Extended Discussion Meeting:

Generalized Langevin Equations in classical and quantum simulations

Organizers: S. Bonella (EPF-Lausanne)
C. Hartmann (BTU Cottbus-Senftenberg)
S. Huppert (Sorbonne Université)
F. Pietrucci (Sorbonne Université)

Date : 11-13 December 2019

Location : ISCD - Sorbonne Université – 4 Place Jussieu, Paris (iscd.sorbonne-universite.fr)

Sponsor: E-CAM European Centre of Excellence / CECAM (www.e-cam2020.eu / www.cecam.org)

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 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, experts will present state-of-the-art methods in GLEs and their applications in 45 min long presentations. Each presentation will be followed by ample discussion time (at least 30 min) to foster interactions among participants in view of possible common work, see below. 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:

Pauline Bacle	(Sorbonne Université)
Michele Ceriotti	(EPF-Lausanne)
Philippe Depondt	(Sorbonne Université)
Fabio Finocchi	(Sorbonne Université)
Ludovic Goudenège	(Centrale Supelec)
Gerhard Hummer	(Max Planck institute of Biophysics)
James Hynes	(Ecole Normale Supérieure)
Frédéric Legoll	(Ecole Nationale des Ponts et Chaussées)
Hugues Meyer	(Université du Luxembourg)
Pierre Monmarché	(Sorbonne Université)
Thomas Plé	(Sorbonne Université)
Benjamin Rotenberg	(Sorbonne Université)
Marco Saitta	(Sorbonne Université)
Tanja Schilling	(University of Freiburg)
Gabriel Stoltz	(Sorbonne Université)
Rodolphe Vuilleumier	(ENS/Sorbonne Université)

Program of the meeting:

Wed Dec 11	
13:00-14:00	**Welcome**
14:00-14:30	**Introduction: scope of the meeting, previous event**
14:30-16:00	**Talk+discussion: Rodolphe Vuilleumier** *Mori-Zwanzing kernels and projected dynamics from molecular dynamics simulations*
16:00-16:30	**Coffee break**
16:30-18:00	**Talk+discussion: Frédéric Legoll** *From slow/fast dynamics to effective equations*
19:00-22:00	**Social dinner**
Thu Dec 12	
9:00-10:30	**Talk+discussion: Gerhard Hummer** *What's wrong with diffusion?*
10:30-11:00	**Coffee break**
11:00-12:30	**Talk+discussion: Tanja Schilling** *Nucleation is neither diffusive nor Markovian*
12:30-14:00	**Lunch break**
14:00-15:30	**Talk+discussion: Michele Ceriotti**
15:30-16:00	**Coffee break**
16:00-18:00	**Discussions**
Fri Dec 13	
9:00-10:30	**Talk+discussion: Gabriel Stoltz** *Effective diffusion and convergence rates of generalized Langevin dynamics*
10:30-11:00	**Coffee break**
11:00-12:30	**Talk+discussion: Hugues Meyer**
12:30-13:00	**Closing remarks**