Molecular Dynamics for Microsystems.
Introduction
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Learning Goals

♦ Why Molecular Simulation?
♦ Molecular Motors
♦ Course Structure
♦ Organizational Details

DNA

polymer brush under shear forces

indentation
Why Molecular Simulation?

The Next Step for MST -> NST

♦ Learning from Nature:
  ♦ Basis for cellular life processes is molecules (proteins)
  ♦ Transcription
  ♦ Decoding
  ♦ Messaging
  ♦ Production

♦ Engineering at the Nanoscale:
  ♦ Discovery/verification of natural molecular processes

♦ Manipulation of existing molecular mechanisms
♦ Design of new molecular mechanisms

♦ Continuum models does not work at nanoscale
♦ Nature is discontinuous at molecular level
♦ Classical laws may be not appropriate any more
Why Molecular Simulation?

Example: Nanobiotechnology

- www.lifesciencesinfo.com/nano, Nanobiotechnology, Where the Science and Applications Drive Change from Discovery through Development, July 16-17, 2001 - San Diego, CA
- Dr. Rashid Bashir, Towards the Use of Biological Entities to Assemble Semiconductor Devices.
- Dr. Ralph C. Merkle, Nanotechnology and Replicating Systems.
- Dr. Steven Smith, Some Implications of Self-Assembling Three-Address Structures in the Construction of Nanoscale Materials and Devices from Proteins and Nucleic Acids.
- Dr. Ricky K. Soong, Engineering Hybrid Organic/Inorganic Nano-Scale Devices Powered by Biomolecular Motors.
Overview

♦ International Workshop “Molecular Motors”, November 2001

♦ Biologists
  ♦ Muscle motor
  ♦ Biological Springs

♦ Chemists
  ♦ Artificial Molecular Machines
  ♦ Light-driven Molecular Switches
  ♦ Polymer Gels as Molecular Motors

DECHEMA / Frankfurt am Main Germany
Molecular Motors

Muscle motor


myosin and actin filaments “cross-bridge” makes a rowing action
Molecular Motors

Biological Springs

♦ P. Matsudaira, web.wi.mit.edu / matsudaira/pub/home.html

♦ 50 µm- long acrosomal process, horseshoe crab, *Limulus polyphemus*
Artificial Molecular Machines


Molecular shuttle

E.B. Rudnyi, J.G. Korvink, Chair for Microsystem Simulation
Molecular Motors

Light-driven Molecular Switches

- B.L. Feringa, www.chem.rug.nl/feringa/
- Monodirectional Rotation
- Molecular Submarine

Polymer Gels as Molecular Motors

Overview

♦ Particle Dynamics (4)
♦ Molecular Models (3)
♦ Statistical Thermodynamics and Monte-Carlo (1)
♦ Molecular Dynamics and Simulation (3)
♦ Empirical Correlations and Chemometrics (1)

♦ (Number of lectures is given in parentheses)
Course Structure

Particle Dynamics

- Classical mechanics of moving particles
- Fast computation of net forces
- Postprocessing and different external conditions
- Stochastic particle dynamics

- Example: MD of crack propagation
  The colors refer to the state of stress at the atomic sites
  www.gre.ac.uk/~rh01/movie/
Course Structure

Molecular Models

- Quantum chemistry
  - Born-Oppenheimer approximation, atomic and molecular orbitals, Hartree-Fock equation. Electron correlation, configuration interaction and DFT.

- Molecular mechanics
  - Empirical chemical bonding and non-bonding interactions. Determining the empirical force field.
  - Quantum corrections and quantum molecular dynamics.

- Exploring the energy surface
Statistical Thermodynamics and Monte-Carlo

- Time average and ensemble average. Monte Carlo method. Solutions in the closed form.

\[ (N_1, V_1, E_1) \]
\[ (N_2, V_2, E_2) \]

Most random points fall in region where \( f(x) \) is almost zero.

Random Points
Molecular Dynamics and Simulation

- Simulating phase equilibria and molecular solutions
- Simulating a partition function. Particle insertion, direct simulation, Gibbs ensemble method. Molecule in solution and in the electrical field. Continuum and discrete solvation models.

- Chemical kinetics: simulating rare events
- Reaction path, transition state, transition state theory. Sampling rare events and transition pathways
- Advanced molecular simulations: Polymers, mesoscale and multiscale modeling

Time evolution of phase partition of a Pluronic 64 and water mixture

GRPOMACS
## Course Structure

- **Empirical Correlations and Chemometrics**

### Quantitative Structure - Activity Relationship (QSAR) and Quantitative Structure - Property Relationship (QSPR)

![Chemical Structures](http://www.accelrys.com/cerius2/images/qsar_1.gif)

### Table: QSAR Analysis

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Organizational Details

Overview

♦ Where and when
♦ Literature
♦ Exercises
♦ Presentation Project
♦ Schein
Organizational Details

Where and when

♦ Lecture: Room # 00-006, Geb. 051, Mo. 14-16
♦ Exercises: Room # 00-006, Geb. 051 or in Comp. Class, Mo 16-17

Lecturers

♦ Prof. Dr. Jan G. Korvink, korvink@imtek.de, 203 7381, 103.03.033
♦ Prof. Dr. Evgenii Rudnyi, rudnyi@imtek.de, 203 7410, 103.03.017

Course Requirements

♦ Recommended: Inorganic Chemistry, Organic Chemistry, Physical Chemistry, Noise and Fluctuations
♦ Required: Simulation I, Mechanics, PDEs
Organizational Details

Literature


♦ Additional literature and online resources in each lecture

Links

♦ Computational Chemistry List, www.ccl.net
♦ Tutorials, cmm.info.nih.gov/modeling/tutorials.html
♦ Leach’s book, www.booksites.net/leach/
♦ MDSalon_Related Sites, www.ks.uiuc.edu/Services/MDSalon/links.php
Organizational Details

Exercises

♦ Software demonstration in Room # 00-006, Geb. 051
♦ Computer labs in Computer Class, Geb. 103

Particle Molecular Dynamics (3)
♦ Object Oriented Molecular Dynamics by David Kauzlaric

Quantum Chemistry (2)
♦ GAMESS, www.msg.ameslab.gov/GAMESS/

Visualizing proteins (2)

♦ Small report for each exercise - send it by e-mail.
Organizational Details

Presentation Project
♦ Present an assignment in a 15 minute oral presentation. Presentations held are during the last two semester weeks. Each member of the team presents 7.5 minutes.

Paper Project
♦ A team is assigned a separate scientific MD paper.
♦ Understand the contents of the paper. Refer to the literature for more detailed explanations, and to discussion during the exercise periods.
♦ Present the paper, as if it was the result of your own research.
Organizational Details

Software Review Project
♦ Instead of paper, a team is assigned a molecular simulation software package.
♦ It is necessary to install it, run the demos, to create your own examples to be used next year.
♦ Present the software.

Programming Project
♦ A team is assigned a task to program a “meter” for David Kauzlaric’s code.
♦ C++ knowledge is required.
♦ Program and make a presentation.

Schein
♦ Completion of the computational exercises and a presentation assignment.
Summary

♦ Why Molecular Simulation?
  ♦ Molecular Motors
♦ Course Structure
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♦ If you would like to attend, please register.
♦ Exercises will be made in pairs, please specify your neighbor.
♦ Choose between paper review, software review or programming.

www.zyvex.com/nanotech/nano4/tuzun