Institute for Multiscale Simulation

MSS

Master Thesis

Hydrodynamic memory effects in fractional Kramers model of chemical reactions

Type

Theoretical & Computational

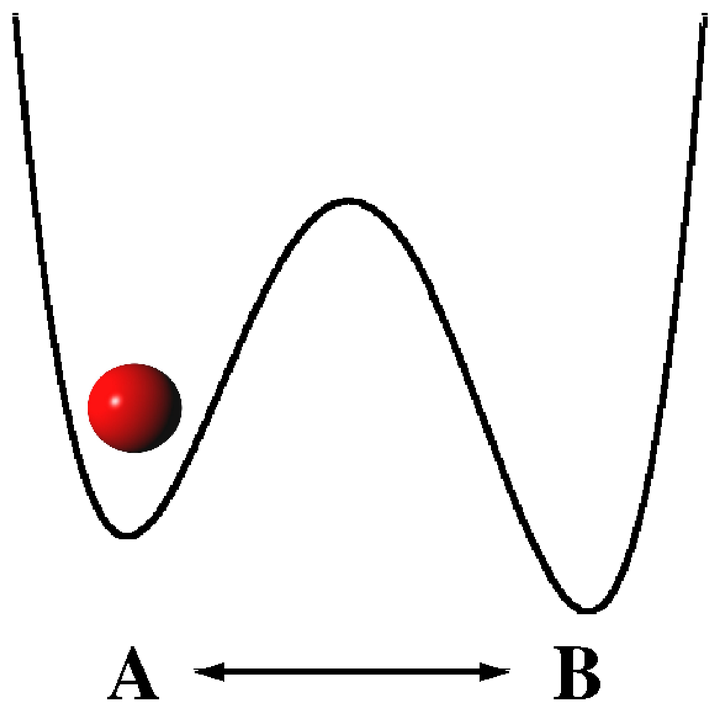
Requirements

- Basic knowledge of statistical physics and chemical kinetics
- Basic knowledge of C/C++/FORTRAN or Matlab

QR code
zum pdf der Ausschreibung

Background

Classical (memoryless) Kramers model presents one of the cornerstone models in the physico-chemical kinetics. Beyond the conventional model, the medium's memory effects make it profoundly non-Markovian. Mathematically, the model is described by a Generalized Langevin Equation (GLE) dynamics in a bistable potential. The project focuses on clarifying the influence of hydrodynamic memory effects (Basset force and accompanying fractional Gaussian thermal noise leading to a Fractional Langevin Equation description) on the chemical kinetics. The numerical approach is based on a Prony series approximation of the memory kernel and the corresponding multi-dimensional Markovian Langevin embedding of GLE dynamics.



Aim

- **Stochastic simulations of a non-Markovian generalization of the Kramers model**
- **Clarifying influence of hydrodynamic memory effects on the reaction kinetics, residence time distributions in chemical states, and dependence of the reaction rate on the medium's viscosity**

For further information please contact:

Priv.-Doz. Dr. Igor Goychuk
Institute for Multiscale Simulation (MSS)
Department of Chemical and Biological Engineering (CBI)
Cauerstrasse 3, IZNF,
91058 Erlangen,
Room 03.156
email: igor.goychuk@fau.de
web: www.mss.cbi.fau.de