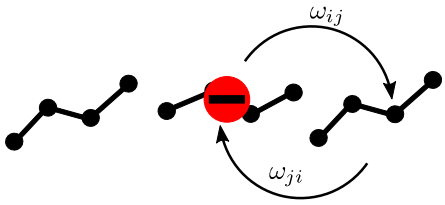
BACHELOR PROJECT SCIENTIFIC COMPUTING

Numerical Integration of Systems of Ordinary Non-linear Differential Equations

Problem Description



Hopping of an electron from one molecule to the next

The movement of electrons inside disordered molecular materials can often be characterized as a hopping process, in which the charge carrier hops from one molecule to the next.
With given hopping rates ω_{ij} for the transition from molecule i to j, the behavior of an electron can be described by a Master equation

$$\frac{\mathrm{d}P_i(t)}{\mathrm{d}t} = \sum_j \omega_{ji} P_j(t) - \omega_{ij} P_i(t), \tag{1}$$

where t is time and $P_i(t)$ is the occupation probability of site i.
If two or more electrons are in the same system, the electrons repel each other. Consequently, two electrons cannot occupy the same site. To first order this can be modelled via

$$\frac{\mathrm{d}P_i(t)}{\mathrm{d}t} = \sum_j \omega_{ji} P_j(t) \left[1 - P_i(t)\right] - \omega_{ij} P_i(t) \left[1 - P_j(t))\right]. \tag{2}$$

This system of equations is often solved via kinetic Monte Carlo (KMC) simulations, where the electrons' dynamics is treated using a stochastic process. As the mean error of KMC scales with $1/\sqrt{N}$, a large number of simulations are required to converge results.

A numerical integration of equation 2 allows for a much faster evaluation of electron properties. Difficulties arise due to the positivity of the occupation probabilities, the range of hopping rates, which spread many orders of magnitude, and finally the non-linearity.

A functioning solver may lead to the implementation in VOTCA-XTP, an open source software package.

Tasks

- Study literature (provided by the supervisor).
- Implement a stable solver in for the linear equation (1) in Matlab or Python
- Implement a stable solver in for the non-linear equation (2) in Matlab or Python
- Analyze results and compare with kinetic Monte Carlo simulations

Requirements

- Linear algebra
- system of ordinary differential equations
- Basic programming skills in Matlab or Python

Supervisor

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