![System requirements](https://img.shields.io/badge/python-3.8-red.svg)

![System requirements](https://img.shields.io/badge/platform-win%2064,%20linux%2064-green.svg)

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# Analysis code for “the role of protein shape in multiphasic separation within condensates”

The GitHub space contains analysis programs for the study “the role of protein shape in multiphasic separation within condensates” by Vikas Pandey, Tomohisa Hosokawa, Yasunori Hayashi, Hidetoshi Urakubo [1].

All programs were written in Python3.8 (Windows) and designed for the analyses of output from LASSI simulation engine [2].

[1] https://www.biorxiv.org/content/10.1101/2024.08.26.606306v1

[2] https://github.com/Pappulab/LASSI

| directory | contents |

| -------- | -------- |

| \*\*`bin`\*\* |Executable programs. |

| \*\*`lib`\*\*| Shared libraries. |

| \*\*`workspace`\*\*| Accessary programs. |

| \*\*`obsolete`\*\*| Obsolete programs. |

Analyses were conducted through two steps: the conversion of lammpstrj files into intermediate data files and the visualization based on the intermediate data.

### specification\_datasets.py

Each method specifies a set of lammpstrj files and the directory/filenames for intermediate data. In the methods of “SpecDatasets” class, the following instance variables should be specified:

| instance variable | variable type | content |

| -------- | -------- | -------- |

| \*\*`self.dir\_lammpstrj`\*\* | str | Directory for target lammpstrj files. |

| \*\*`self.dir\_edited\_data`\*\*| str |Directory for intermediate data files. |

| \*\*`self.dir\_imgs\_root`\*\*| str | Directory for image files. |

| \*\*`self.filenames\_lammpstrj`\*\*| list/tuple | Filenames of target lammpstrj files. |

| \*\*`self.filenames\_edited`\*\*| list/tuple | Filenames of intermediate data files. |

The "SpecDatasets" is a superclass of executable programs, and all the executable refer the above variables.

### lib/paramters.py

It defined basic parameters such as “ID versus molecular name“, “the size of lattice space” and so on. Defined variables are referred as p.space.

### lib/colormap.py

Colors were specified.

Under documentation...

### lib directory files

Files in this directory are shared by the following executable Python files.

### all1\_edit\_data.py

All of the beginning, Simulated lammpstrj files were translated into the dict variable d that contains many.

### all2\_edit\_connectivity\_graph.py

All of the beginning, Simulated lammpstrj files were translated into the dict variable d that contains a network multigraph and generated connectivity info.

### all3\_plot\_profile.py

### all4\_plot\_profile\_3d\_ovito.py

### all5\_plot\_profile\_3d\_pyvista.py

### all6\_plot\_video\_3d\_ovito.py

### all7\_plot\_profile\_shared\_PSD95.py

### both1\_plot\_matrix.py

### both1\_plot\_matrix\_3d\_pyvista.py