

Project Progress - Week 3 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 third 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 second week of March 2025. The key achievements include:

- Interface of the `get_mobility_tensor` function has been updated and corrected.
- Preliminary structure of modules for the particle class has been established.

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 the week of March 10th to March 15th, 2025:

- Check of the `setup.py` installing issues.
- Reading of Raúl's documents on software development.
- 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.
- Brenner's paper [1] reading.

3 Week Progress

3.1 Wednesday, March 19th, 2025

The week tasks and current progress have been reviewed.

3.2 Thursday, March 20th, 2025

Raúl's documents on python packages development have been read.

3.3 Friday, March 21st, 2025

Based on Raúl's documents, the strcture of the repository 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.

4 Summary

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.

5 Current Status of the Project

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.

6 Next Steps

The next steps for the project are:

- 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].

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](https://doi.org/10.1016/0009-2509(61)80035-3). URL: <https://www.sciencedirect.com/science/article/pii/0009250961800353>.