Oberseminar Numerik am 31.01.13

Dr. Tony Lelievre CERMICS - Ecole des Ponts ParisTech

Title: Sampling metastable trajectories: numerical techniques and mathematical analysis

Abstract:

I will present numerical methods which are used in molecular dynamics to generate efficiently trajectories in metastable situations.

Metastability is a common feature of many molecular dynamics simulations: the system remains for a very long time in a so-called metastable state before hopping to another one. This limits the interest of naive molecular simulations, since the time scales associated to macroscopically relevant changes of conformations are much larger than the typical time step used to discretize the molecular dynamics trajectory. I will present numerical techniques which have been proposed to obtain an accurate simulation of a coarse-grained representation of the trajectory