

SIMULATION TECHNIQUES FOR NANO- AND BIO-TECHNOLOGY APPLICATION

dr inż. Justyna Czerwinska email: jczer@ippt.gov.pl
IPPT PAN, Świętokrzyska 21, 00-049 Warszawa
Mondays 1400-1600 room 108

1. Introduction
2. Motivation
3. Physics of Continuum
 - Fluids Continuum Description
 - Solid State
 - Fluid-Solid Phenomena
4. Molecular Physics
 - Condensed Matter
 - Gas Matter
 - Chemical Reaction
 - Quantum Description
5. Mathematical and Numerical Basics
 - Basic Theory
 - Numerical Methods for Partial Differential Equations
 - Numerical Methods for Stochastic Differential Equations
6. Continuum description
 - Finite Volume Method
 - Finite Elements Method
 - Finite Difference Method

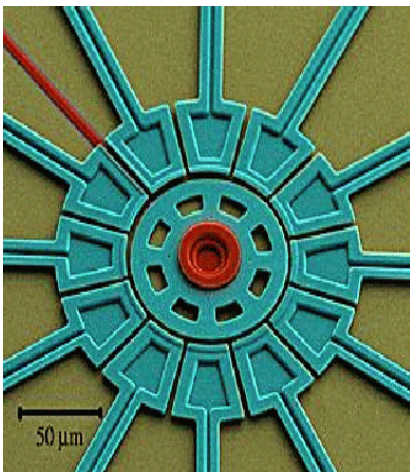


Illustration 2: Micro-motor

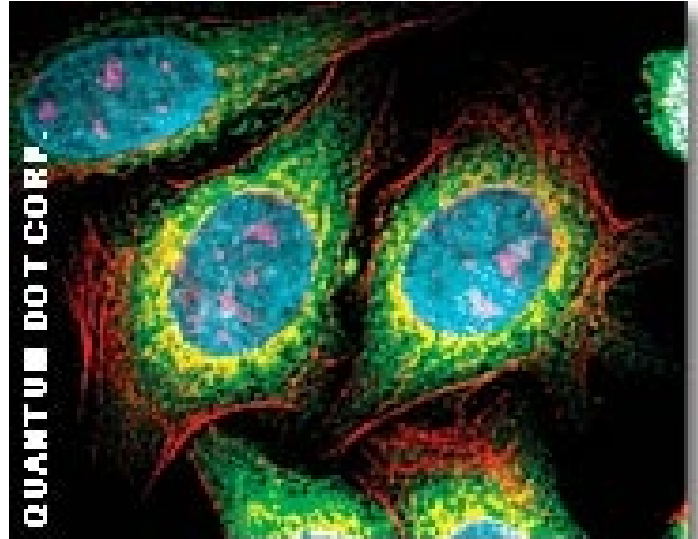


Illustration 1: Cells colored by quantum dots

7. Molecular Description
 - Molecular Dynamics
 - Molecular Dynamics with Lennard -Jones potential
 - ab initio Molecular Dynamics
 - Monte Carlo Methods
8. Mesoscale Models
 - Lattice Boltzmann Method
 - Particle Dynamics
 - Dissipative Particle Dynamics,
 - Smoothed Particle Dynamics
 - Rotational Dynamics
 - Direct Simulation Monte Carlo
 - Boundary Methods
9. Optimization Methods
 - Heterogeneous Multiscale Method
 - Genetic Algorithms
 - Variable Optimization
10. Standard Computations and Validation
 - Carbo Nano Tubes
 - Biological Membranes
 - Cell Engineering
 - DNA Interactions
 - Mesoscale Blood Flow
11. Future Directions in Simulations