Adapt your dataset for visualization

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Adjust 'input_column_names' in run.sh to match your dataset column

To visualize particles, the input column must have the coordinate of particles (x, y, z).

Other parameters such as the normal vector (nx, ny, nz) to determine the shape of particles or the size of the particles 'scale' can be added. If they are not specified, the default shape and size are going to be used for visualization which is sphere with radius 1.

Example of run.sh

```
#!/bin/bash
python3 pipeline.py \
 --input_dir data \
 --vtk_saved_dir . \
 --input_column_names x y z nx ny nz \
```

dataframe

Based on the given data from MD output files, you can add more features into the dataframe.

Some examples include

- size and shape of particles
- color of particles
- only visualize certain particles

Common errors

- **"x", "y", "z" is not used in 'input_column_names', instead "pos_x", "rx" are used. It is case sensitive**

- The program is not reading the .dat file correctly. → adjust separator in pipeline.py depending on the space in .dat file