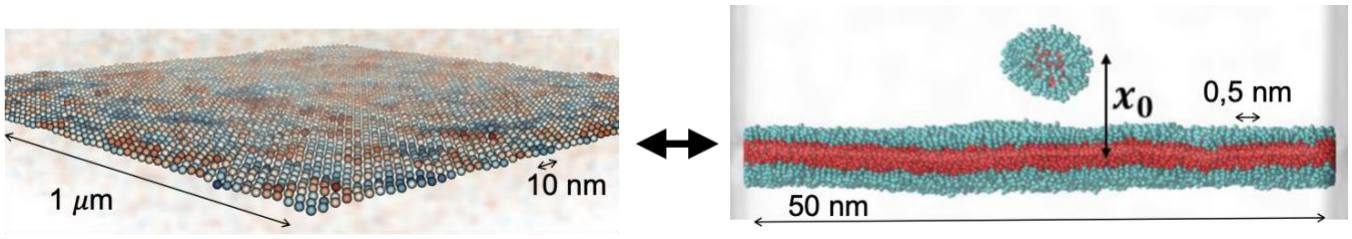
Transport near Wiggly Membranes

Membranes are at the heart of environmental and medical applications. From the environmental point of view, they are key in water desalination, filtration, and the generation of renewable, so called “blue energy” from salt concentration differences. From a medical point of view, membranes regulate transport to and in between cells, and are also used in drug carrier or virus detection applications. In all of these diverse membrane systems, mixing, separation, and diffusion are all transport phenomena that are strongly modified by membrane fluctuations. Indeed, as membranes are soft and deformable, they fluctuate, affecting the motion of water molecules and, hence, of potentially larger particles nearby. For instance, fluctuations in the inner membrane of a biological pore can dramatically modify the passage of molecules. Experiments in nanofluidics show mechanical vibrations can couple to fluid particle transport in specific geometries. This diversity of results typically shows how little we know about the mechanisms that can modify transport near wiggly membranes [1,2].



Visualization of the 2 membranes used to investigate nearby transport at complementary scales. Right hand side from [3]

How is the diffusion of particles, individual or collective, modified by the presence of the membrane? How do weak interactions with the membrane affect transport? How do these corrections depend on the distance to the interface? And are these different effects coupled?

To investigate the motion of particles near wiggly membranes, we will use a combo of 2 simulation techniques at small and large scales, and investigate the motion of diverse particle suspensions in the vicinity of a wiggly membrane (as illustrated in Fig. 1, see also [3]). We will then analyse the results with various data analysis tools: from single particle trajectories, to structure factors, and an innovative method of counting particles in virtual observation boxes (``The Countoscope'') [4]. The internship will be in collaboration between Micheline Abbas and Sophie Marbach, offering the possibility to work either in Toulouse or Paris.

Tools learned/used: Simulations: Molecular Dynamics/Dissipative particle dynamics/Stochastic simulations & Data Analysis & Using or Deriving theories based on Statistical Physics and Mechanics

A few references

[1] S. Marbach, D. Dean, L. Bocquet, Nature Phys. 2018, https://doi.org/10.1038/s41567-018-0239-0
[2] Zhang, Z., Bertin, V., Arshad, M., Raphael, E., Salez, T., & Maali, A. , *Phys Rev. Lett.* 2020 https://doi.org/10.1103/PhysRevLett.124.054502
[3] Sheikh, S., Lonetti, B., Touche, I., Mohammadi, A., Li, Z., & Abbas, M , *J Chem Phys* 2023 https://doi.org/10.1063/5.0182499
[4] E.K.MacKay, S. Marbach, B. Sprinkle, A. Thorneywork, ArXiv 2024 https://doi.org/10.48550/arXiv.2311.00647

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