Praktikum Theoretische Chemie II: Moleküldynamik-Simulationen

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1. INTRODUCTION

1.1. Molecular simulation

Molecular simulation of fluids is having an increasingly significant impact on the chemical, pharmaceutical, materials and related industries. This is because molecular simulation provides a set of tools for predicting entirely computationally many useful functional properties of systems of interest to these industries. These properties include thermodynamic properties (such as equations of state, phase equilibria, and critical constants), mechanical properties (such as stress- strain relationships, and elastic moduli), transport properties (such as viscosity, diffusion and thermal conductivity), and morphological information (such as location and shape of binding sites on a biomolecule and crystal structure).

Consider Fig. 1, beginning at the lowest level of description, the electronic structure/quantum mechanics level–the domain of computational quantum chemistry. Calculations at this level can predict, for example, molecular structure, free energies of formation and of reaction, dipole moments and other spectroscopic properties, and reaction rates in the gas phase and on the surfaces.

Above this level, the Car-Parrinello method is representative of *ab initio* molecular dynamics techniques, in which the atoms undergo motion described by classical dynamics in response to forcers computed on the fly at each time step by one of the computational quantum chemistry methods, such as density functional theory. In particular, it has play an important role in deepening our fundamental understanding of water and aqueous solutions.

At the next highest level of description, the atomistic and united atom levels, the two main molecular simulation techniques are molecular dynamics (MD) and Monte Carlo (MC) methods, both of which have their origin and justification in classical statistical mechanics. Given mathematical models for the internal structure of each molecule and the interaction between molecules, through classical statistical averaging over the possible microscopic states of the system as it evolves under the rules of classical mechanics. Thus, the building blocks are molecules, the dynamics are described by classical mechanics, and the key concept is statistical averaging. MD and MC may be summarized as follows:

- In MD, solving the classical equations of motions as a function of time (typically over a period limited to tens of nanoseconds) generates the microscopic states of the system. Thus, in MD one can observe the relaxation of a system to equilibrium (provided the time for the relaxation falls within the time accessible to MD simulation), and so

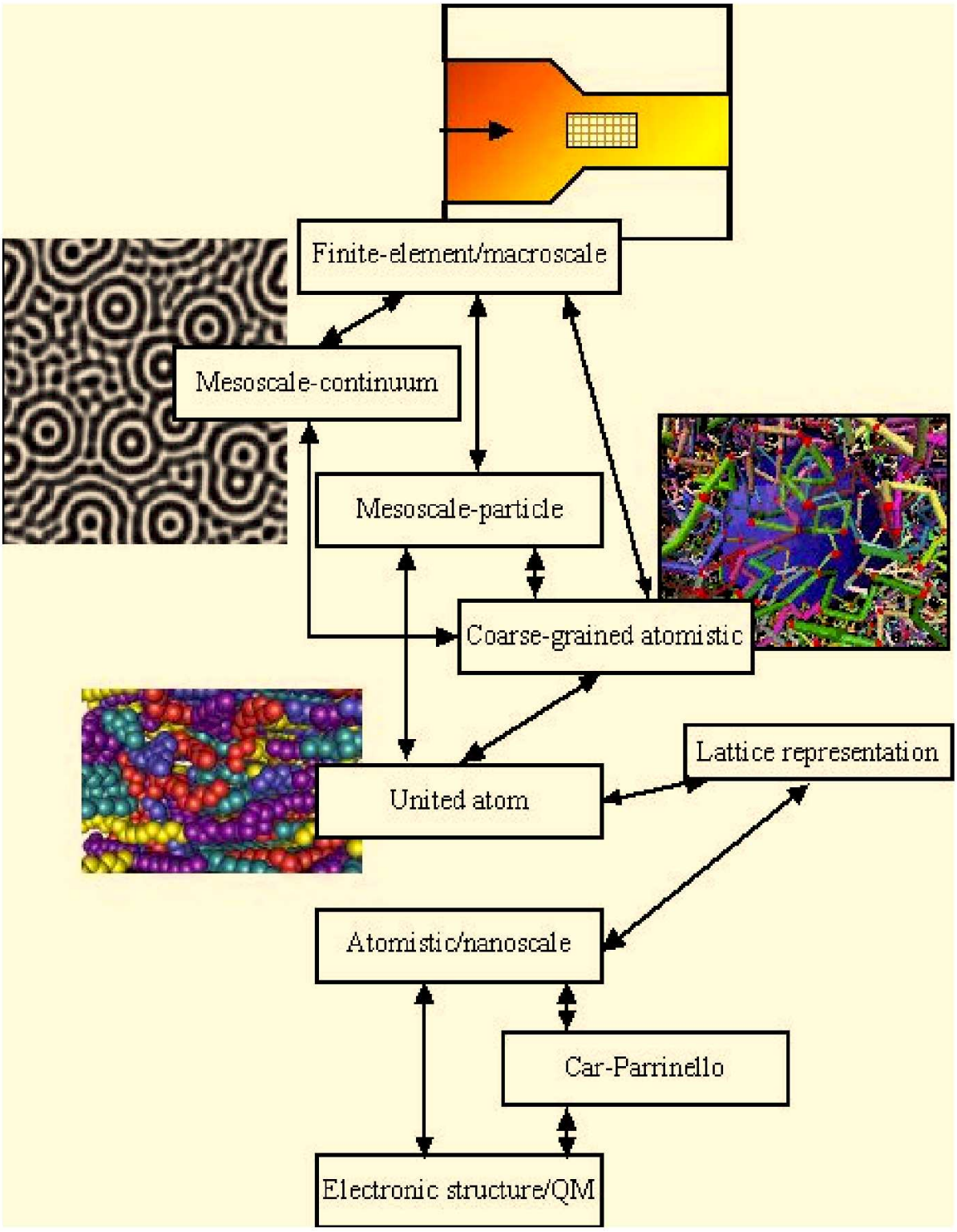

FIG. 1: Molecular modeling methods

determine transport properties, which at the macroscopic scale decribe the relaxation

of the system in response to inhomogeneities.

- IN MC, equilibrium configurations are generated stochastically according to the probabilities rigorously known from statistical mechanics. Thus, MC generates equilibrium states directly (which has many advantages, including bypassing configurations which are not characteristic of equilibrium but which may be difficult to escape dynamically) and so can be used to study the equilibrium configurations of systems which may be expensive or impossible to access via MD. The drawback of MC is that it cannot yield the kind of dynamical response information that leads directly to transport properties.

- Mesoscale methods apply MD or MC techniques in domains too large for individual molecules and atoms to be included explicitly. Coarse-graining techniques are examples.

1.2. Purpose

The Praktikum consists of a general computer introduction (1 lecture), a number of molecular-dynamics excercises (10 lectures), a "question-answer" week on research projects, and a seminar (about 14 weeks in total). The goal is (i) to obtain an idea on how molecular-dynamics simulations work in practice and (ii) to provide an impression on what can be confidently calculated by state-of-the-art simulation methods and what not.

- First a brief introduction to the computer environment such as editing, plotting, printing is given. It's assumed that you have worked with computers before. Some knowledge on programming is helpful but not mandatory.

- Next follows a set of molecular-dynamics excercises, using empirical force fields. The goals are (i) to gain a basic understanding of the practical issues of a computer simulations, (ii) to obtain some experience with standard program packages such AMBER and MOLDEN, and (iii) to simulate simple biomolecular systems. It's assumed that you have attended a basic course on statistical thermodynamics (e.g., PC III).

- The seminar accompaning the Praktikum a short presentation is to be given on a (a bit advanced) computational project. We have prepared several suggestions for research projects, however, you are invited to come up with a better idea.

1.3. Recommended literature

- General Computer stuff:

  E. Siever, S. Spainhour, S. Figgins, and J. P. Hekman, *Linux in a N utshell* (O'Reilly, Köln, 2001). A good textbook, 2 copies available.

  H. Wehnes, *Fortran 77* (Hanser, München, 1992).
  A good textbook, 1 copy available.

  Online AWK MANUAL, http://www.cs.uu.nl/docs/vakken/st/nawk/nawk_toc.html#TOC95

- Molecular Dynamics:

  D. Frenkel and B. Smit, *Understanding Molecular Simulations* (Academic Press, San Diego, 1996). A good textbook, 3 copies available.

  A. R. Leach, *Molecular Modeling* (1996)

  Online book, *Molecular Simulation* (http://boltzmann.vuse.vanderbilt.edu/ w3press/)

1.4. General organisation

The Praktikum takes place one afternoon a week in the rooms N120/120. At the beginning of each class, the adivisor in charge (i) gives an introduction of the exercises of the day, (ii) gets you started on the project, and (iii) remains available for further questions. Moreover, a key to the rooms is available from Ms. Madic for further studies during the rest of the week.
The Praktikum team is:
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  Secretary

Note: The Praktikum is still under development. Please report any errors, inconsistencies, obscurities or suggestions for improvement. For the convenience of foreign users, the description of the Praktikum is in English.

Have fun computing!
Frankfurt, SS 2003

Your Praktikum team
Yuguang Mu
Rainer Hegger
Gerhard Stock