MATH CCES Center for Computational Engineering Science Mathematics Division | RWTH AACHEN UNIVERSITY

Master Thesis

Dynamic Mode Decomposition for Molecular Dynamics Simulations

Course of study:	Computer Science, Applied Mathematics
Kind of thesis:	Theoretical Analysis, Programming and Simulation
Programming language:	C++
Start:	April 2017

Problem

By solving classical Hamiltonian equations of motion, a high-dimensional probability density distribution is sampled efficiently. For these Hamiltonian equations of motion frequently nonlinear potentials are used. Koopman operator theory states, that the computation of these nonlinearities is equivalent to the action of an infinite-dimensional linear operator on the state.

Approximating this infinite-dimensional operator numerically leads to a procedure, which potentially reduces simulation time. Dynamic Mode Decomposition (DMD) is a numerical method to approximate the infinite-dimensional linear Koopman operator.

Applications

Within the molecular dynamics community DMD is a hot topic. Also in the field of financial trading strategies and neural sciences DMD is revealing great potential, because the algorithm enables a short time future prediction.

Task

The student will make himself/herself familiar with the concept of numerical solution techniques of Hamiltonian equations of motion, DMD, Koopman operator theory and programming with C++.

$$X = [\boldsymbol{x}_0, \boldsymbol{x}_1, \cdots, \boldsymbol{x}_{n-1}]$$
$$X' = [\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n]$$
$$A = X' X^+$$
$$A\boldsymbol{x}_k = \boldsymbol{x}_{k+1}$$

After diving into these topics the student implements the DMD as given in common literature in C++ or uses a code, which is already available within the work group. The student uses the implementation to perform molecular dynamics simulations. After reaching this point empirical cases and theoretical considerations are studied.

Supervision

This thesis belongs to the research of the group headed by Prof. Dr. Benjamin Stamm at the MATHCCES. The project will be supervised by the doctoral candidate

Contact: **M. Sc. Andreas Smolenko**
Adress: MATHCCES
Schinkelstr. 2, 52062 Aachen
Room: 216a (Rogowski building, 2nd floor)
Tel.: (+49) (241) 80-98675
Email: smolenko@mathcces.rwth-aachen.de