SORBONNE UNIVERSITÉ

Laboratoire
PHENIX

Master thesis proposal

Campus Pierre et Marie Curie,
Sorbonne Université
Director: Laurent Michot

Title: Modeling droplet growth on chromosomes

Keywords: Simulations, polymers, phase transition, biophysics

Scientific description:

Recent innovations in imaging techniques have led to the discovery of new types of structural organization inside cells [1]. Similar to liquid-liquid emulsions, intracellular fluids separate to form liquid or solid droplets. Specifically, **protein droplets form on the surface of chromosomes**, at a scale of about 100 nm (see Figure 1. A-B). The underlying physics and chemistry are still poorly understood. A better understanding could, however, shed light on some intriguing experimental results, such as the observed propulsion of droplets [2].

In our team, we model and simulate these phenomena numerically. We develop simple models of the wetting of fibers by droplets. The fibers model chromosomes, and the droplet material is made of spherical particles. **We can simulate the trajectories of individual particles**, which has already allowed us to study the influence of molecular interactions on droplet growth dynamics and shape (Figure 1, C). Currently, we are working on extending these models to study complex dynamics around many concentrated fibers, analogous to the behavior of a liquid evolving on a spider web

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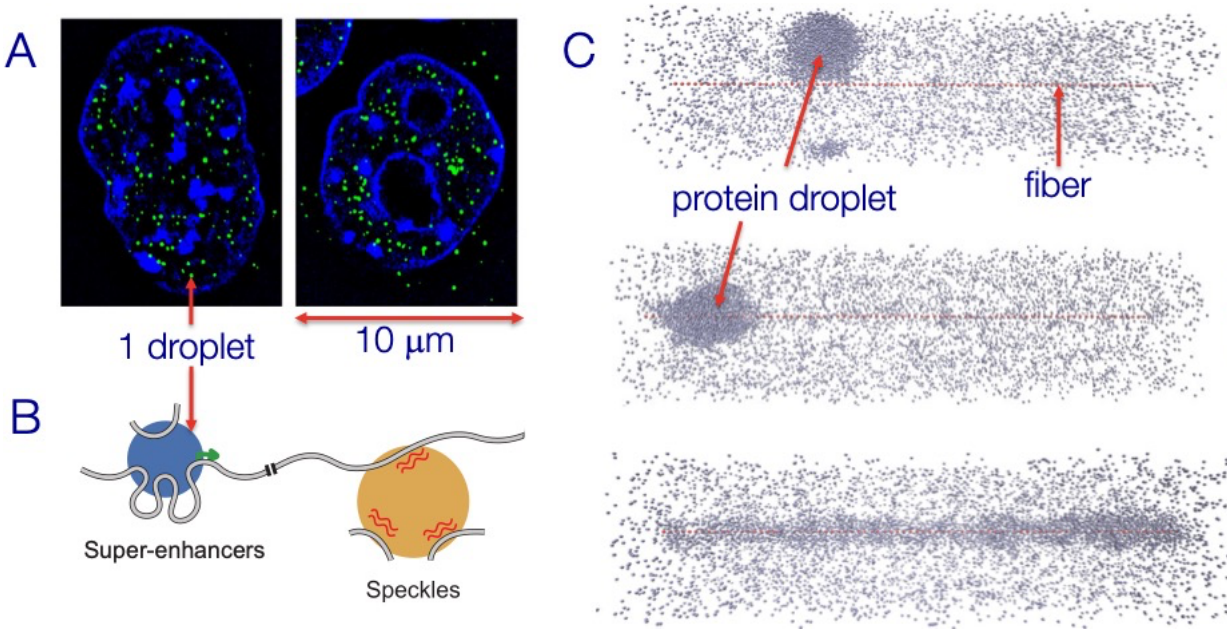

Figure 1: Biomolecular droplets around chromosomes: imaging and simulations. *(A) Super-resolution microscopy of fluorescently labelled DNA-binding proteins (from Ref [1]). The green dots show droplets, that form around a fiber of DNA as drawn in (B). (C) Preliminary investigation of protein droplet formation around DNA : Snapshots from Brownian Dynamics simulations (The DNA-protein interaction increases from top to bottom).*

During this internship, we will add *chemical reactivity* to our models of droplets on chromosomes. In previous projects, we have already included chemical reactions in models of self-propelled colloids [3] and active emulsions [4]. It is known that the droplet contains proteins that catalyze reactions on the surface of chromosomes. We hypothesize that such reactions will influence the wettability of the surface and thus be strongly correlated with the dynamics and structure of the droplets.

References

[1] B. R. Sabari et al, Trends in Biochemical Sciences, 2020, 45-11
[2] J. Kim, K. Y. Han et al, Journal of Cell Science, 2019, 132
[3] J. Decayeux, V. Dahirel, M. Jardat, P. Illien, Phys. Rev. E, 2021, 104(3)
[4] R. Berthin, J. Fries, M. Jardat, V. Dahirel, P. Illien, arXiv, 2024, preprint arXiv:2406.14256.

Techniques/methods in use:
This internship consists in a theoretical work based on numerical simulations. **Reactive Brownian Dynamics simulations** will be handled, as in [3-4].

Applicant skills: Basic coding skills (C, python…).

Internship supervisor(s) (name, email, phone, …):
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Internship location: UMR PHENIX Campus Pierre et Marie Curie, Sorbonne Université

Possibility for a Doctoral thesis: Y