Project Progress - Week 4 of March 2025

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This is a file that contains the tracking of the activities related to the Hydrodynamic Interactions project during the fourth week of March 2025. The activities are divided into groups and a summary of the progress is provided.

1   Initial Status of the Project

The project has made significant progress during the third week of March 2025. The key achievements include:

- The repository structure has been updated and checked.

- The dependencies have been updated in `environment.yml`.

- The setup.py file has been substituted by a pyproject.toml file, enabling developer mode installation.

- Metadata of the modules and packages have been added.

- The particles module has been modified with different classes for particle and particle sets.

- Fundamental attributes and methods have been added to the classes.

- The tests have been updated to check the new classes.

So far, the project is developing in some areas:

- The development of the Python module with the implementation functions for mobility tensor calculations.

- The development of theory to express vectors in VSH basis.

- The initial functions to establish specific particle arrangements and geometries.

2   Potential Tasks for the Week

The following tasks are proposed for this week:

- Reading of Raúl's documents on GitHub basics.

- Studying the convenience of class/functions for particle arrangements and geometries.

- Exploration/creation of Python functions that allow specific particle arrays and geometries to be established.

- Exploration/creation of Python functions that handle vector spherical harmonics (VSH) and their properties. Study of the convenience of a class.

- Creation of Python functions that allow the mobility tensor to be obtained in the basis of VSH.

- Reading of Brenner's paper [1].

3 Week Progress

3.1 Monday, March 24, 2025

The SSH connection of the new laptop to the office server has been successfully configured. The connection name is "office" and can be accessed using the command "ssh office". In addition, the connection can be activated from the VSCode command palette. The particle's module has been updated, simplifying the particles' class (Structure of Arrays philosophy). An initial structure for the geometry main class has been created, yet not tested.
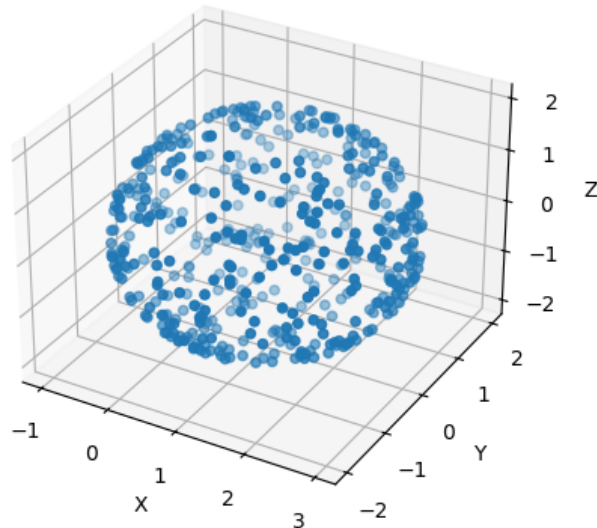

Figure 1: Plot of a 500 particle sphere.

3.2 Tuesday, March 25, 2025

The Geometry general class has been tested, and the data parameter of the particles' class has been updated. Now the initialization is better automated and the data is a list of lists, being each list composed by particle's properties. A `SphereGeometry` subclass has been created A `get_position` method have been added to the geomtry classes, and plotting and setting position methods have been added to the particles class. All test have been passed and a plot of a 500 particle sphere has been created as exposed in Figure 1. The graphs and plotting scripts should be moved to a plotting module, and examples directory or compiled as commands/executables.

4 Current Next Steps

The next steps for the project are:

- The managing of plotting outputs

- The development of the geometry module.

- The development of the VSH module.

- Reading of Brenner's paper [1].

- Reading of Raúl's documents on GitHub basics and documentation generation.

5 Summary

The project has made significant progress during the fourth week of March 2025. The key achievements include:

6 Current Status of the Project

The project is developing in some areas:

7 Next Steps

The next steps for the project are:

References

[1] Howard Brenner. "The slow motion of a sphere through a viscous fluid towards a plane surface". In: *Chemical Engineering Science* 16.3 (1961), pp. 242–251. ISSN: 0009-2509. DOI: https://doi.org/10.1016/0009-2509(61)80035-3. URL: https://www.sciencedirect.com/science/article/pii/0009250961800353.