Course title: Computational Methods for Rare Events

Description: The course will cover theoretical and computational topics relevant to computational investigation of rare events, starting from standard reaction rate theory, and modelling of dynamics in terms of the Langevin equation, to first passage times, collective variables, commmittors, methods for enhanced sampling methods and efficient methods for estimating rates.

Topics: Barrier crossing, transition state theory, Kramers theory, collective variables, first passage, committors, umbrella sampling, replica exchange, metadynamics, Bennett-Chandler approach, transition path sampling, steered MD, and other methods.

Format: Class room lectures, with some hands-on exercises, during April-May.

Credits: 1 credit as "Special Topics in Statistical Mechanics (JT 216)"