



Multiscale modelling of actin filaments

We are currently seeking a highly motivated postdoctoral fellow who will be mentored by Dr. Matthieu Chavent (IPBS, Toulouse, <http://matthieuchavent.com>) and Prof Jean-Philip Piquemal (Sorbonne University, Paris, <https://piquemalresearch.com>). The researcher will be hosted in Dr Chavent's lab in Toulouse and will regularly visit Prof Piquemal in Paris. The **postdoc** will be funded for **2 years** with a possibility of extension **starting January 2021**. The deadline to send an application is the **1st of December 2020**.

Project:

The goal of this project is to investigate, at the atomistic level, the mechanics of actin filaments and understand how external forces can modulate them. To do that, the candidate will perform high performance computing of polarizable forcefield using Tinker-HP [1], atomistic simulations, and up to coarse-grain models [2]. The results will then be combined to numerical and analytical models developed by our collaborator Dr Dmitrieff to design new mesoscale models [3]. The models will be validated at different scales by our collaborator experimentalists (see below).

- [1] L. Lagardère, L.-H. Jolly, F. Lipparini, F. Aviat, B. Stamm, Z. F. Jing, M. Harger, H. Torabifard, G. A. Cisneros, M. J. Schnieders, N. Gresh, Y. Maday, P. Y. Ren, J. W. Ponder, and J.-P. Piquemal, "Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields" *Chem. Sci.*, vol. 9, no. 4, pp. 956–972, Jan. 2018.
- [2] M. Chavent, E. Seiradake, E. Y. Jones, and M. Sansom, "Structures of the EphA2 Receptor at the Membrane: Role of Lipid Interactions" *Structure* (London, England : 1993), 2016.
- [3] M. Mund, J. A. van der Beek, J. Deschamps, S. Dmitrieff, P. Hoess, J. L. Monster, A. Picco, F. Nédélec, M. Kaksonen, and J. Ries, "Systematic Nanoscale Analysis of Endocytosis Links Efficient Vesicle Formation to Patterned Actin Nucleation" *Cell*, vol. 174, no. 4, pp. 884–896.e17, Aug. 2018.

Team and collaborations:

The fellow will be hosted in the team of Matthieu Chavent (<http://matthieuchavent.com>) in Toulouse, south west of France. The IPBS (<http://www.ipbs.fr>) and the Toulouse Paul Sabatier University nearby host teams constituted by both experimental and theoretical researchers with a long collaborative and interdisciplinary history, which will be beneficial for researchers working at the interface of mathematics, informatics and structural biology. Development and applications of polarizable forcefield will be done in the team of Prof Jean-Philip Piquemal (<https://piquemalresearch.com>) at Sorbonne University, Paris, France.

Close collaborations will be established with Serge Dmitrieff (<http://biophysics.fr>, Institut Jacques Monod, Paris) to refine his meso-scale models of actin filaments and develop a multiscale framework to link polarizable simulations up to mesoscale model. The multiscale modeling strategy will be validated thanks to interactions with Antoine Jégou and Guillaume Romet-Lemonne team (<https://www.actindynamics.net>, Institut Jacques Monod, Paris) and Renaud Poincloux (IPBS, Toulouse, <http://www.ipbs.fr/member/renaud-poincloux>).

Minimum Requirements

- Ph.D. in Computational Structural Biology, Biophysics or closely related disciplines.
- Familiarity of Linux operating systems.
- Experience with at least one of the following programming languages: python, tcl, C++.
- Experience with molecular dynamics simulations.
- Experience with high-performance computing environments.
- Record of published peer-reviewed research articles.
- Ability to work independently and communicate effectively.

Desired Qualifications

- Graduate training in biophysics, physical chemistry, and/or structural biology.
- Experience with computational studies of biological systems at different scales (QM-AT, AT-CG, CG-Meso).

Required Application Materials to send to M. Chavent and J.P. Piquemal by email

- Curriculum vitae
- List of two references
- List of peer-reviewed publications

Dr. Matthieu Chavent

IPBS institute, UPS university, Toulouse, France.

E-mail : matthieu.chavent@ipbs.fr

Website: <http://matthieuchavent.com>

Prof. Jean-Philip Piquemal

Laboratoire de Chimie Théorique, Sorbonne
Université, Paris, France,

& Institut Universitaire de France,

& UT Austin, Department of Biomedical Engineering,
USA.

E-mail : jean-philip.piquemal@sorbonne-universite.fr

Website: <http://piquemalresearch.com>