Introduction to Ovito

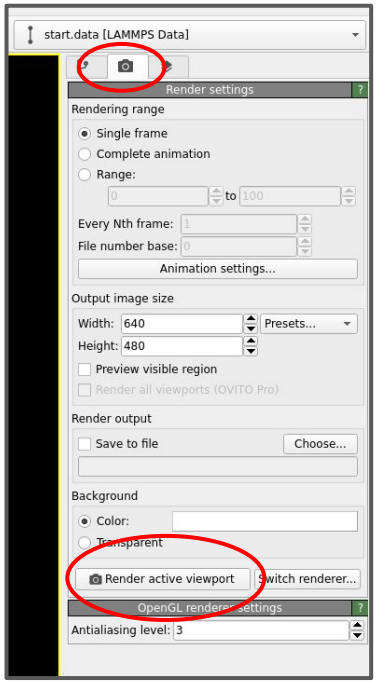
The basic functionalities of ovito is described in this Youtube video: Introduction to Ovito.
Further explanation can be found in the official user manual of Ovito.

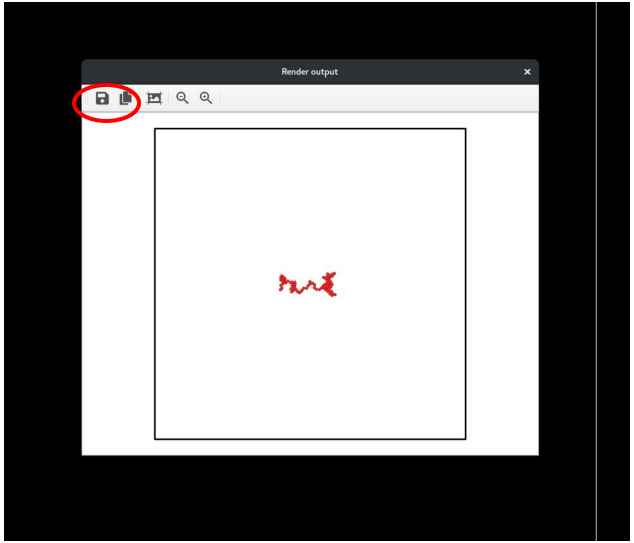
This tutorial contains the instructions on how to generate snapshots of a simulation file (start.data) using Ovito. Save the image/video file you obtained at the end of each slide to your computer. And make a powerpoint presentation with those files.

A template for the powerpoint presentation can be found at the end of this document.
You can find Ovito icon in the Desktop.

Slide 1: How to render images using Ovito

1) Open *start.data* file in ovito (follow the instructions in the video)
2) Enlarge the *Left viewport* (follow the instructions in the video)
3) Render the viewport (instructions below)
4) Save the render output to the computer (instructions below)

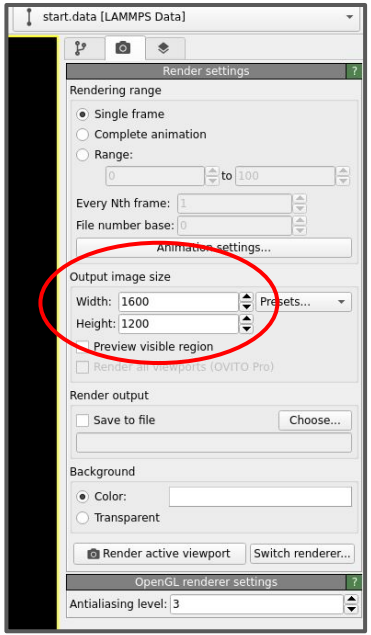




Slide 2: High resolution rendering

The image resolution in the previous slide poor. Let's remedy that:

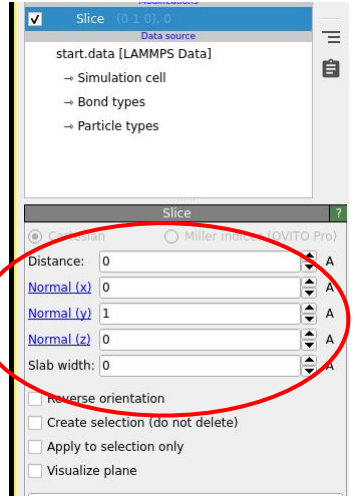
1) Repeat steps 1 & 2 from before
2) Change the *output image size* to 1600 x 1200
3) Render and save the image as before



Slide 3: Adding modifiers

Let's add some filters (also called modifiers according to Ovito) before we render the snapshot:

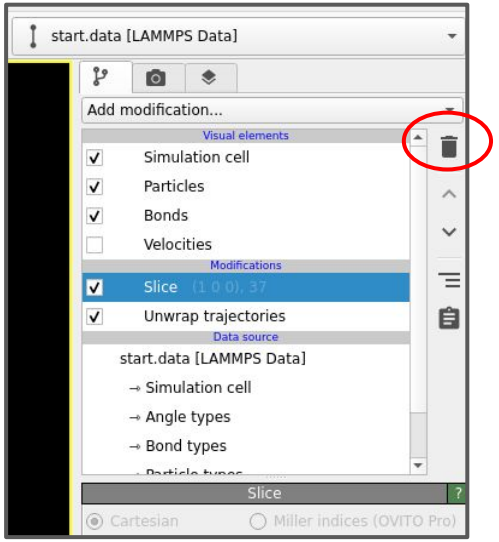
1) Open a fresh copy of start.data.
2) Add the modifier called *Slice* (see the modifiers section in the video)
3) Change the parameters of the modifier as below so that only half the box is visible
4) Render a high resolution snapshot



How to delete modifiers

Instead of opening new windows, we can remove the modifiers by deleting them.

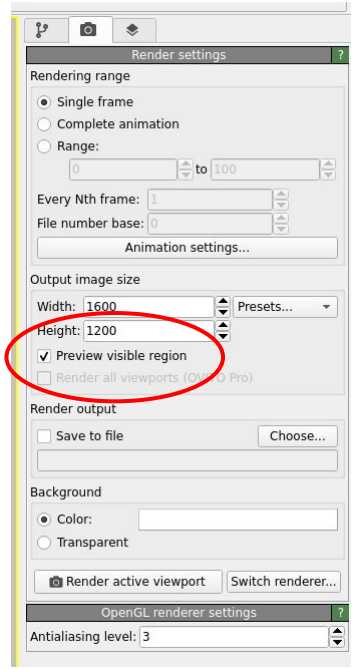
1) select a modifier and press the delete button
2) Repeat until all modifiers are deleted



Slide-4: Perspective view of the system

It is hard to see the orientation of the polymer chains from a Left view snapshot. So let's take a snapshot from a side angle.

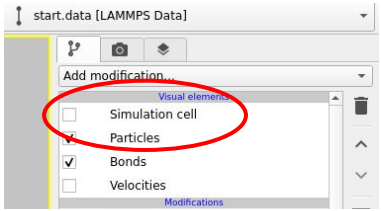
1) check the *Preview visible region* button in the render settings
2) press and hold the left mouse button to rotate the box
3) press and hold the right mouse button to position the box in the center
4) use mouse scroll to zoom in and out
5) Render the snapshot as before



Slide-5: Close-up snapshot of the molecule

If we really want to see a molecule, we need to take a closer snapshot and not show the entire empty box!

1) double click on the molecule to set the origin of the viewport to the molecule.
2) Use right, left and scroll mouse buttons to zoom in on the molecule (see the slide Perspective view of the system)
3) Hide the simulation box by unchecking the box called Simulation cell
4) Render the snapshot



Slide 6: A sequence of modifiers

The objective of this task is to capture a snapshot of only some of the particles and hide the others. This is possible by splitting it into two subtasks:

1) select the particles we want to hide
2) delete the selected particles from view

Subtask-1:

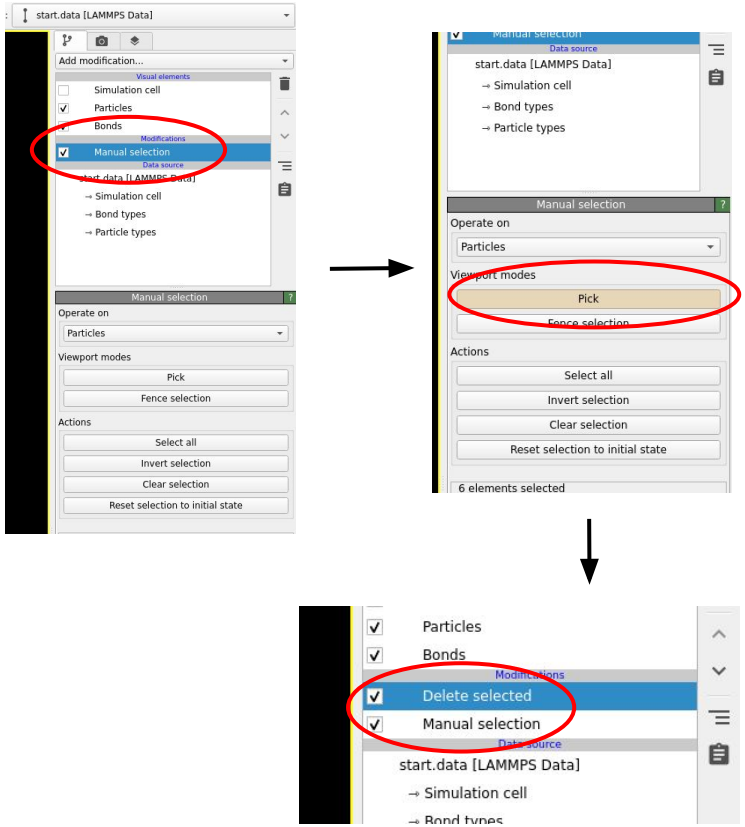
A. select the *Manual selection* modifier
B. Click on the Pick button
C. Select a few particles by clicking on the them (zoom in and you will see the selected particles turn darker red)
D. Deselect the Pick button

Subtask-2:

A. select the *Delete selected* modifier without changing the previous modifier.

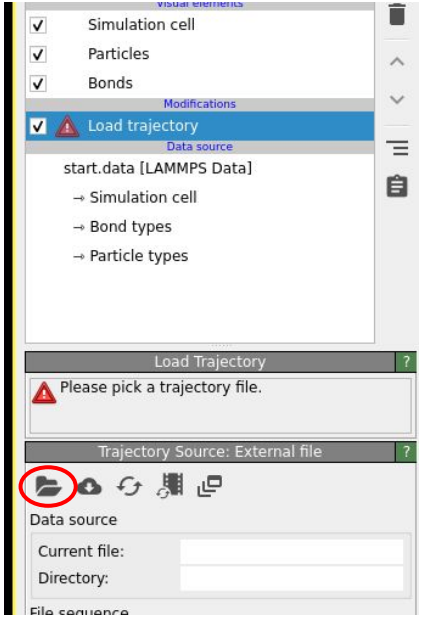
Now we can get a snapshot of a subset of particles.

Render the snapshot of the molecule (zoomed in) as before.



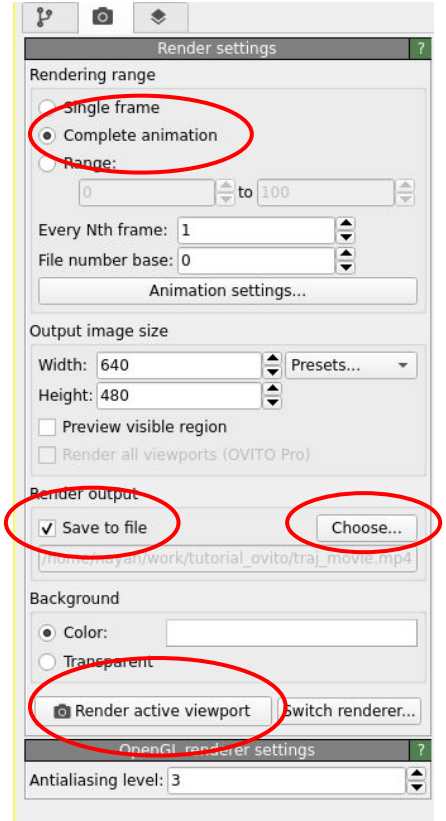
How to load trajectory file

1) Open the start.data as before
2) Select the Load trajectory modifier
3) Open the trajectory file as shown



Slide-7: Creating a video of the trajectory

1) Open the start.data and trajectory file as before
2) Select Complete animation
3) Check Save to file option
4) Click on the Choose button and write a file name (traj_movie.mp4) and save
5) Click on Render active viewport

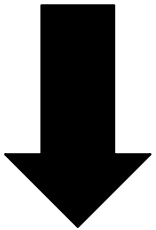


Slide-8: video with wrapped trajectory

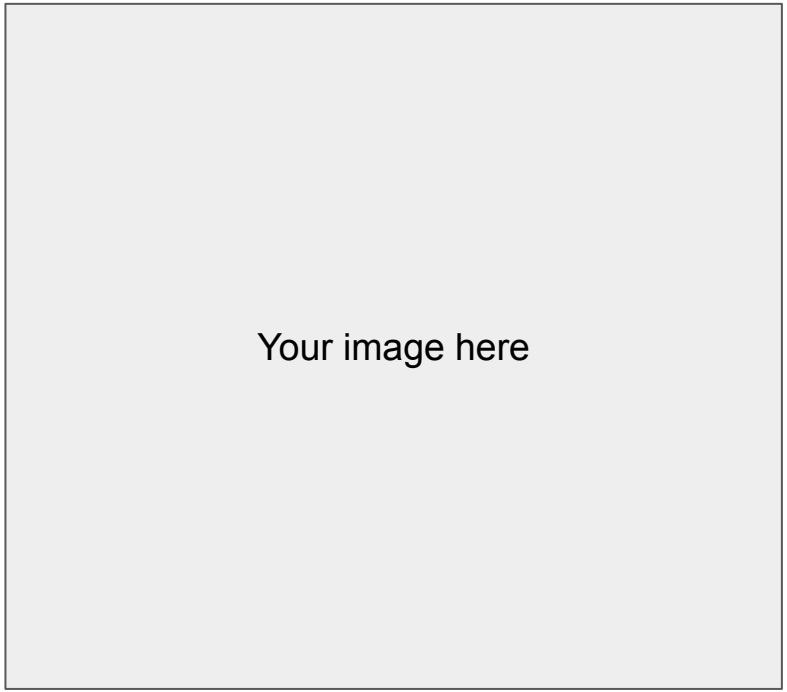
The chain went outside the box in the previous trajectory. To see the movement of the chain better, we first need to wrap the trajectory to the simulation box.

1) Open the start.data and trajectory file as before
2) Add the Wrap at periodic boundaries modifier
3) Verify that the chain remains in the box by playing the trajectory once
4) Render the video of the trajectory as before

TEMPLATE



Left view of the system



High resolution snapshot