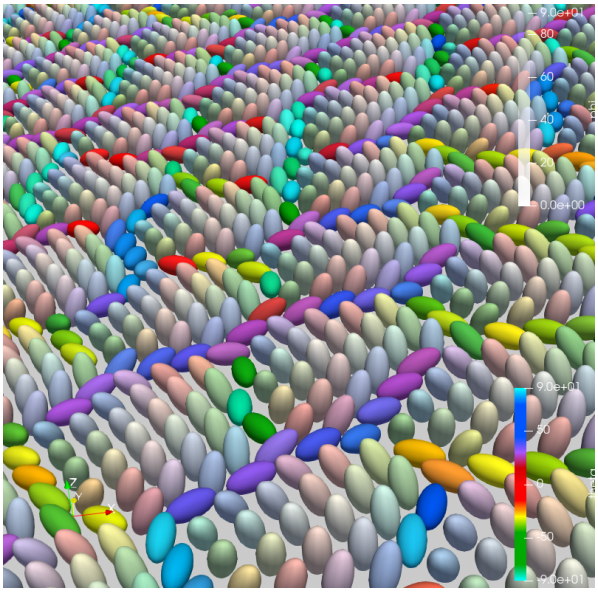
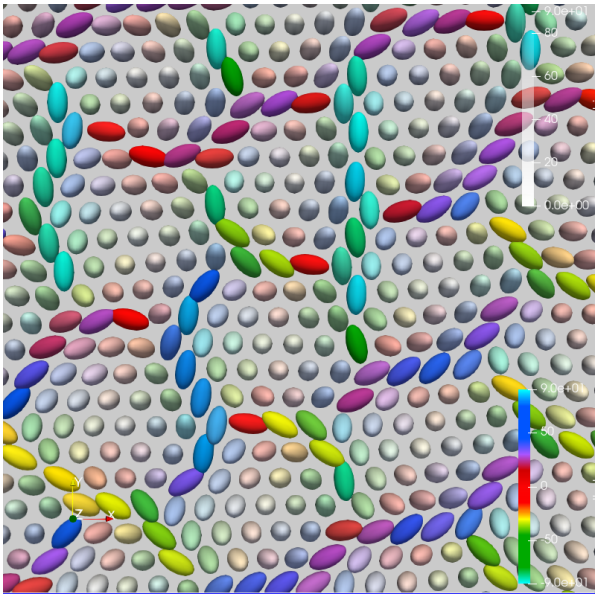
Overview

Created	@May 18, 2022 2:00 AM
Tags	

This is the user manual and reference guide to visualize ellipsoids in Paraview.

One of the goals of the project is to enable researchers to visualize the result of molecular dynamic(MD) simulation easily with Paraview.





Breakdown of directories

`data` - where input data need to be stored

`Paraview_macro` - python macro can be loaded and run in Paraview. Detail on macros is on this page

`utils` - contains helper functions to process dataframe, converting vtk file etc

Command to run

1. `git clone` `https://gitlab.com/amorphousmlops/skyrmion-visualisation.git`

2. `python pipeline.py --input_dir <data>` and generate vtk file

If you want to see the cross section of the system using plane

`python pipeline.py --input_dir <data> --plane_grad <a, b, c, d> --plane_width <> --plane_origin <x0, y0, z0>`

3. load macro `visualiseVTK.py` on Paraview
4. run `visualiseVTK.py` on Paraview

Arguments

`input_dir` - path to the directory containing input data

`vtk_dir` - path to store output vtk files

`save_csv` - If ‘on’, the program saves the processed dataframes into csv file

`video` - If ‘on’, the program creates a .vtk.series file which combines all the vtk files, which can be animated in Paraview

`scale` - Scale determines the radius of particles. This parameter is used unless scale is not specified in dataframe for each particles. Every particle will have the same scale in this way.

`ratio` - Ratio determines the shape of particles. The parameter is the ratio of the long and short axis(long/short), which are the length of the eigenvectors. This parameter is used unless ratio is not specified in dataframe for each particles. Every particle will have the same ratio in this way

Plane equation: $a \cdot (x - x0) + b \cdot (y - y0) + c \cdot (z - z0) + d = 0$

more detail on this page

`plane_grad` - parameter(a, b, c, d) to define the gradient of the plane

`plane_width` - width of 2 planes cutting the 3D particle models

`plane_origin` - origin of the plane(x0, y0, z0)

packages required

- numpy
- pandas