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**SEMINAIRE**

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**« Modelling F-actin bundles pushing hard obstacles and flexible membranes »**

With the aim of predicting the polymerization force of a F-actin bundle in various situations, we have studied bundles interacting with various kind of obstacles during the actin polymerization process (supercritical conditions).

In presence of a hard smooth obstacles, like in optical trap experiments, we employed a Fokker-Plank approach based on the number of monomers per filaments and the obstacle position. We developed an original model to introduce filament flexibility based on the discrete-Wormlike-chain model and show how the behavior of this model is considerably richer than the simpler Brownian Ratchet model predictions used in interpreting experiments. In particular we show how flexibility enhances the transduction of chemical into mechanical energy, hence the ability of a bundle to displace the obstacle.[1,2,3,4]

A different coarse-grained particle-based model has been developed to study bundles interacting with a flexible fluid membrane. The fluid membrane is represented as a triangulated surface with bond-flips to model fluidity and with grandcanonical bond insertion-deletion moves to allow the membrane to grow under the pushing action of the filaments. Filaments are modeled as semi-flexible assemblies of monomers and the (de)polymerization events are assumed to occur with fixed rates. Preliminary results show that specific characteristics of the bundles, rather important for hard obstacles, are less relevant for flexible obstacles.[5]

**REFERENCES**

- [1] C. Pierleoni, G. Ciccotti and J.-P. Ryckaert, "A semi-flexible model prediction for the polymerization force exerted by a living F-actin filament on a fixed wall", *J. Chem Phys.* **143**, 145101 (2015).
- [2] A. Perilli, C. Pierleoni, G. Ciccotti and J.-P. Ryckaert, "On the properties of a bundle of flexible actin filaments in an optical trap", *J. Chem Phys.* **144**, 245102 (2016).
- [3] A. Perilli, C. Pierleoni, G. Ciccotti and J.-P. Ryckaert, "On the force-velocity relationship of a bundle of rigid bio-filaments", *J. Chem Phys.* **148**, 095101 (2018).
- [4] A. Perilli, C. Pierleoni, and J.-P. Ryckaert, "Filament flexibility enhances power transduction of F-actin bundles", arXiv:1806.08767v2
- [5] A. Perilli, C. Pierleoni, and J.-P. Ryckaert, in preparation.

**Jeudi 13 décembre 2018**

**14h30**

**Salle de conférences**