ESPResSo Tutorial

Visualization of simulation results obtained with ESPResSo

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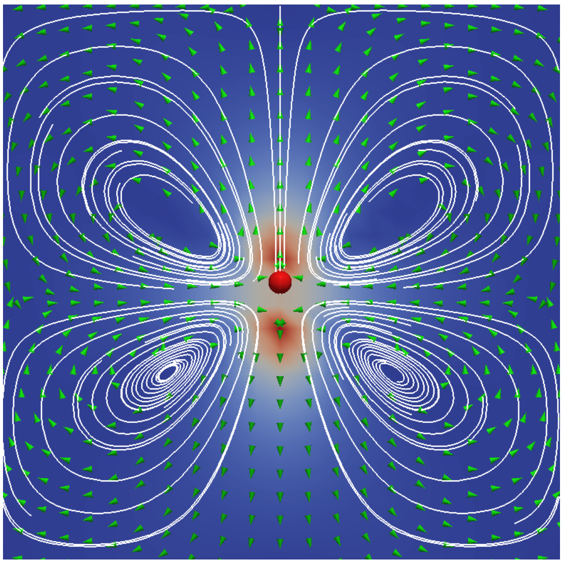

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1 Introduction

Whether you are debugging a crashing simulation, trying to understand your simulation results, or create material to explain your findings to fellow researchers – you are going to require ways to visualize what is going on in your system. Traditionally **ESPResSo** has offered an interface to VMD (Visual Molecular Dynamics), a visualization package developed with NIH support by the Theoretical and Computational Biophysics group at the Beckman Institute, University of Illinois at Urbana-Champaign [1].

While VMD is an incredibly powerful tool to visualize particle based data, it does not allow the user to include field data such as flow fields produced by coupled MD-LB simulations. To overcome this limitation, the lattice-Boltzmann and electrokinetics implementations in **ESPResSo** contain output routines producing Paraview compatible VTK files. Routines to output particle positions exist as well, which allow the user to produce images and videos of coupled MD-continuum simulations.

Tutorial Outline

At this stage, the tutorial only contains instructions on how to use Paraview with **ESPResSo** generated data. Please to the User's Guide for information on how to visualize **ESPResSo** simulations with VMD.

2 Paraview

For this part of the tutorial we are going to use Paraview, an easy to use, open source visualization program for scientific data. You should find a preinstalled version on the CIP pool computers, which you can execute with the command

```
paraview
```

If you want to use it on other computers, it is part of most Linux distributions' repositories or you can get a copy at http://www.paraview.org/.

You can output the LB velocity field and the boundary geometry from **ESPResSo** in a Paraview compatible format with the following commands

- `lbfluid print vtk boundary` *`filename`*
- `lbfluid print vtk velocity` *`filename`*

while the particle coordinates can be output using

- `writevtk` *`filename`* `[`*`particle-type`*`]`

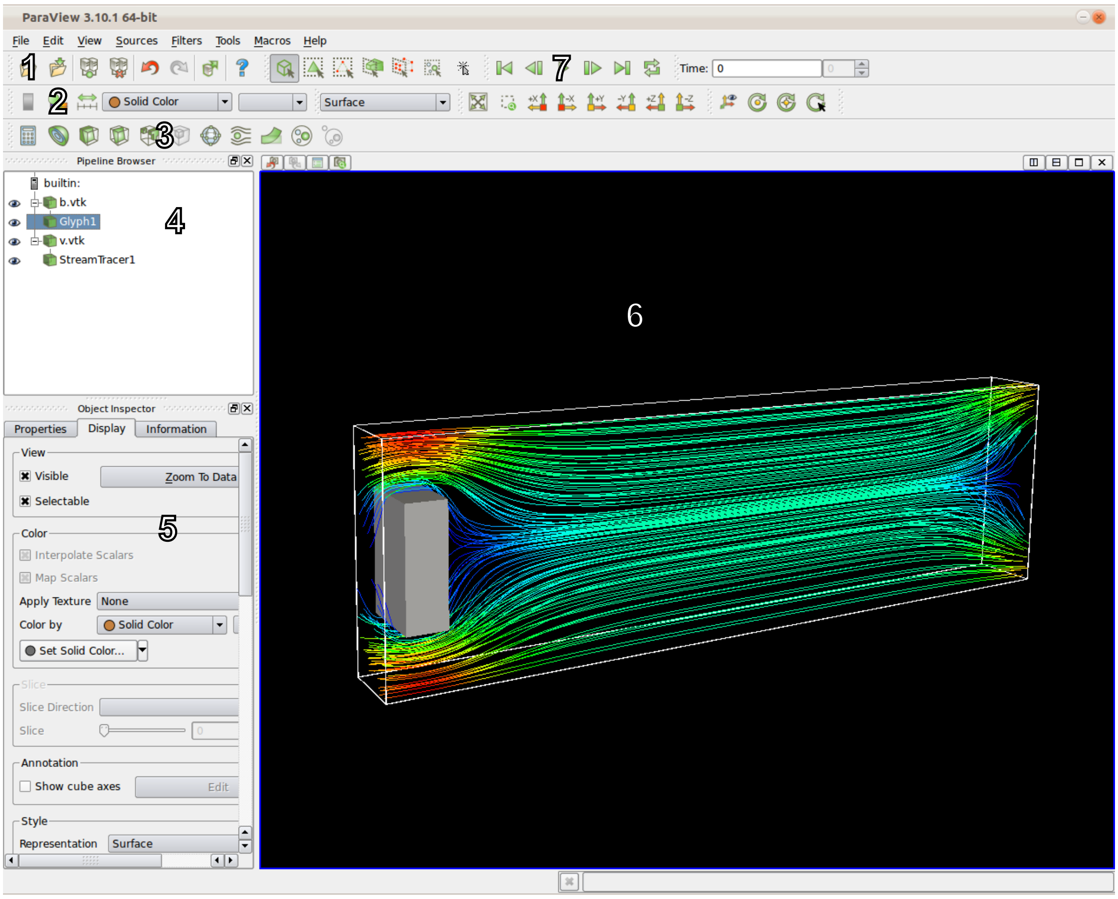
If no particle type id is given, all particle coordinates are written.

Filenames should always carry the suffix `.vtk`, so that Paraview automatically selects the correct reader upon opening. If you want to create a time series (video), you should name your files `filename_CTR.vtk` with CTR a number incremented for every frame. You can then load all these files at one with Paraview and use the video controls to step through time.

Paraview is a very flexible visualization program. You can use the GUI to create very specific visualizations for your data. Visualization methods and data post processing algorithms are contained in so-called *filters*. Filters can be chained and filter chains form a *pipeline* which can be manipulated using the *pipeline-browser*. For a start, it will be sufficient to know about the 7 Paraview controls shown in Figure 1.

1. Load data files into the pipeline for visualization
2. Adjust color settings of the filter selected in the pipeline browser
3. Add one of the most used filters to the element selected in the pipeline browser
4. The pipeline browser – shows loaded data files and filter applied to them for visualization
5. Configuration panel for the filter chosen in the pipeline browser
6. The preview panel – you can rotate, zoom and move this with the mouse
7. Controls for videos

For a start it makes sense to use a *Glyph* filter to visualize particle positions and a *Slice*, *Streamline*, or *Glyph* filter for LB velocity fields. With a little exploration, these controls should be self explanatory. If you need help, don't hesitate to consult your tutor, the Paraview help (F1) or the Paraview online documentation at http://www.paraview.org.



Time: 0

builtin:
b.vtk
Glyph1
v.vtk
StreamTracer1

☒ Visible

☒ Selectable

☒ Interpolate Scalars

☒ Map Scalars

Apply Texture None

Color by Solid Color

Slice Direction

Slice 0

□ Show cube axes

Representation Surface

Figure 1: Paraview with a sample visualization and the most important controls.

References

[1] Theoretical and University of Illinois at Urbana-Champaign Computational Biophysics group at the Beckman Institute. VMD visual molecular dynamics, 2015.