chemisch physikalische gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum Vortrag
von

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Bridging Time Scales with Variationally Enhanced Sampling

am Dienstag, 15. Oktober 2019, um 17:30 Uhr

Ort: Lise-Meitner-Hörsaal, Fakultät für Physik, Universität Wien,
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Barrierefreier Zugang: Boltzmanngasse 5, Lift, 1. Stock rechts über den Gang zum Hintereingang des Hörsaals

Abstract

The usefulness of atomistic simulations is generally hampered by the presence of several metastable states separated by high barriers leading to kinetic bottlenecks. Transitions between metastable states thus occur on much longer time scales than one can simulate in practice. Numerous enhanced sampling methods have been introduced to alleviate this time scale problem, including methods based on identifying a few crucial order parameters (generally called collective variables) and enhancing their sampling through the introduction of an external biasing potential [1].

Variationally Enhanced Sampling [2,3] is one such enhanced sampling method that is based on a variational principle where an external bias potential is constructed by minimizing a convex functional. The method is generally applicable where one can define good collective variables and allows for obtaining both free energy landscapes and kinetics of rare events. Variationally Enhanced Sampling is implemented in the VES code [4], which is an open-source library for the PLUMED 2 plugin, allowing usage of the method in a wide range of molecular dynamics codes.

In this talk I will review the theory behind Variationally Enhanced Sampling, and present numerous examples from physics and chemistry which show the flexibility and practicality of the method. I will then present various new developments and applications of the method. This includes for example wavelet-based bias potentials, and an extension for biasing permutationally invariant local collective variables.

[1] O. Valsson, P. Tiwary, and M. Parrinello, Annu. Rev. Phys. Chem. 67 159-184 (2016) [doi: 10.1146/annurev-physchem-040215-112229]
[2] O. Valsson and M. Parrinello, Phys. Rev. Lett. 113 090601 (2014) [doi: 10.1103/ PhysRevLett.113.090601]
[3] O. Valsson and M. Parrinello, Handbook of Materials Modeling, Methods: Theory and Modeling (Vol. I) [doi: 10.1007/978-3-319-42913-7_50-1]
[4] http://www.ves-code.org

Kaffee und Getränke werden bereitgestellt