27th September 2017 - 2:00 p.m.
CFEL-bldg. 99, seminar room IV

Michele Ceriotti

Laboratory of Computational Science and Modelling (COSMO),
École Polytechnique Fédérale de Lausanne (EPFL)

Fine-grained control of sampling and dynamics with a generalized Langevin equation

Molecular dynamics provides an efficient, general framework to probe the thermodynamic and dynamical properties of matter at finite temperature. The Langevin equation has been used for a long time as a device to achieve sampling that is consistent with a classical Boltzmann distribution.

I will discuss how a framework based on a generalized Langevin Equations can be used to exquisitely control the sampling behavior of a molecular dynamics trajectory, so as to converge averages more efficiently, but also to include quantum mechanical fluctuation effects. Furthermore I will show that the considerable disruption to the dynamical properties that is typically introduced by Langevin dynamics can be controlled and corrected to a large extent within this framework.

Host: Robin Santra – CFEL-DESY Theory Division