Computational Techniques for Molecular Modeling

First Ed. Spring Semester, AY 2020/2021

Computational Techniques for Molecular Modeling

- NUMERICAL METHODS FOR MOLECULAR SIMULATION
- Contents
  - Models
  - Equations
  - Numerical Challenges / Techniques
  - Software Tools / Utilities
- Hands-on Approach
  - Presentation of general model framework
  - Choice of model problem
  - Guided group projects

Models

- Classical Molecular Dynamics
- Protein Solvation Electrostatics (Poisson-Boltzmann Model)
- Brownian Dynamics (Langevin Model)

Equations

- Classical Hamiltonian Dynamics
- Nonlinear Elliptic PDEs (with discontinuos equations and point sources)
- Stochastic Differential Equations
- Diffusion-Advection PDEs (possibly Advection dominated)

Numerical Challenges/Techniques

- Particle-particle interactions, Space Filling Curves, Fast Multipole Method
- Consistent simulation of Hamiltonian systems, Symplectic/Geometric Integrators, handling of stiff modes/internal constraints
- Lattice Kinetic Monte Carlo, Stable discretizations for Advection-Dominated Advection Diffusion PDEs

Tools

- GNU Linux
- Octave
- Gromacs
- APBS
- Nanoshaper
- ...

Exam / Evaluation

- Tasks for group projects
- Problem Presentation
- Code implementation
- Result presentation and discussion