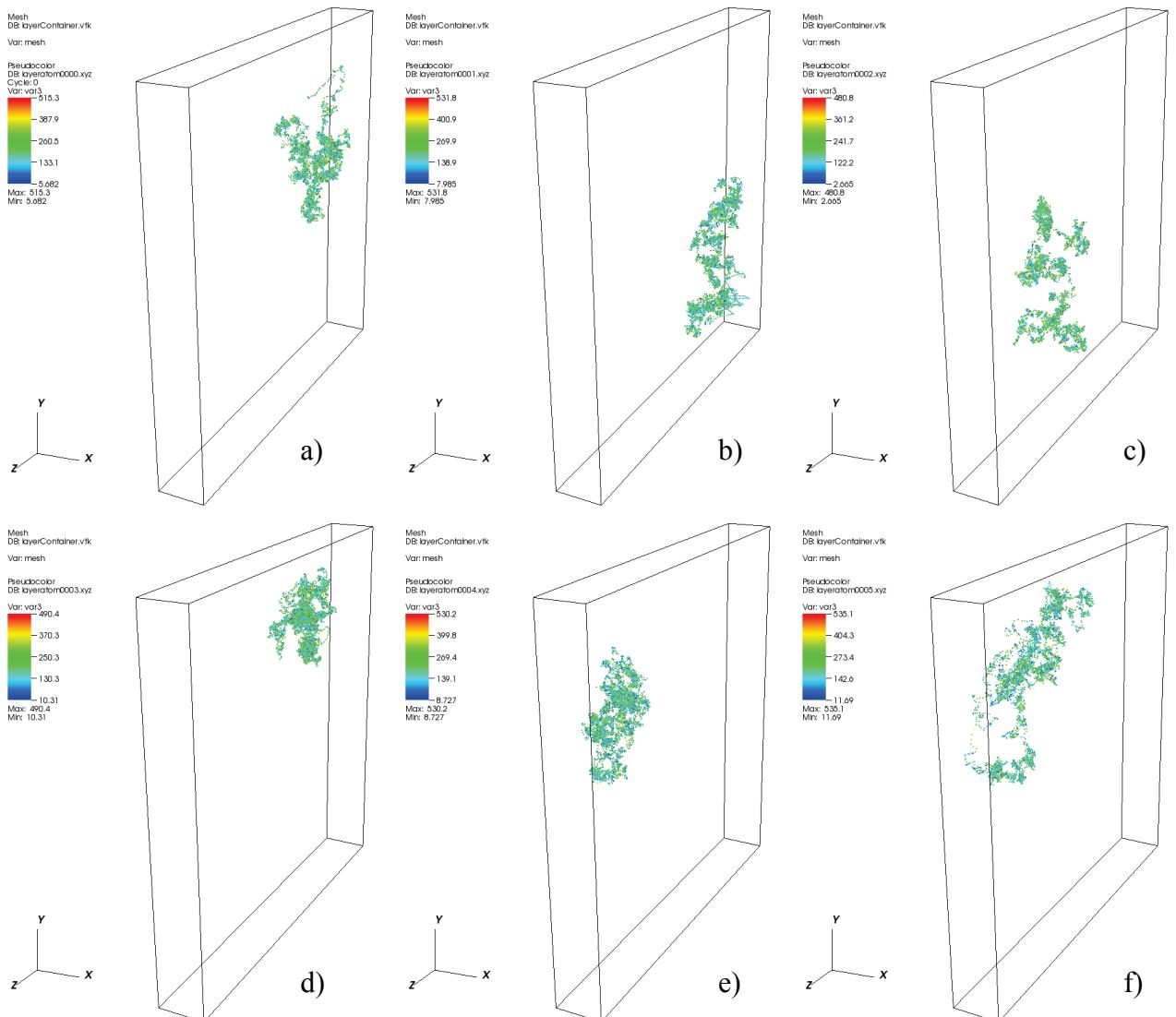


Figure 24. Trajectory of tracked atoms: a) Atom 2000; b) Atom 20; c) Atom 380; d) Atom 400; e) Atom 760; f) Atom 762.