Project Progress - Week 2 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 second 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 first week of March 2025. The key achievements include:

- Implementation of the .gitignore, setup.py, and __init__.py files for modular development.
- Creation, check and improvement of the test_RPY_distance.py script to obtain the RPY mobility for two particles as a function of the distance between them.
- Meeting with Rafa to discuss the creation of specific particle configurations and geometries, particularly the configuration of a sphere near a horizontal wall.

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:

- Modification of the structure of the get_mobility_tensor function, establishing default arguments and eliminating external initialization.
- 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 Monday, March 10th, 2025

The project status and potential tasks for the week have been established. The definition/interface (arguments) of the <code>get_mobility_tensor</code> function has been updated and corrected by making a copy with the name <code>get_mobility_tensor_RPY</code>. The external initialization of the variables has been removed and default values have been set for the arguments. The <code>test_RPY_distance.py</code> script tests this function.

3.2 Wednesday, March 12th, 2025

A preliminary structure of modules has been established for the particle class (possibly with methods to create arrays). Several problems have been found with the configuration of a general package for src from setup.py, and the update of dependencies in the created virtual environment, having modified the environment.yml.

4 Next Steps

The next steps for the project are:

- 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.
- 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. URL: https://www.sciencedirect.com/science/article/pii/0009250961800353.