Bachelor thesis: Numerical methods for molecular dynamics

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Prerequisites: Good knowledge of undergraduate numerical analysis, interest in programming

Language: English or German

Topic: In molecular dynamics we are interested in the classic description of microscopic ensembles of atoms. Thus, our goal is to determine the position of the i-th atom by solving the ordinary differential equations

$$m_i \ddot{x}_i = F(x_1, \ldots, x_n),$$

where $i \in \{1, \ldots, n\}$ and n is large.

The goal of this bachelor thesis is

- Obtain an understanding of the qualitative features of a force field F that is used in practice (for example, the Lennard-Jones potential).
- Conduct an (assisted) literature research on so-called symplectic integrators. Explain why this class of methods are appropriate for molecular dynamics.
- Implement two or three numerical integrators and compare their performance (such as the leapfrog method, classic Runge–Kutta methods, and symplectic integrators of high order) in a programming language of your choice.
- Thermodynamic properties of the bulk system (such as density) can be calculated from such simulations. This requires the computation of an ensemble average that is replaced by a time average (the ergodic hypothesis). The convergence behavior of this procedure should be studied numerically.