Simulation in Chemistry

General information

Asdrubal Lozada

Techniques

1. Stochastic Simulation
2. Molecular Dynamics
3. Quantum Chemistry
4. Edition & Visualization

About

This document provides an overview of computational simulation techniques commonly used in condensed matter physics, chemistry, and materials science. It also provides a lists the programs, software packages, or frameworks employed for such simulations.

Stochastic

Overview

Monte Carlo Methods

- Crude Monte Carlo
- Stratified Sampling
- Importance Sampling
- Control variates
- Antithetic variates
- Metropolis Algorithm (Metropolis-Hastings)
- Gibbs Sampling
- Perfect Sampling
- Gillespie Algorithm

Programs

- Melquiades (GPL) [Fortran]
- DL-Monte (BSD) [Fortran]
- Cassandra (GPL) [Fortran]
- GOMC (MIT) [CPP]
- Dice (GPL) [FORTRAN]

Dynamics

Programs

- Gromacs (LGPL) [CPP]
- Lammps (GPL) [CPP]
- CP2K (GPL) [Fortran]
- Tinker (Tinker license) [Fortran - C]

Quantum

Programs

- CP2K (GPL) [Fortran]
- ORCA (Academic) [C]
- MOPAC (LGPL) [Fortran]
- Quantum Espresso (GPL) [Fortran]
- Octopus (GPL) [Fortran]
- XTB (LGPL) [Fortran]
- DFTB (LGPL) [Fortran]

Edit

Programs

- Molden (Molden license) [FORTRAN]
- Travis (GPL) [CPP]
- Gabedit (Gabedit license) [CPP]
- Jmol (LGPL) [JavaScript]
- Avogadro (GPL) [CPP]
- VMD (VMD license) [CPP]
- Molekel (GPL) [CPP]
- EasyHibrid (Open) [python]

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