Molecular Dynamics for Microsystems. Introduction

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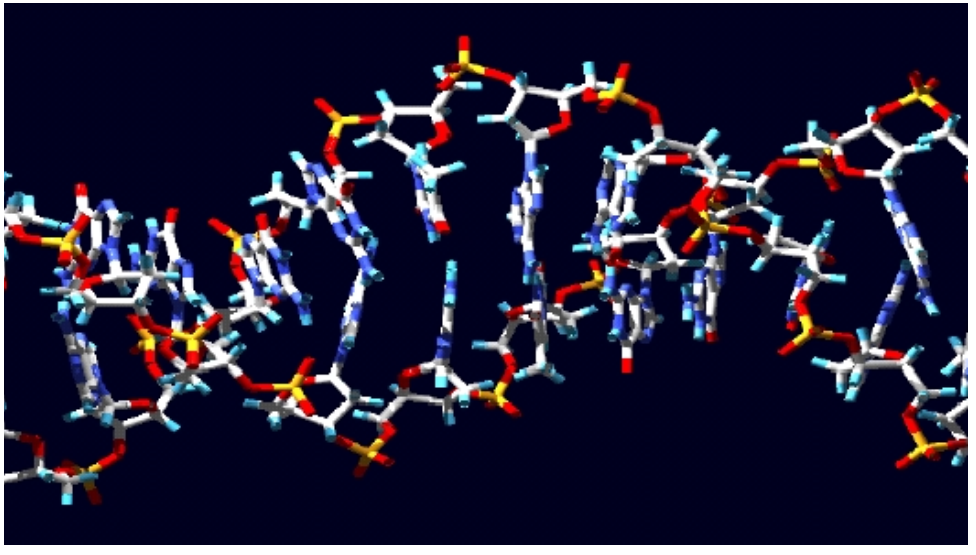
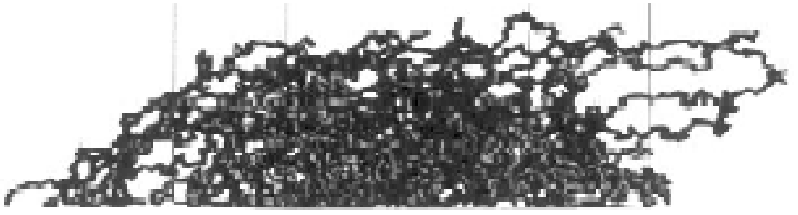
Learning Goals

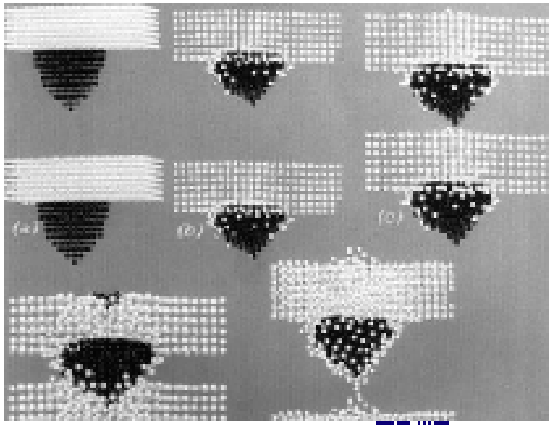
- Why Molecular Simulation?
  - Molecular Motors
- Course Structure
- Organizational Details



DNA



polymer brush under shear forces



identation

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?

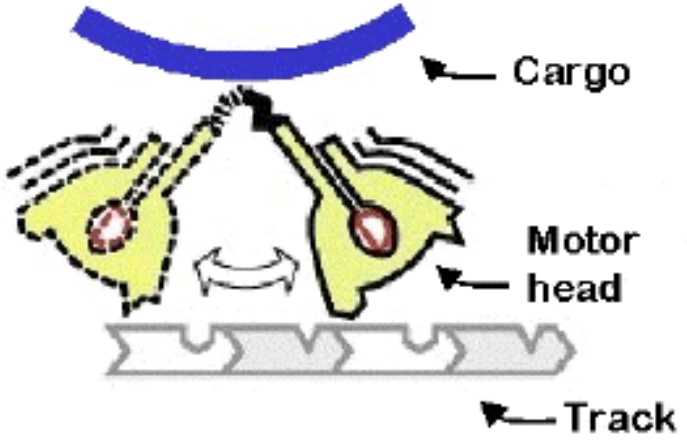
Example: Nanobiotechnology

- 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.

Molecular Motors

Overview

- International Workshop *"Molecular Motors"*, November 2001



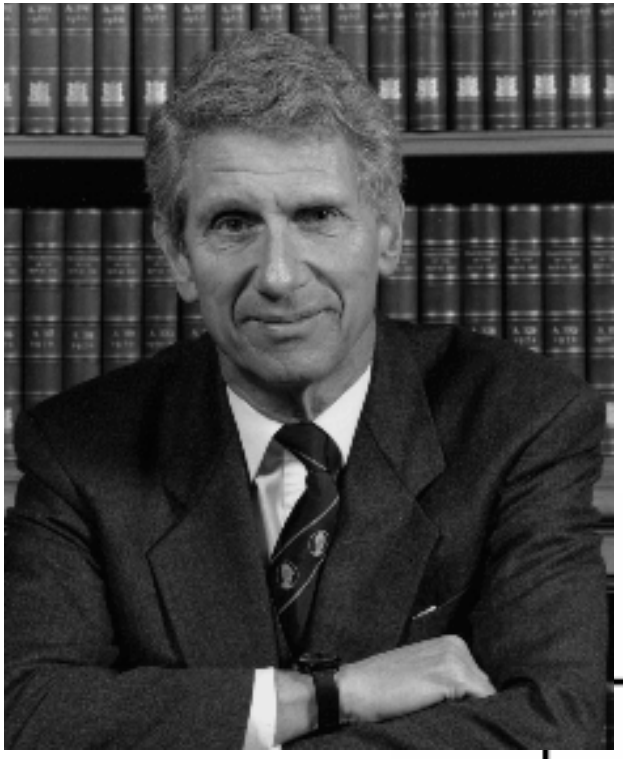
DECHEMA / Frankfurt am Main
Germany

- Biologists
  - Muscle motor
  - Biological Springs
- Chemists
  - Artificial Molecular Machines
  - Light-driven Molecular Switches
  - Polymer Gels as Molecular Motors

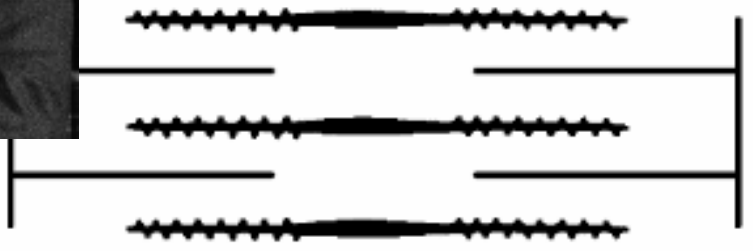
Molecular Motors

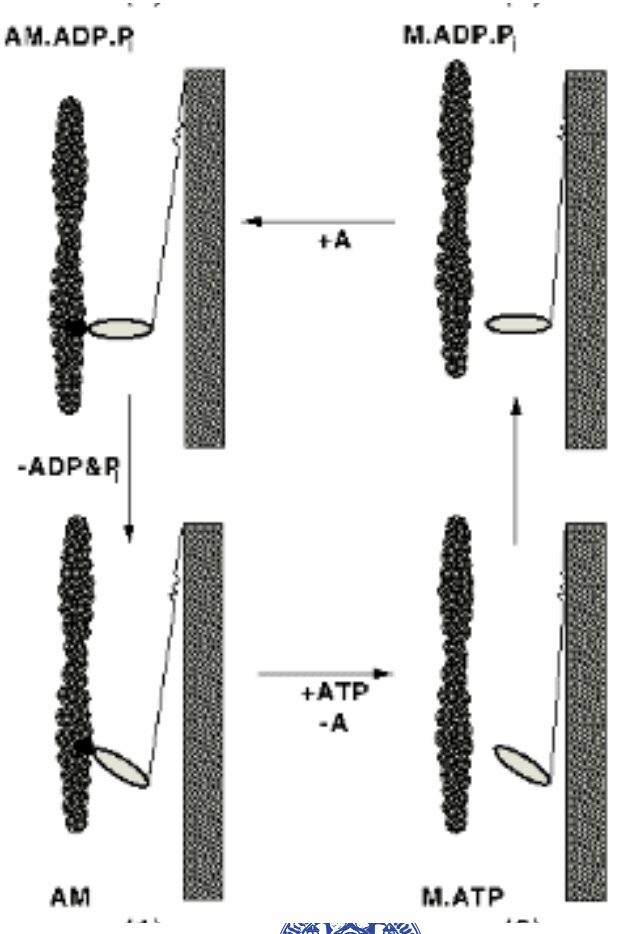
Muscle motor

- K.C. Holmes, www.mpimf-heidelberg.mpg.de/~holmes/



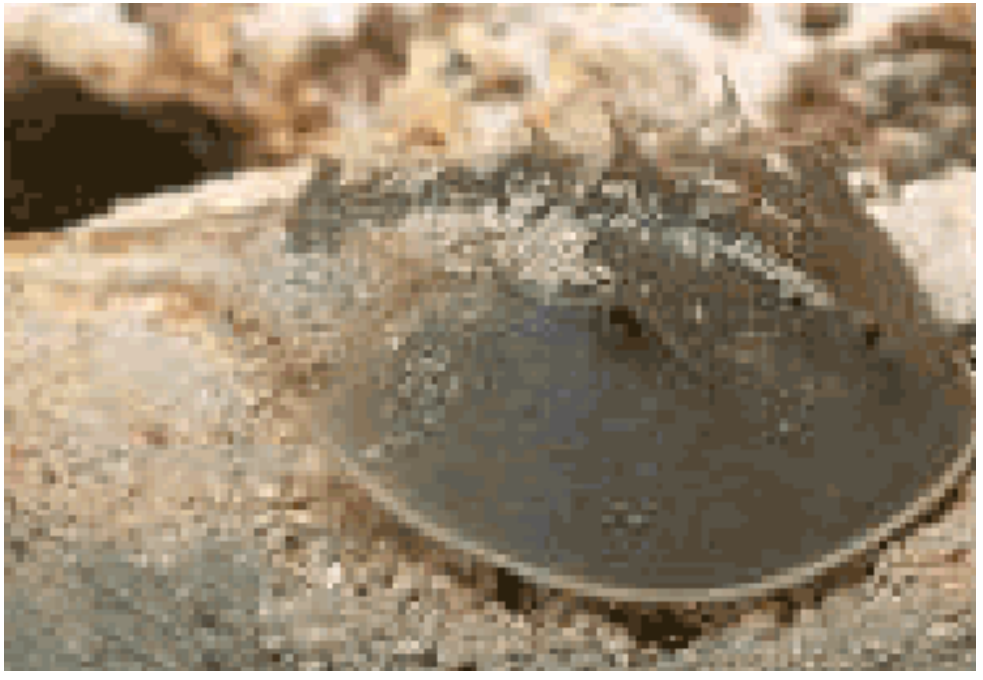
myosin and actin filaments
"cross-bridge" makes a rowing action

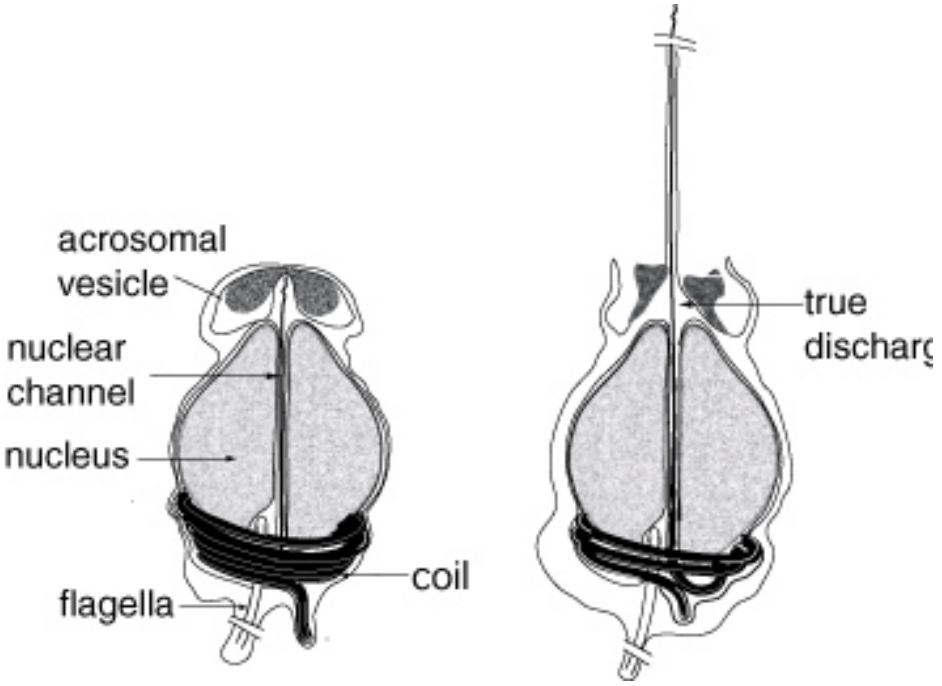


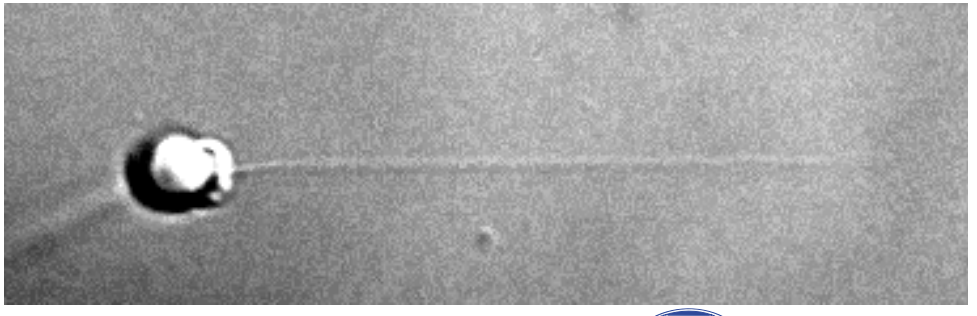


Biological Springs

- P. Matsudaira, web.wi.mit.edu / matsudaira/pub/home.html
- 50 μm- long acrosomal process, horseshoe crab, Limulus polyphemus



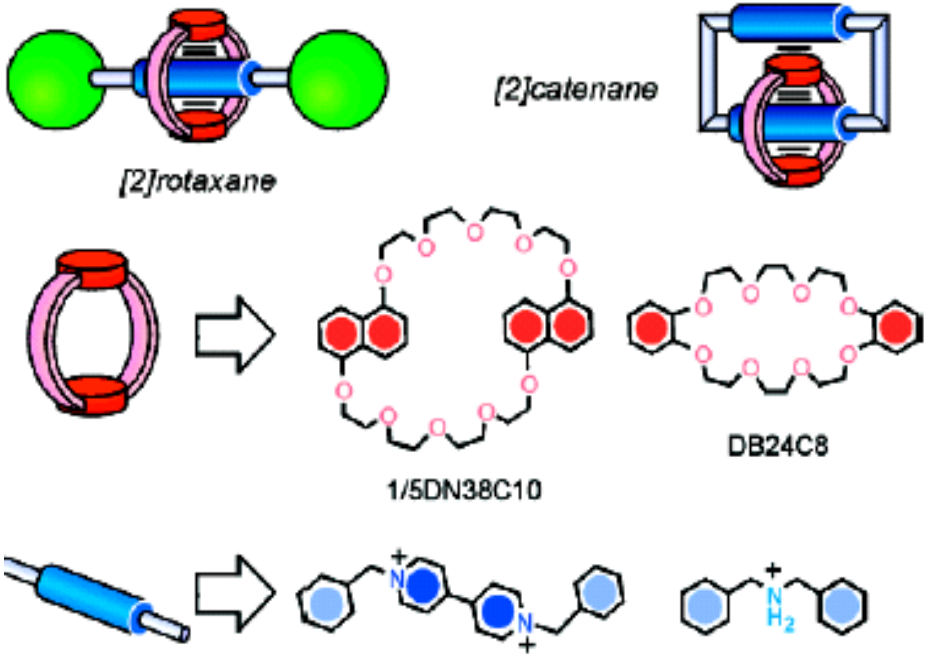




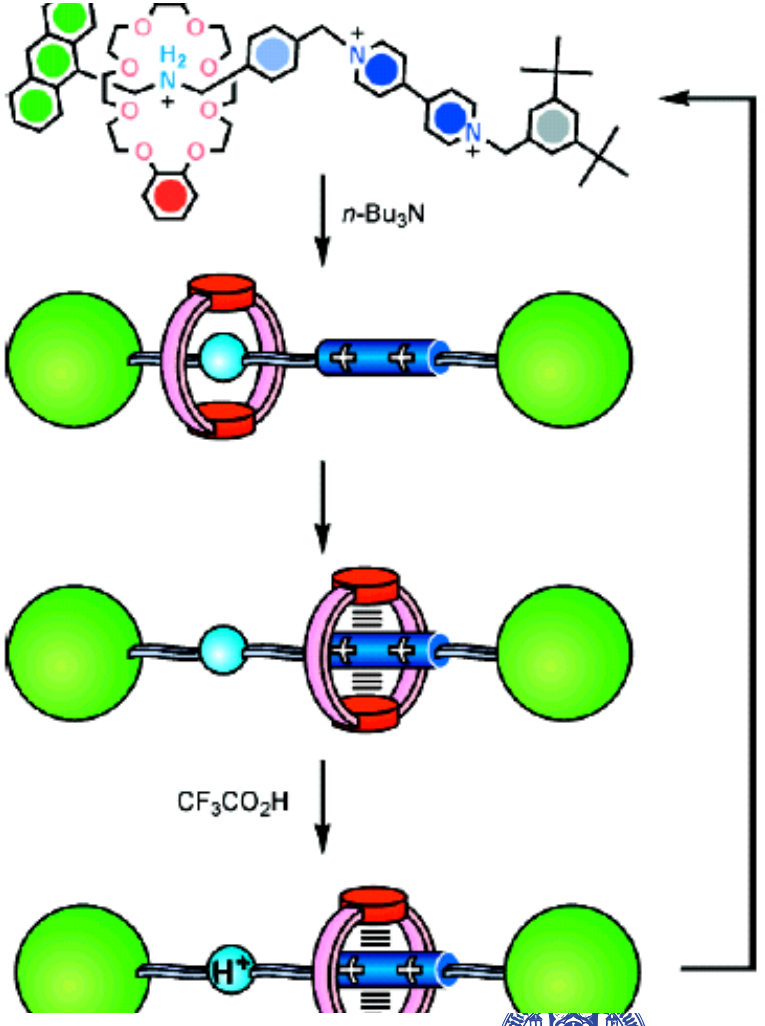
Molecular Motors

Artificial Molecular Machines

- V. Balzani, *Acc. Chem. Res*, 2001, 34, 445-455.



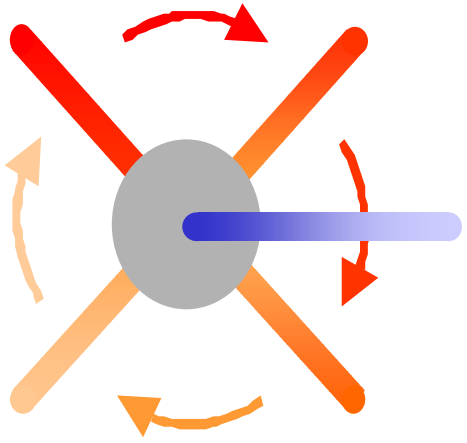
- Molecular shuttle

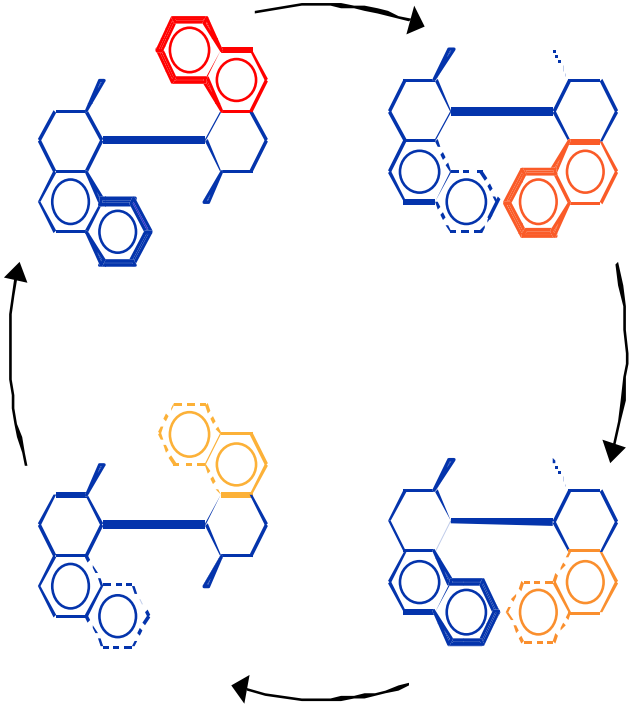


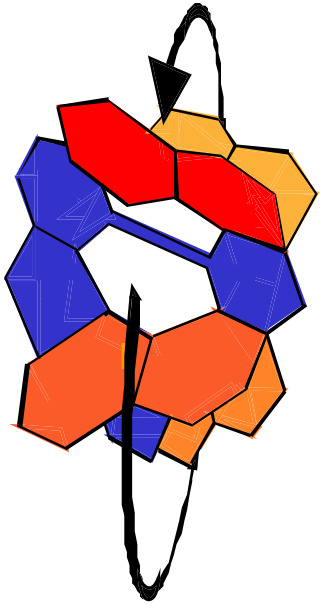
Molecular Motors

Light-driven Molecular Switches

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



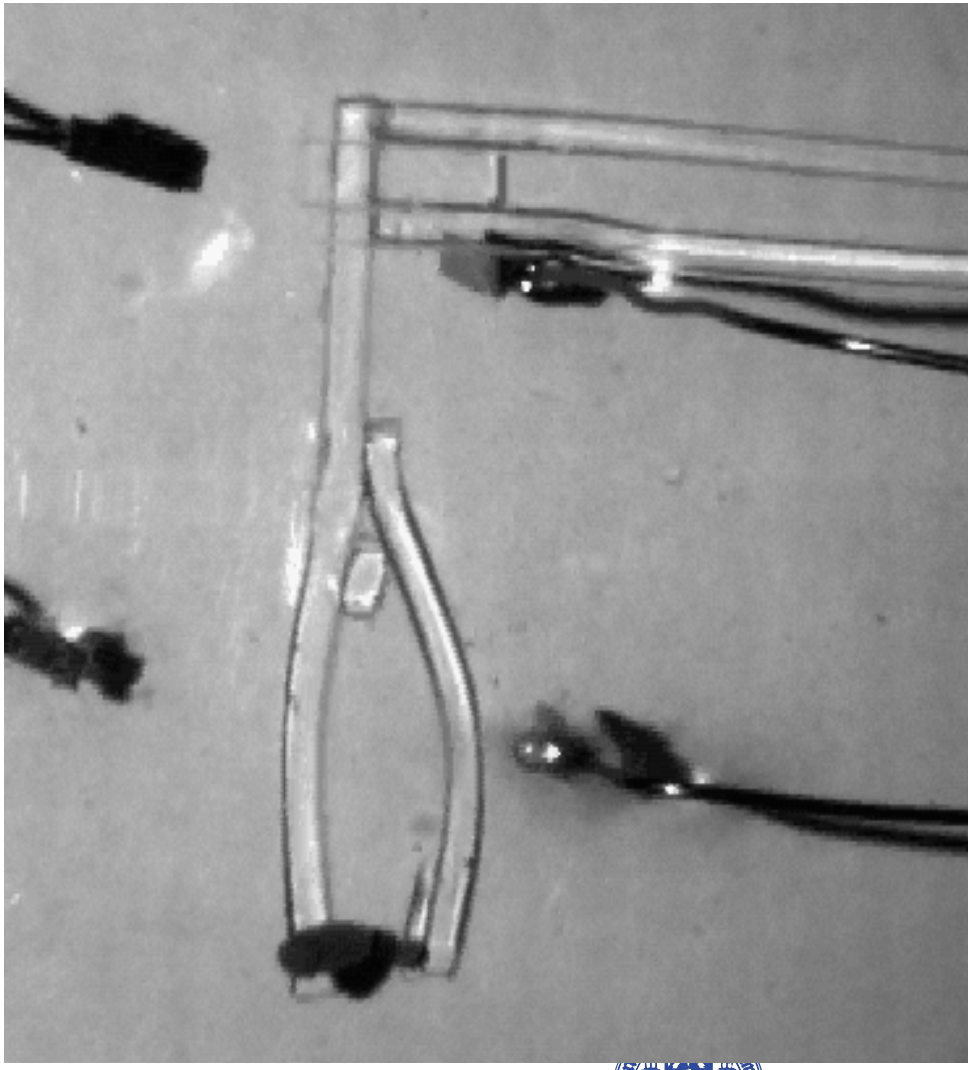




Koumura, N.; Zijlstra, R.W.J.; van Delden, R.A.; Harada, N.; Feringa, B.L. Nature 1999, 401, 152.

Polymer Gels as Molecular Motors

- Gülch, R. W., Holdenried, J., Weible, A., Wallmersperger, T., Kröplin, B.: *Electrochemical stimulation and control of electro-active polymer gels*. In Smart Structures and Materials 2001. Y. Bar-Cohen (Ed.), Proceedings of SPIE 4329, 328-334 (2001)

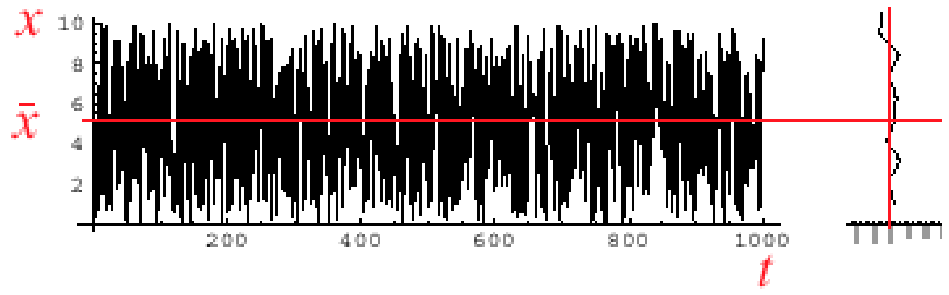


Course Structure

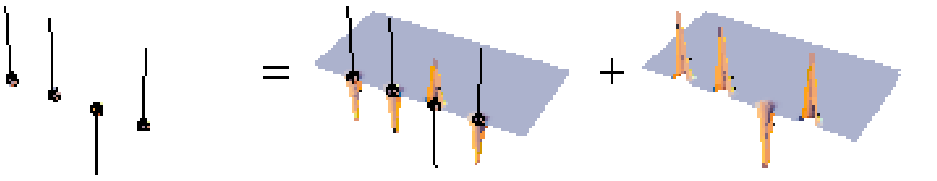
Overview

- 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)

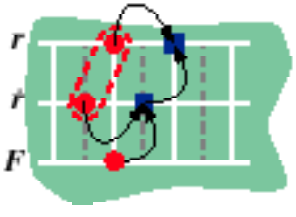


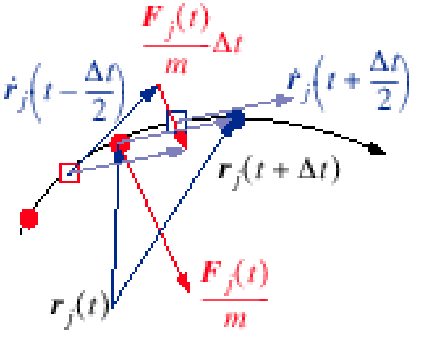
Time average



Ewald Summation

Leap Frog

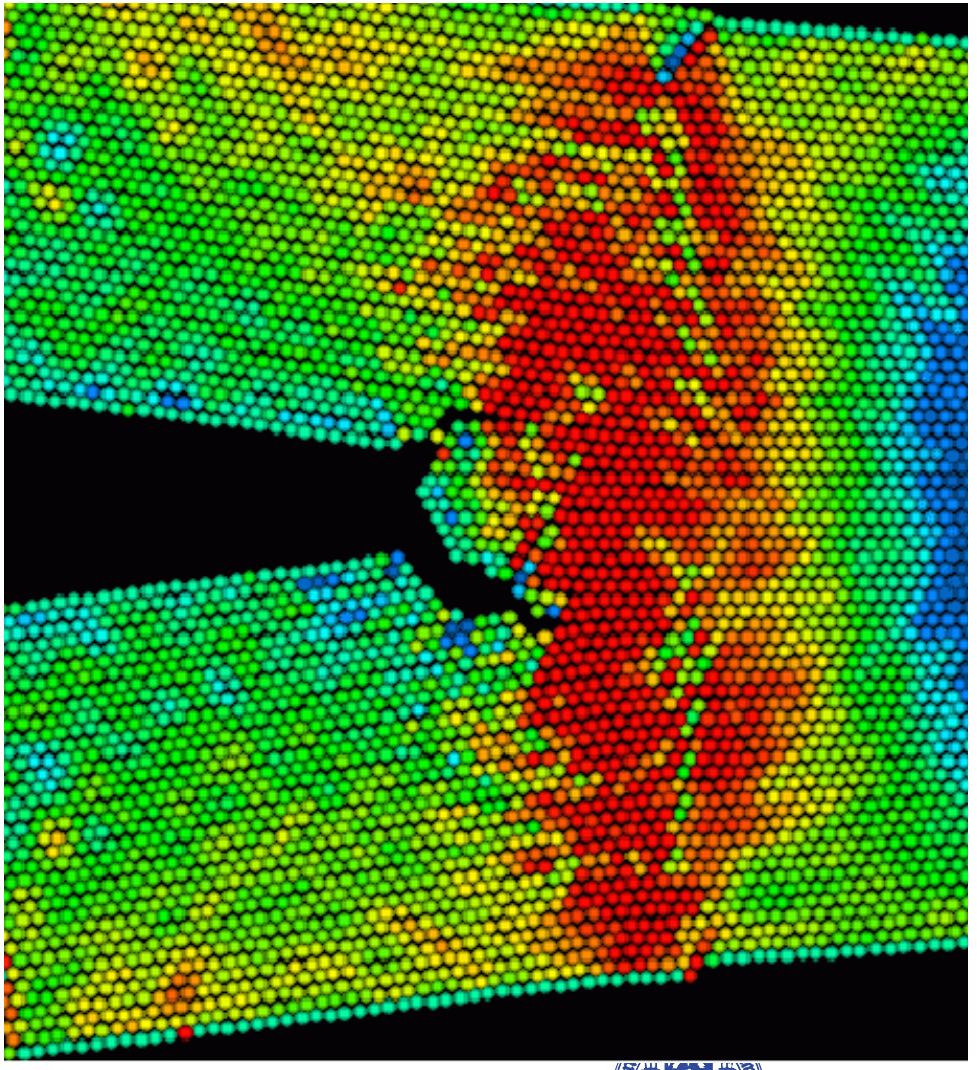




Course Structure

Particle Dynamics

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

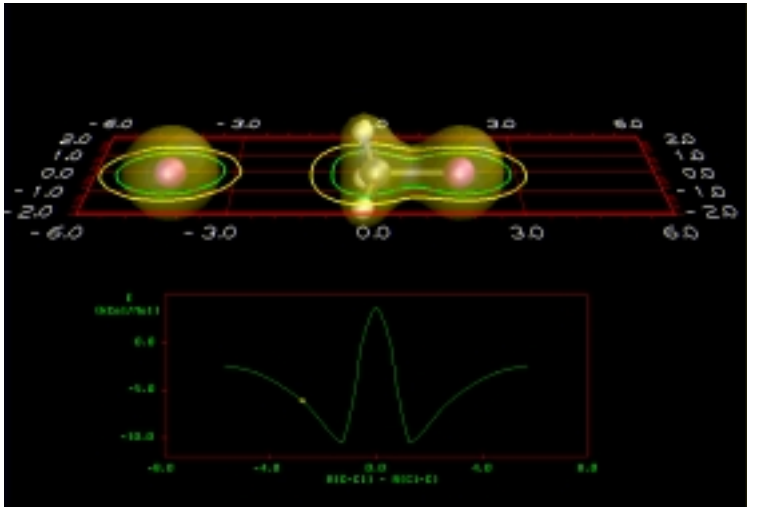


- Example: MD of crack propagation
  The colors refer to the state of stress at the atomic sites
  www.gre.ac.uk/~rh01/movie/

Course Structure

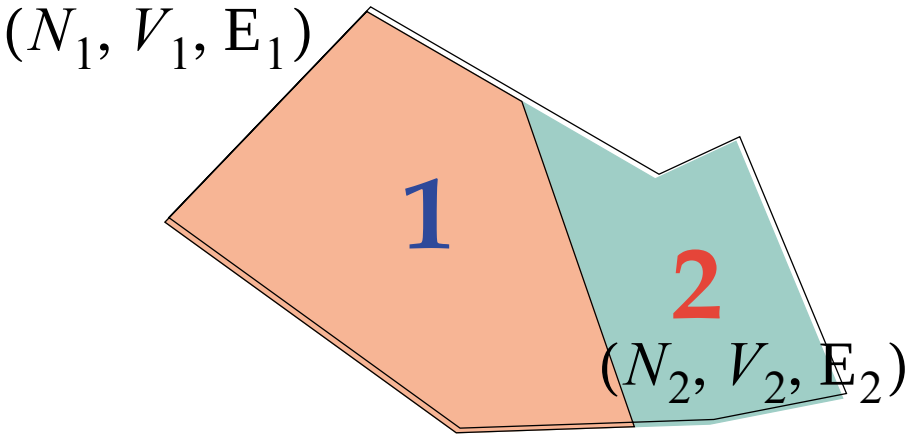
Molecular Models

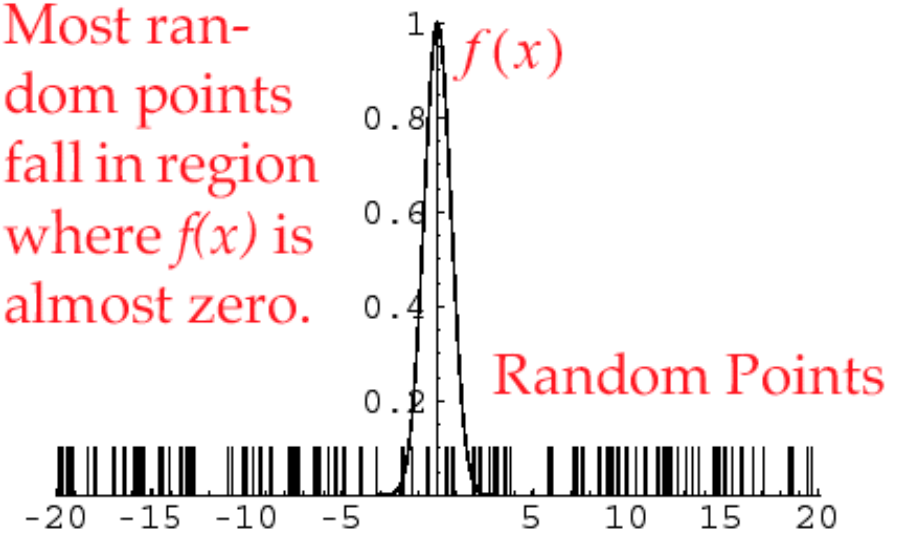
- Quantum chemistry
  - Born-Oppenheimer approximation, atomic and molecular orbitals, Hartree-Fock equation. Electron correlation, configuration interaction and DFT.
- Molecular mechanics
  - Empirical chemical bonding and non-bonding interactions. Determining the empirical force field. Quantum corrections and quantum molecular dynamics.
- Exploring the energy surface
  - Conformational analysis. Local and global optimization. Structure of proteins. Proteins folding and docking.



Statistical Thermodynamics and Monte-Carlo

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

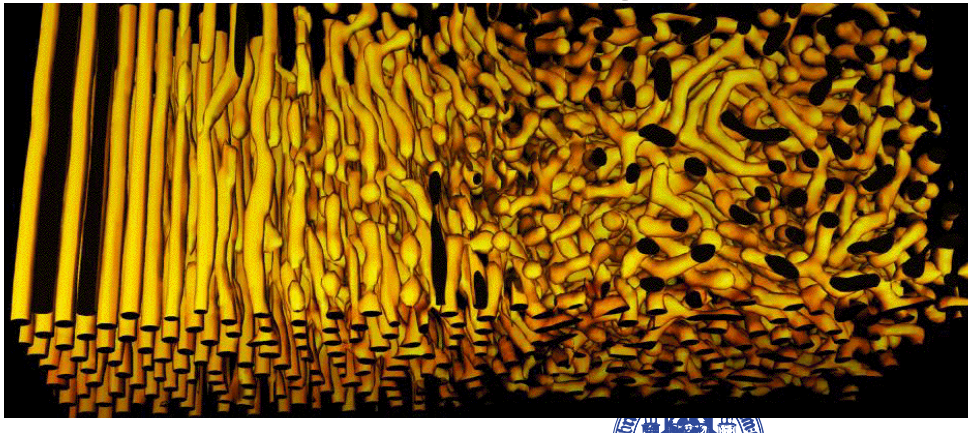




Course Structure

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

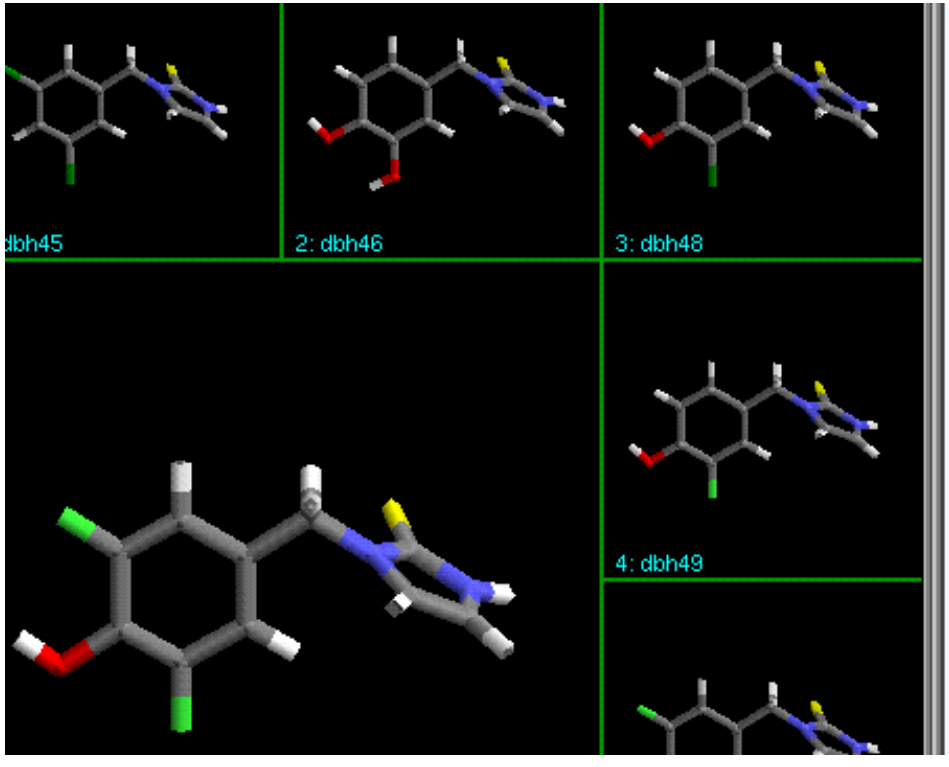


Time evolution of phase partition of a Pluronic 64 and water mixture
GRPOMACS

Course Structure

Empirical Correlations and Chemometrics

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



RUN | GFA | Current Defaults Set: QSAR

http://www.accelrys.com/cerius2/images/qsar_1.gif

R1 C3 (Derived): ==3.14769 + 0.028503 * col "Pi-0^2" + 1.0661 * SP

	Y1 -log(IC50)	GFA Predicte	GFA Residual	STEPWISE Pr	STEF
1.	3.00	3.71	-0.71	2.84	
2.	3.15	3.75	-0.60	3.64	
3.	3.30	3.43	-0.13	2.32	
4.	3.45	3.95	-0.50	3.94	
5.	3.47	3.69	-0.22	3.68	
6.	3.47	3.61	-0.14	3.78	
7.	3.70	3.86	-0.16	3.74	
8.	3.76	3.67	0.09	3.61	
9.	3.81	3.80	0.01	3.32	

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

- J. M. Haile, *Molecular Dynamics Simulation: Elementary Methods*, John Wiley & Sons, Inc., New York (1992)
- D.C. Rapaport, T*he Art of Molecular Dynamics Simulation*, Cambridge University Press, (1995)
- A. R. Leach, *Molecular Modelling: Principles and Applications*, Addison Wesley Longman Limited, Harlow (1996)
- 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)

- Swiss-PdbViewer, www.expasy.ch/spdbv/

- 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

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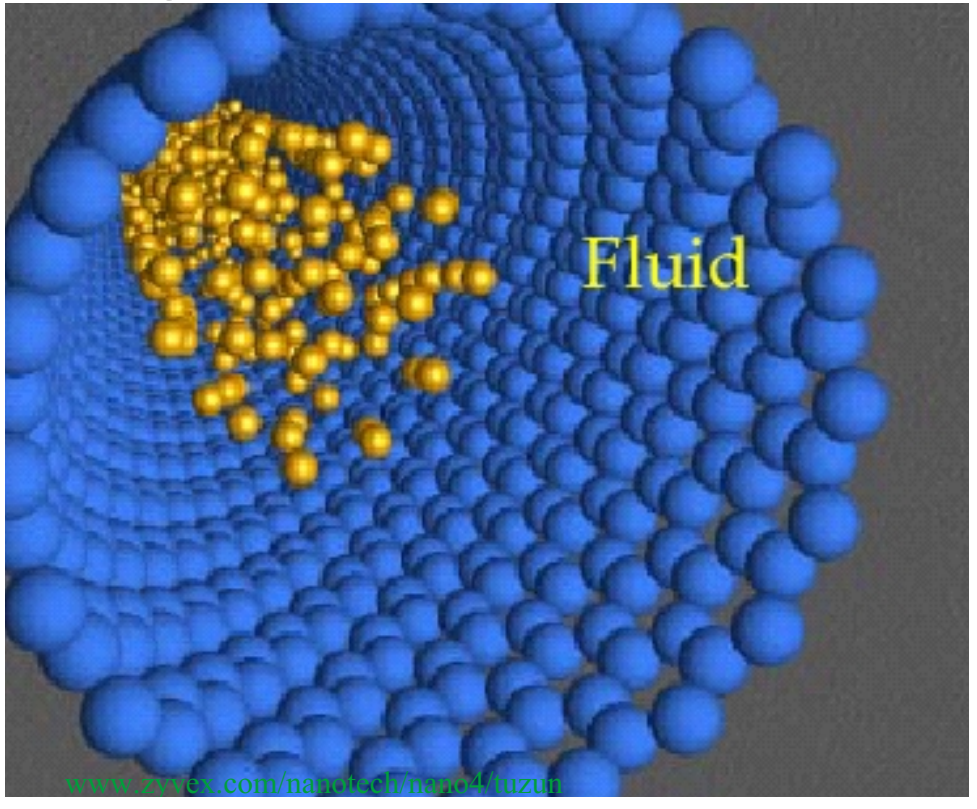

- If you would like to attend, please register.
- Exercises will be made in pairs, please specify your neighbor.
- Choose between paper review, software review or programming.