Project Progress - Week 1 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 first 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 up until the first week of March 2025. The key achievements include:

- Meetings with Raúl to discuss the hydrodynamic interactions.
- Documentation in Notion of the basic theory behind hydrodynamic interactions.
- Preliminary exploration of the "spreadinterp" repository.
- Creation of a general function to obtain the mobility tensor given a solver and a set of particle positions.
- Initial tests for obtaining the "Self-Mobility Tensor".

2 Potential Tasks for the Week

The following tasks have been identified as potential areas of focus for the first week of March 2025:

- Development of the Python module with the implementation functions.
- Tests for obtaining the RPY tensor. Discussion of the representation and its properties.
- Initial functions to establish specific particle arrangements and geometries.

3 Week Tracking

3.1 Monday - March 3, 2025

The repository has been reorganized, and the functionalities of `.gitignore`, `setup.py`, and `__init__.py` have been discussed to manage the import of functions and modules. The use of pytest and the inclusion of asserts in the test functions are emphasized. The correct functioning of the self-mobility tensor test is verified.

3.2 Tuesday - March 4, 2025

I have been learning how to compile LaTeX projects located inside the repository. The pdf tab viewer in VSCode has been installed and configured to facilitate the visualization of the documents. This document serves as an example of the compilation process.

3.3 Wednesday - March 5, 2025

The tasks for the week have been specified and the progress in documentation, code, and testing has been tracked. The script `test/test_RPY_distance.py` has been created to obtain the RPY mobility for two particles as a function of the distance between them. The script checks the symmetry of the tensor, the reproduction of the self-mobility elements on the diagonal, the symmetry of the elements of the off-diagonal blocks of cross mobility, the nullity of the elements corresponding to crossed coordinates (the particles are on the x-axis), and the equivalence between the two yy, zz terms (perpendicular to the axis that joins the particles) of the cross mobility diagonal. The script also generates a graph with the dependence of the non-zero elements of the cross mobility with the distance between the particles, from 0.1 to 10 times the hydrodynamic radius of the particles. The ordering and storage of this type of graphs in the repository must still be studied.

3.4 Thursday - March 6, 2025

Added checks to the test file `test_RPY_distance.py` that include the equivalence between the analytical result and the matrix obtained in the numerical calculation. The code has been refactored to separate functions, with one function for generating the graph and another for the array of analytical tensors. Additionally, the `output/` directory has been created to store the graphs generated by the test scripts. The figure shown in

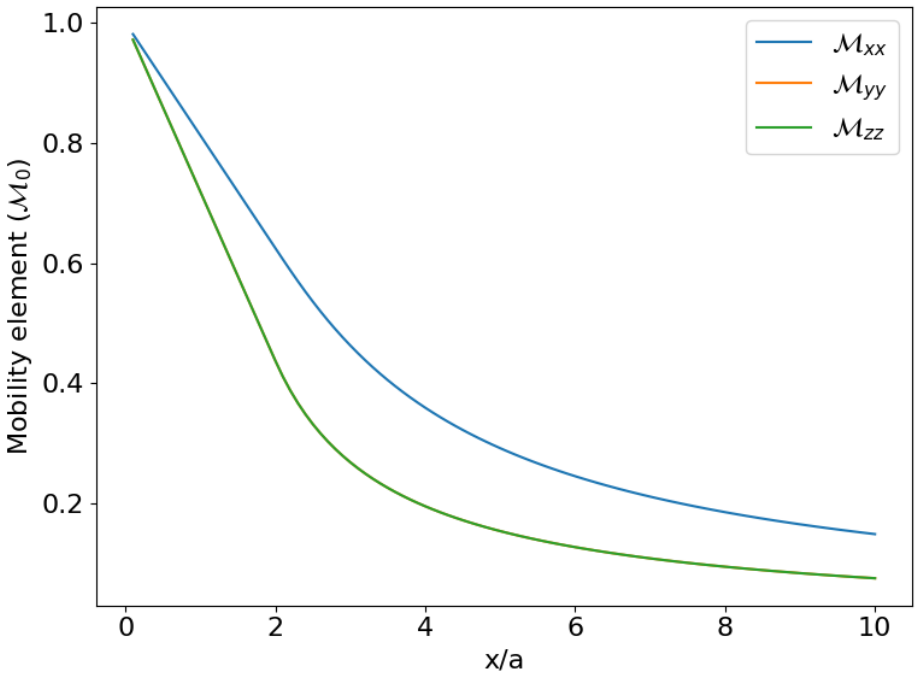

Figure 1: RPY mobility for two particles as a function of the distance between them.

Figure 1 depicts the RPY mobility for two particles as a function of the distance between them. The mobility decreases with distance, decaying exponentially when the particles do not overlap. It can be observed that the mobility is higher in the direction of the line connecting the particles and lower in the perpendicular directions. When the particles overlap, the mobility decreases linearly with distance. In the case of complete overlap where the particles are in the same position, the mobility is the same as the self-mobility of an isolated particle. No singularities in the mobility are observed in the case of complete overlap.

Doubt

What does the overlap of the particles mean?

3.5 Friday - March 7, 2025

The plot functionality has been removed from the testing code, as discussed with Raúl regarding the convenience of creating plots in non-testing scripts. Additionally, emphasis has been placed on the importance of building good function interfaces (declarations, arguments, and returns) that simplify and minimize complexity for ease of use and scalability. A meeting with Rafa was held to provide an overview of the current project status, with a focus on tasks such as creating specific particle configurations and geometries, particularly the configuration of a sphere near a horizontal wall (potentially a liposome system). The idea is to apply an external force to the sphere and observe its displacement and deformation. This can be useful for future treatment of surface interactions and the modes of vibration of an immersed or nearby liposome in relation to a surface, as well as the decomposition of forces and velocities in the basis of vector spherical harmonics.

4 Next week tasks

The next steps for the project include:

- 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.
- Brennan's paper reading.