

4:30-5:05 Erwin Luesink (University of Utrecht, Netherland)

Underdamped Langevin dynamics on the rotation group

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Langevin equations are ubiquitous in molecular dynamics, interacting particle systems and sampling. The underdamped Langevin equations can be viewed as a stochastic perturbation of a Hamiltonian system, which helps to design numerical methods. In this talk, we focus on the underdamped Langevin equations on the group of rotation matrices. This is not a Euclidean space, which means one has to be careful with the interpretation of the stochastic differential equation, as naive approaches will instantly leave the correct space. We discuss appropriate numerical methods, some of their analyses and show simulations.