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**Directorate of studies
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Physics**

<http://ssc-physik.univie.ac.at>

Univ.-Prof. Mag. Dr. Thomas Pichler
Boltzmannngasse 5, 1090 Vienna

Phone +43(1) 4277 51466
dspl.physics@univie.ac.at

To all members of the
Faculty of Physics

Vienna, 14 October 2024

Invitation to the public defense of the doctoral thesis

**“Monte Carlo methods and machine learning for rare
event sampling”**

by

Sebastian Falkner

Friday, 22 November 2024, 14:00 p.m.

Schrödinger Lecture Hall, ESI, Boltzmannngasse 9A, 1090 Vienna

In all domains of natural sciences, we encounter rare events such as phase transitions, chemical reactions, or protein folding. Molecular simulations of these processes can lead to invaluable insights into their kinetics, thermodynamics, and mechanisms. However, the timescale disparity between the fastest molecular motions and the rate at which these processes occur renders it nearly impossible to observe rare events in unbiased equilibrium simulations. For these cases, transition path sampling is a method that focuses the computational resources on the ensemble of reactive trajectories that connect arbitrary states. The ensemble is sampled by repeatedly generating a new path from a point on a previous or initial path in the so-called shooting move. While this significantly reduces the computational resources necessary to obtain a reactive path, the shooting move introduces correlations between subsequently generated paths. Reducing these correlations is vital for any efficient path sampling scheme, particularly in complex systems with different reaction channels and many short-lived intermediate states. This thesis focuses on developing shooting schemes with the primary goal of reducing correlations between sampled paths. That includes the proposal of new shooting schemes using generative models, advancing replica exchange methods for path sampling, and revisiting shooting methods that evolve the shooting point from trial to trial.

Defense committee:

Jutta Rogal, New York University, USA (reviewer)

Titus Sebastian van Erp, Norwegian University of Science and Technology, NO (reviewer)

Christoph Dellago (supervisor)

Thomas Pichler (chair)