

**RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM****Field: Mathematics and their applications****Subfield:** (Statistical mechanics, statistics, applied mathematics)**Title:** Irreversible algorithms for molecular modeling**ParisTech School:** ESPCI Paris | PSL**Advisor(s) Name:** Anthony Maggs**Advisor(s) Email:** anthony.maggs@espci.fr**Research group/Lab:** Gulliver**Lab location:** ESPCI, 10 rue Vauquelin Paris 75005**(Lab/Advisor website):** <https://www.gulliver.espci.fr/>**Short description of possible research topics for a PhD:**

Molecular modeling (research rooted in particle-based computation) is central to our understanding of the material world. Its methods allow one to investigate complex phenomena in biophysics and materials research, and to describe the fundamental phase behavior of the universe that surrounds us. Molecular modeling has provided methods for many other fields, from astrophysics to hydrodynamics, statistical mechanics and field theory. Molecular modeling is an interdisciplinary research field, in which the development of algorithms plays an important role. Improved sampling methods, constrained ensembles, and novel approaches beyond molecular dynamics stand out in their promise for the future.

Although the principal methods have been developed for over half a century, disruptive development continues to take place. An example is the irreversible Markov-chain Monte Carlo methods which violate the fundamental detailed-balance condition yet converge towards equilibrium. They illustrate that past algorithms were overly restrictive. Radically new Markov-chain Monte Carlo algorithms have already led to the resolution of long-standing controversies (as for example in two-dimensional melting studied through the use of irreversible Markov chains). We wish to extend these methods to standard interaction potentials in soft-matter physics, in the belief that this can lead to highly efficient codes that explore equilibrium configurations using irreversibility flows.

**Required background of the student:**

We are looking for students with background in statistical mechanics, applied mathematics or statistics who are interested in joining an open collaboration between several groups in the historic center of Paris.

**A list of 5 (max.) representative publications of the group:**

[All-atom computations with irreversible Markov chains](#), M.F. Faulkner, Liang Qin, A.C.

Maggs and Werner Krauth, J.Chem Phys (2018).

<https://aip.scitation.org/doi/10.1063/1.5036638>

Event-chain Monte Carlo with factor fields, Ze Lei, Werner Krauth, and A. C. Maggs, PRE (2019). <https://doi.org/10.1103/PhysRevE.99.043301>

