Multiscale modeling of soft and biological matter

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1 Workshop Details

1.1 Details

Timing
Number of days : 3
Start : 2006-10-18
end : 2006-10-20

Location of the activity

Motivation for a different location

1.2 Description

No description provided

2 Requested Support

CECAM

Simbioma

3 Participant List

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4 Presentation List

Replication in micelle formation
Peter Bolhuis
University of Amsterdam, Netherlands
Abstract
In a dilute aqueous surfactant solution the majority of surfactant molecules are single, while above the critical micelle concentration they self-assemble into micellar clusters of a well defined size, driven by the hydrophobicity of the tails and the hydrophilic nature of the headgroups. This process is akin to nucleation in a first order phase transition. Several decades of theory suggests that the mechanism of micellar growth takes place by diffussion, adding one surfactant to the cluster at a time. The kinetics of micelle formation thus slows down exponentially with the height of the nucleation barrier, representing the least likely cluster size.
We report molecular simulations suggesting that the kinetics of surfactant micelle formation can be sped up significantly by a replication mechanism, in which growing micelles become unstable and split into two similar sized micelles. We argue that for certain surfactants types around the critical micelle concentration such a mechanism becomes more dominant than the commonly accepted nucleation pathway.

References
René Pool and Peter G. Bolhuis, Phys. Rev. Lett. 97 018302 (2006)

Computational tools for modeling and simulation of nanoscale systems
Reinier Akkermans
Accelrys Ltd, United Kingdom
Abstract
We present various computational tools that can aid research of nanoscale systems, by providing concrete examples of multiscale modeling workflows, in which mesoscale models are contructed from atomistic data, and mesoscale simulation methods are used to generate input for finite-element calculations. The link between the micro- and mesoscale is discussed into more detail, in particular the coarse-graining route via the Flory-Huggins theory of mixtures. We investigate a simple method to estimate the Flory-Huggins interaction parameters from force field calculations, based on sampling the density-of-states of molecular clusters in the space spanned by coarse-grained coordinates. We show how we use the density-of-states to calculate the excess free energy of mixing, and how this leads to mesoscale interaction parameters. The role of entropy introduced by the process of coarse-graining and ways to calculate this contribution are discussed.

Numerical Simulations of Polymer Translocation Through Nanopores
Tapio Ala-Nissila
Helsinki University of Technology, Finland

Investigation of lipid monolayers with coarse-grained models

Svetlana Baoukina
Dept. of Biological Sciences, University of Calgary, Canada

Exploring nucleic acid structure at the atomic level: Can this be the foundation for multi-scale modeling of RNA
Thomas Cheatham III
University of Utah, United States

Modelling nano-scale objects in a continuum description of a complex fluid
Colin Denniston
The University of Western Ontario Department of Applied Mathematics, Canada

Multiple scale modelling of lipid membranes: bridging atomistic models to macroscopic experiments
Alex de Vries
Univ. Groningen, Netherlands
Abstract
The quadrupole splitting of deuterated lipid chains provides a beautiful non-invasive probe of lipid structure, and can be measured using NMR techniques. Reproduction of the order parameter profile along the lipid chains is an important objective in simulation models of lipid membranes. There are two gaps to be bridged, however, between the experiment and the atomistic model calculations. (1) time-scale: the order parameters should be calculated by first averaging the orientation of each C-D vector with respect to the magnetic field over the time of interaction of the field with the magnetic quadrupole (of the order of a microsecond). Atomistic models typically average over tens of nanoseconds. (2) length scale: experimental samples are often multilamellar stacks of millimeter dimension. Atomistic models typically model a single bilayer of even less than 10 nanometer, suppressing longer wavelength undulations.
Coarse-graining helps in bridging both gaps and results will be presented of long-time multilamellar lipid membranes. An attempt will be made to develop models to correct the order parameter profile calculated using atomistic models to reflect those of macroscopic systems.

Curvature-mediated interactions between membrane proteins lead to aggregation and vesiculation
Markus Deserno
MPIP Mainz, Germany
Abstract
Cellular tasks such as endocytosis, vesiculation, and protein sorting, or the biogenesis of organelles such as the endoplasmic reticulum or the Golgi apparatus rely on significant protein-assisted membrane remodeling. Special curvature-sensitive proteins may both experience geometry-driven forces and, conversely, induce major changes in membrane shape and topology. Yet, owing to the lipid bilayer's bending stiffness, the latter requires a cooperative action of many

individual proteins. Effecting their aggregation and subsequent function at a specific location thus poses not only a regulatory but also a physical challenge. Using large-scale coarse grained membrane simulations we demonstrate that even in the absence of any direct protein interactions curvature-mediated forces alone constitute a robust mechanism for aggregation, which due to positive feedback can suffice to trigger vesiculation.

Phase Field Crystal Modeling in Material Science

Ken Elder
Oakland University, United States

Abstract

The vast majority of naturally occurring or man-made solids are not in equilibrium and contain complex spatial structures on nanometer, micron or millimeter length scales. This is particularly important since these morphologies often determine the mechanical, electrical and optical properties of the material. In this talk I would like to discuss a continuum field theory approach to modeling the formation of these structures. This approach bridges the gap between atomic scale models and mesoscopic continuum elasticity theory. For illustrative purposes a number of applications will be considered including liquid phase epitaxial growth, spinodal decomposition, eutectic solidification, dendritic growth and material hardness.

Multiscale Studies into Structure and Dynamics of Lipid Membranes

Emma Falck
UIUC, United States

Abstract

In this talk, I will describe multiscale simulation studies into the structure and dynamics of lipid membranes. Membrane structure is the target of intense investigation: new insights into the presence of rafts and microdomains in multicomponent lipid bilayers are frequently reported. Our coarse-grained studies of lipid bilayers revealed surprising features in the lateral structural properties of the bilayer. This finding was verified by atomic-scale studies of large bilayer systems, confirming that coarse-grained models, whose parameters are rigorously derived from more detailed descriptions, can indeed be expected to reproduce the relevant physics and chemistry of the original system. Knowing (transient) membrane structures is a very good starting point. However, since cellular membranes are always under non-equilibrium conditions, understanding their dynamics is at least as crucial. Unfortunately, the dynamics of cell membranes has received considerably less attention than membrane structure, indeed, one could say there is no comprehensive model for membrane dynamics. Even seemingly simple basic dynamic processes, such as the lateral diffusion of lipids in one-component lipid bilayers, are not fully understood. In the second part of my talk, I will describe simulations that have shed new light on the lateral diffusion of lipids.

Heterogeneous Lipid Bilayers: Evolving Microstructures in Biology

Mikko Haataja
Princeton University, United States

Abstract

The design and processing of materials with novel physical and mechanical properties requires a fundamental understanding of the connections between processing, microstructure, and properties. For example, mechanical properties in pure metals and alloys can be varied by manipulating the polycrystalline grain size or the size of the compositional domains through heat treatment, while elastic strain provides a way to tune the optical properties of self-assembled quantum dots during growth. In an analogous manner, the biological function of cell membranes is strongly affected by the details of the local Ã'microstructureÃ".
Typically, microstructural evolution takes place across multiple length and time scales, ranging from atomistic to mesoscopic ones. In this talk I will describe our recent efforts in developing physically-based, coarse-grained continuum models, which bridge the atomistic and mesoscopic scales, to elucidate the self-assembly and non-equilibrium dynamics of heterogeneous lipid bilayers.

t.b.a.
Jesus Izaguirre
Univ. of Notre Dame, United States

Adaptive Resolution Simulation Approach
Kurt Kremer
MPI fuer Polymerforschung, Germany

Multiscale modelling based on effective potentials
Alexander Lyubartsev
Stockholm University, Sweden

Towards consistent parametrization of coarse-grained models of DNA
Filip Lankas
EPFL, Switzerland

Continuum mechanics models of DNA looping probabilities
John H. Maddocks
EPFL, FSB-IMB, Switzerland

Multiscale Monte Carlo for simple fluids
Anthony C. Maggs
ESPCI France, France

Abstract
We introduce a multiscale Monte Carlo algorithm to simulate simple fluids. The probability of an update follows a power law distribution in its length scale. The collective motion of clusters of particles requires generalization of the Metropolis update rule to impose detailed balance. We apply the method to the simulation of a Lennard-Jones fluid and show substantial improvements in efficiency over conventional methods, eliminating hydrodynamic slowing down.

Coarse-grained simulations of liposomes
Albert Jan Markvoort
Eindhoven University of Technology, Netherlands
Abstract
Lipid bilayer membranes are known to form various structures like large sheets or vesicles. To bridge the gap between what can be studied experimentally and what can be studied using atomistic models, we study these structures using coarse-grained molecular dynamics simulations. In first instance, we have used our coarse-grained lipid model to study spontaneous vesicle formation [1], showing the role of entropy in the bilayer-vesicle transition. Subsequently, such spontaneously formed vesicles have been used to study fusion [2,3] in which various mechanisms can be discerned. Finally, our coarse grained model is used to study mixtures of lipids. This shows that the positioning of domains with different lipid types opposite to each other induces spontaneous curvature in a membrane and that even small differences in the lipid-solvent interactions already result in such spontaneous curvature. This has a tremendous influence on vesicle shapes, resulting in ellipsoids, discoids, pear-shaped vesicles, cup- shaped vesicles, as well as budded vesicles [4].

References
[1] A.J. Markvoort et al., J. Phys. Chem. B, 2005, 109, 22649-22654
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[3] A.F. Smeijers et al., J. Phys. Chem. B, 2006, 110, 13614-13623
[4] A.J. Markvoort et al., J. Phys. Chem. B, 2006 (In press)

t.b.a.
Teemu murtola
Helsinki University of Technology, Finland

Assembly of Diblock Copolymers on Patterned Substrates: A "Single-Chain-in-Mean-Field-Simulation" Study
Marcus Muller
Georg-August Universitaet, Goettingen, Germany
Abstract
The directed assembly of diblock copolymers on patterned substrates is a way to create nanoscopically structured materials [1-3]. We study the structure and kinetics of diblock copolymers on patterned substrates by simulating a large ensemble of independent chains in an external field [4,5]. This external field depends on the density created by the ensemble of molecules and it is

frequently updated as to mimic the instantaneous interactions of a molecule with its neighbors. This approximate, particle-based self-consistent field method allows to (i) incorporate arbitrary chain architecture (ii) includes fluctuations and (iii) the explicit propagation of the chain conformations in time permits us to study the kinetics of structure formation. The factors that control the accuracy of the method are quantitatively discussed [6].

References

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K. Ch. Daoulas, M. Mü ller, J.J. de Pablo, P.F. Nealey, and G.D. Smith, Soft Matter 2, 573 (2006)
K. Ch. Daoulas, M. Mü ller, preprint (2006)

Two new (and unrelated) efforts to overcome length scales in MD

Martin Mueser
Department of Applied Mathematics, University of Western Ontario, London, Ontario, Canada, Canada

References

One of the two topics alluded to in the title deals with a new method for the parameterization of electrostatic interactions. The starting point is to rewrite regular charge equilibration models in terms of bond variables rather than as atomic variables. While the original charge equilibration method can be obtained as a limiting case, it is possible to introduce a new bond term, which effectively introduces a band gap. The band gap is present in nature but not in the original charge equilibration method. The hope is that a successful parameterization will allow us to tackle more problems with force fields than currently possible.

The other topic (provided there is time left) deals with ways how to efficiently solve for elastic deformation when an object is contact with a semi-infinite, elastic manifold, e.g., the situation of a soft, elastic solid (or membrane) pressed against a hard corrugated substrate. We worked out the details of a Green's function formulation, in which only the outermost atoms of the elastic solids need to be considered. The effects of all bulk atoms is encoded in the Green's functions. The method allows us to simulate systems with atomic resolution, whose linear length approaches 1 micron.

Simulation of fluctuating hydrodynamics on a mesocopic scale

Frank (E.A.J.F.) Peters
Department of Chemical Engineering, Eindhoven University of Technology, Netherlands

t.b.a.

Jelger Risselada

RUG, Netherlands

Local algorithms for long ranged interactions

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Bowen Hall, 70 Prospect Ave, Princeton University, Princeton, NJ 08544, USA, United States

Abstract

The computation of Coulombic interactions forms one of the major bottlenecks in soft matter and biomolecular simulations. Most current fast Coulomb techniques rely on Fourier methods that do not parallelize well on large compute clusters, have difficulty treating inhomogeneous dielectric environments and only work well in molecular dynamics. We discuss a new class of (real-space) linear (i.e. O(N)) scaling algorithms that mediate the Coulomb interaction through a thermalized auxiliary field that is dynamically constrained to obey Gauss' law. Instead of globally optimizing the field configuration as in conventional approaches, the algorithm performs a partial integration over the transverse degrees of freedom of the electric field, which requires only local operations. The method is particularly powerful in Monte Carlo (MC) simulations, but has also been fruitfully extended to molecular dynamics (MD). We present continuum (off-flattice) implementations for both MC and MD and discuss recently developed strategies for achieving high accuracy and efficiency. In addition to the ease of parallelization, the approach holds the promise of a more accurate treatment of polarization effects in coarse-grained simulations that rely on implicit solvent models.

Modeling coarse-grained polymer with entanglements by using stochastic slip-links

Jay Schieber
Illinois Institute of Technology, United States

Abstract

Traditionally there have been two distinct classes of mathematical or conceptual models to describe the behavior of entangled polymers: temporary network models and tube models. We have taken an approach that marries these two different views, using the idea of a slip-link. Key to this novel development is the use of monomer density between entanglements as a stochastic variable. The resulting model contains only a single phenomenological parameter (a time constant), which is determined by linear viscoelastic experiments (or possibly by molecular dynamics). All nonlinear flow dynamics are then described without adjusting parameters. This approach offers a way to model systems that have been modeled by separate equations, to date. The resulting theory has given excellent predictions of all known shear data, and steady elongational data. However, it has not been able to describe transient elongational data. We will examine and eliminate the use of simplifying assumptions in previous implementations of the theory as a possible cause of the remaining discrepancy with data. We will also show how the current theory can incorporate semi-flexibity, branching and even cross- linking without a significant change to the underlying mathematical structure, making it a useful bridge between atomistic and macroscopic descriptions for soft biological materials.

Spontaneous nanostructure formation in copolymer systems

Friederike Schmid
Universitat Bielefeld, Fakultat fur Physik, Germany

Abstract

Block copolymers are chain molecules containing blocks of two or several chemically incompatible components. Much like smaller amphiphiles (e.g., lipids in water), copolymers in melt or solution spontaneously aggregate into a variety of nanostructures, e.g., lamellar phases or polymeric vesicles, which can be tuned by tuning system parameters such as the chain lengths, the block lengths, the composition, the temperature, etc. This can be used to prepare nanoscaled materials with well-defined properties. To simulate these processes on a mesoscopic scale, it is often efficient to use field-based methods where the polymers are no longer treated individually (as single chains). We will briefly introduce the concept of field-based polymer simulations and present two applications: The formation of a microemulsion in a ternary copolymer/homopolymer system [1,2] and the dynamics of spontaneous vesicle formation in a dilute copolymer solution [3,4]

References

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D. Dü chs, F. Schmid, Formation and structure of the microemulsion phase in ternary AB + A + B polymeric microemulsions, J. Chem. Phys. 121, 2798 (2004).
X. H. He, F. Schmid, Dynamics of spontaneous vesicle formation in dilute solutions of amphiphilic diblock copolymers, Macromolecules 39, 2654 (2006).
X. H. He, F. Schmid, in preparation (2006).

Spanning length and time scales in simulations of membrane-associated processes

Julian Shillcock
MPI of Colloids and Interfaces, Germany

A guided tour through the landscape of coarse-grain models for biomembranes

Maria Maddalena Sperotto
Biocentrum, DTU, Denmark

Abstract

Biomembranes are multi component systems which show a complex behaviour. To understand this behaviour and how it may be related to biological functions, it is often necessary to consider simplified reconstituted membranes, i.e., lipid bilayers and lipid vesicles.
These have been a subject of experimental and theoretical investigations, the latter based on theories and modeling which cover time and length scales ranging from the atomistic to the mesoscopic ones.
The aim of this contribution is to give a short and schematic overview [1] of the coarse-grain mesoscopic models which have been developed to study reconstituted membrane systems.
We will start with classifying the models in two groups, depending on whether the solvent, i.e., water, is treated implicitly or explicitly.
Then, we will briefly describe some of the models, and how they have been used, together with

simulations techniques, to investigate both bilayer related processes – ranging from gel-to-fluid phase changes and the formation of pores, to the structural changes due to impurities like alcohols, cholesterol and proteins – and vesicle related processes such as fusion and fission.

References

[1] Venturoli et al.,Physics Reports, 2006 (in press)

Interaction of cyclic peptide nanotubes with membranes

Mounir Tarek
CNRS / Université Henri-Poincaré , France

Computer simulations of ABC transporters

Peter Tieleman
University of Calgary, Canada

Abstract

ABC transporters are modular proteins that use ATP hydrolysis as a power source to pump a broad range of substrates across membranes. They play critical roles in all forms of life and in humans are primarily known for their role in cystic fibrosis and multidrug resistance in cancer therapy. Computationally, the problem is how to study the mechanism of proteins that in their mechanism combine nanosecond events with millisecond or slower functional motions. We are using a combination of quantum calculations, molecular dynamics, normal mode analysis and homology modeling to understand the modes of action of a number of ABC transporters. An approach which combines normal modes and perturbed normal modes as biasing potential in molecular dynamics to investigate the response of transmembrane domains to motions in the ATP-binding domains seems of particular interest at the moment.

Systematic Multiscale Coarse-graining of Biomolecular and Soft Matter Systems

Gregory Voth
University of Utah, United States

Low Reynolds Number Swimmers

Julia Yeomans
Oxford University, United Kingdom

Abstract

We use three numerical methods to explore the motion of low Reynolds number swimmers, modelling the hydrodynamic interactions by means of the Oseen tensor approximation, lattice Boltzmann simulations and multiparticle collision dynamics. By applying the methods to a three bead linear swimmer, for which exact results are known, we are able to compare and assess the effectiveness of the different approaches. We use the algorithms to explore the interactions between swimmers. We shall also discuss a continuum model for swimmers which shows a rich rheology and point out the current gap between explicitly modelling individual swimmers and the continuum approach.

Multiscale Modeling of structure and phase behavior in heterogeneous lipid bilayers
Roland Faller
UC Davis, United States

5 Program

Day 1: Oct. 18 2006

Session : 1
08:55 to 09:00 : Welcome

09:00 to 09:30 : Presentation
Multiscale Monte Carlo for simple fluids
Anthony C. Maggs

09:30 to 10:00 : Presentation
Adaptive Resolution Simulation Approach
Kurt Kremer

10:00 to 10:30 : Coffee Break

10:30 to 11:00 : Presentation
Replication in micelle formation
Peter Bolhuis

11:00 to 11:30 : Presentation
Multiscale Studies into Structure and Dynamics of Lipid Membranes
Emma Falck

11:30 to 12:00 : Presentation
Modelling nano-scale objects in a continuum description of a complex fluid
Colin Denniston

12:00 to 12:30 : Presentation
Continuum mechanics models of DNA looping probabilities
John H. Maddocks

12:30 to 14:30 : Lunch Break

14:30 to 15:00 : Presentation
Numerical Simulations of Polymer Translocation Through Nanopores
Tapio Ala-Nissila

15:00 to 15:30 : Presentation
Low Reynolds Number Swimmers
Julia Yeomans

15:30 to 16:00 : Presentation
Local algorithms for long ranged interactions

Jö rg Rottler

16:00 to 16:30 : Presentation
Interaction of cyclic peptide nanotubes with membranes
Mounir Tarek

16:30 to 17:00 : Coffee Break

17:00 to 17:30 : Presentation
Multiple scale modelling of lipid membranes: bridging atomistic models to macroscopic experiments
Alex de Vries

17:30 to 18:00 : Presentation
Investigation of lipid monolayers with coarse-grained models
Svetlana Baoukina

18:00 to 18:30 : Presentation
Computational tools for modeling and simulation of nanoscale systems
Reinier Akkermans

Day 2: Oct. 19 2006

Session : 1
09:00 to 09:30 : Presentation
Phase Field Crystal Modeling in Material Science
Ken Elder

09:30 to 10:00 : Presentation
Two new (and unrelated) efforts to overcome length scales in MD
Martin Mueser

10:00 to 10:30 : Coffee Break

10:30 to 11:00 : Presentation
Curvature-mediated interactions between membrane proteins lead to aggregation and vesiculation
Markus Deserno

11:00 to 11:30 : Presentation
Heterogeneous Lipid Bilayers: Evolving Microstructures in Biology
Mikko Haataja

11:30 to 12:00 : Presentation
t.b.a.

Jesus Izaguirre

12:00 to 12:30 : Presentation
Coarse-grained simulations of liposomes
Albert Jan Markvoort

12:30 to 14:30 : Lunch Break

14:30 to 15:00 : Presentation
Assembly of Diblock Copolymers on Patterned Substrates: A "Single-Chain-in-Mean-Field-Simulation" Study
Marcus Muller

15:00 to 15:30 : Presentation
Spontaneous nanostructure formation in copolymer systems
Friederike Schmid

15:30 to 16:00 : Presentation
Multiscale Modeling of structure and phase behavior in heterogeneous lipid bilayers
Roland Faller

16:00 to 16:30 : Presentation
Towards consistent parametrization of coarse-grained models of DNA
Filip Lankas

16:30 to 17:00 : Coffee Break

17:00 to 17:30 : Presentation
Exploring nucleic acid structure at the atomic level: Can this be the foundation for multi-scale modeling of RNA
Thomas Cheatham III

17:30 to 18:00 : Presentation
Multiscale modelling based on effective potentials
Alexander Lyubartsev

20:00 to 22:00 : Dinner

Day 3: Oct. 20 2006

Session : 1
09:00 to 09:30 : Presentation
Spanning length and time scales in simulations of membrane-associated processes
Julian Shillcock

09:30 to 10:00 : Presentation
Systematic Multiscale Coarse-graining of Biomolecular and Soft Matter Systems
Gregory Voth

10:00 to 10:30 : Coffee Break

10:30 to 11:00 : Presentation
Computer simulations of ABC transporters
Peter Tieleman

11:00 to 11:30 : Presentation
Modeling coarse-grained polymer with entanglements by using stochastic slip-links
Jay Schieber

11:30 to 12:00 : Presentation
Simulation of fluctuating hydrodynamics on a mesocopic scale
Frank (E.A.J.F.) Peters

12:00 to 12:25 : Discussion

12:25 to 12:30 : Closing word

6 Key references

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