ESI Erwin Schrödinger International Institute for Mathematics and Physics

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ESI Senior Research Fellow Lecture Course
Summer Term 2026

The Erwin Schrödinger International Institute for Mathematics and Physics (ESI) of the University of Vienna offers the following Lecture Course held by a Senior Research Fellow in residence during the Summer Term 2026:

Langevin Sampling Algorithms
Benedict Leimkuhler (U of Edinburgh)

Lecture Course (260079 VU)
Time: 10:30 - 12:00 h
Start: Thursday, April 16, 2026
Further dates: Every Thursday till May 28, 2026
End: Thursday, May 28, 2026

Venue: Erwin Schrödinger Institute, Schrödinger Lecture Hall

Abstract:
Langevin dynamics is a physical model which replaces a complex, often high-dimensional system by a system interacting with an artificial stochastic "heat bath." While originally conceived as a reducedorder physical model, the Langevin framework has increasingly been put to work for the computation of generic statistical calculation in a high-dimensional setting. While Langevin dynamics methods are in widespread use in chemistry and physics (e.g. molecular dynamics), they are now also important tools for data science and artificial intelligence where they allow efficient statistical inference and uncertainty quantification based on Bayesian inversion.

An important challenge in both physical and data science applications is to select (or engineer) the right model system for the purpose. First order (Brownian) dynamics, kinetic Langevin dynamics, generalized Langevin dynamics and stochastic thermostats all can be used for similar calculations, but some are more suitable than others depending on the task at hand.

Because a complicated dynamical system can only be implemented through discretization, model selection is also intertwined with issues of numerical analysis. For example, constraints can be incorporated into numerical methods and this may allow computations to be performed with larger timesteps, ultimately providing "more bang for the buck" in large scale computing. Thermostats and adaptive stepsizes can further stabilize Langevin dynamics or improve robustness in systems with noisy gradients. In these lectures I will try to unravel some of the mysteries in Langevin dynamics and generalizations and their use for statistical (and statistical physics) calculations, juggling dynamical properties with classical numerical analysis considerations like accuracy and stability.

Contents of the course:
*P*art I Preliminaries in dynamical systems and numerical analysis

- L1 Deterministic (Hamiltonian, Reversible) systems, symplectic and time-reversible numerical methods, experiments

- L2 Stochastic differential equations, numerical methods, types of error, examples, software and numerical issues

*P*art II Contemporary issues in Langevin sampling algorithms

- L3 Discretization schemes for stochastic differential equations of Brownian and Langevin dynamics type, bias and convergence

- L4 Constraints and confinement (working on manifolds and regions with boundary)

- L5 Extended SDE systems (thermostats, generalized Langevin equaCons)

- L6 Adaptive stepsize and adaptive preconditioning of Langevin diffusions

- L7 Applications and numerical studies in molecular modelling and data science

Course website: https://www.esi.ac.at/events/e598/

Christoph Dellago
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