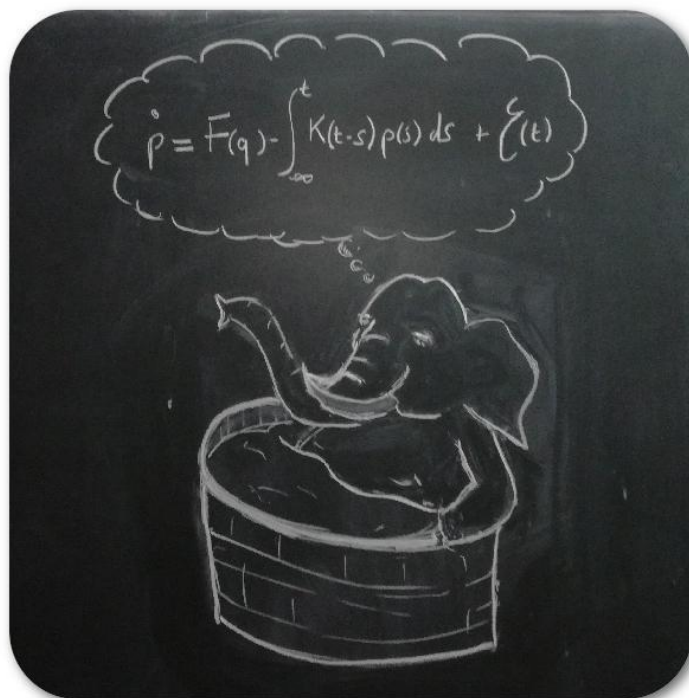


Extended Discussion Meeting:  
***Generalized Langevin Equations  
in classical and quantum simulations***



**Organizers:** Sara Bonella (EPF-Lausanne)  
Carsten Hartmann (BTU Cottbus-Senftenberg)  
Simon Huppert (Sorbonne Université)  
Fabio Pietrucci (Sorbonne Université)

**Date :** 4-6 October 2021

**Location :** ISCD - Sorbonne Université – 4 Place Jussieu, Paris  
([iscd.sorbonne-universite.fr/events](https://iscd.sorbonne-universite.fr/events))



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## Purpose of the meeting:

Underdamped Langevin dynamics is a well-established tool to sample the classical Boltzmann distribution, or its path integral generalization by adding appropriate friction and random forcing terms to the underlying Hamiltonian equations of motion. In most implementations, the friction coefficient is position-independent and Markovian and the random force is a Gaussian white noise. Well-established theoretical results on the properties of the dynamics exist, together with effective algorithms to implement it in computer simulations of general systems.

More recently, different groups have suggested adopting Generalized Langevin equations (GLE) for a variety of purposes in atomistic and multiscale simulations. Of particular interest for this meeting are:

- Projection of high-dimensional dynamics on collective variables
- The quantum thermal bath/quantum thermostat methods
- Generalised thermostats in classical or path integral calculations

GLEs represent an effective mathematical approach to model dynamical trajectories of high-dimensional complex atomic systems projected on a low-dimensional space of collective variables. Due to the projection, Hamilton's equations of motion can be approximated by a stochastic differential equation that in general is non-Markovian. Compared to alternative approaches to model kinetics, a clear physical picture of the process is preserved. An other category of methods, like the quantum thermal bath, make use of a non-Markovian GLEs to approximate zero-point energy effects in complex systems. In spite of several applications of GLEs, considerably less formal and algorithmic works exists compared to the standard case. Suggestions for additional topics of discussion from participants are also welcome.

In this extended discussion meeting, following on a previous meeting in June 2019 in Lausanne with a similar format, we shall gather experts from applied mathematics, physics, and chemistry to address the formal properties of GLEs in different contexts. We plan in-depth discussion of the state-of-the-art and the open issues. In addition to its theoretical interest, this discussion would pave the way for improved numerical implementations, fully establishing GLEs as a simulation tool and enabling to further explore their potential in new challenging applications. For example, specific items of interest will be the definition of numerical methods to reconstruct optimal GLE models from simulation (or experimental) data, and the control of the accuracy of quantum thermostat methods.



## Format of the meeting:

During the meeting, a large amount of time will be devoted to discussion, to foster interactions among participants, also in view of possible common work. Experts will present state-of-the-art methods in GLEs and their applications in 30 min long presentations, followed by 15 min of discussion time. Speakers will be asked to dedicate a specific section of their presentation to indicating open issues (both theoretical and in implementations) and outline possible new lines of research. A large part of the workshop will be devoted to collaborative work in smaller workgroups focused on specific topics that will emerge from the presentations. Each workgroup will organize its collaboration depending on the best format for the specific topic. This might range from the discussion of formal properties of specific GLEs, to the development of new algorithms, to coding. On the final day, a closing discussion will be held to share the outcome of the work and, if useful, discuss plans for continuing the collaborations initiated.



## List of participants:

Michele Casula	(Sorbonne Université)
Michele Ceriotti	(EPF-Lausanne)
Philippe Depondt	(Sorbonne Université)
Fabio Finocchi	(Sorbonne Université)
Arthur France-Lanord	(Sorbonne Université)
Fabian Glatzel	(University of Freiburg)
Ludovic Goudenège	(Centrale Supélec)
Martin Hanke-Bourgeois	(Johannes Gutenberg-Universität Mainz)
Gerhard Hummer	(Max Planck Institute of Biophysics)
James Hynes	(Ecole Normale Supérieure)
Bettina Keller	(Freie Universität Berlin)
Frédéric Legoll	(Ecole Nationale des Ponts et Chaussées)
Tony Lelièvre	(Ecole Nationale des Ponts et Chaussées)
Pierre Monmarché	(Sorbonne Université)
Tommaso Morresi	(Sorbonne Université)
Karen Palacio-Rodriguez	(Sorbonne Université)
Thomas Plé	(Sorbonne Université)
Benjamin Rotenberg	(Sorbonne Université)
A. Marco Saitta	(Sorbonne Université)
Tanja Schilling	(University of Freiburg)
Urbain Vaes	(Ecole Nationale des Ponts et Chaussées)
Hadrien Vroylandt	(Sorbonne Université)
Rodolphe Vuilleumier	(ENS/Sorbonne Université)

<b>Mon Oct 4</b>	
10:30	welcome
11:00	introduction, talk: S. Bonella
11:45	talk: T. Lelièvre
12:30	lunch break
14:00	talk: T. Schilling
14:45	talk: J. Hynes
15:30	coffee break
16:00	talk: G. Hummer
16:45	discussions
19:00	social dinner
<b>Tue Oct 5</b>	
9:00	talk: L. Goudenège
9:45	talk: C. Hartmann
10:30	coffee break
11:00	talk: T. Morresi
11:45	talk: M. Hanke-Bourgeois
12:30	lunch break
14:00	talk: M. Ceriotti
14:45	talk: H. Vroylandt
15:30	coffee break
16:00	talk: F. Finocchi
16:45	discussions
<b>Wed Oct 6</b>	
9:00	talk: B. Keller
9:45	talk: F. Legoll
10:30	coffee break
11:00	discussions
12:30	lunch break
14:00	talk: U. Vaes
14:45	talk: P. Monmarché
15:30	coffee break
16:00	discussions and closing remarks

