NSDL Materials Digital Library Pathway

Materials Informatics Workshop: Definition, Theory and Application

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Cincinnati, Ohio USA

Outline

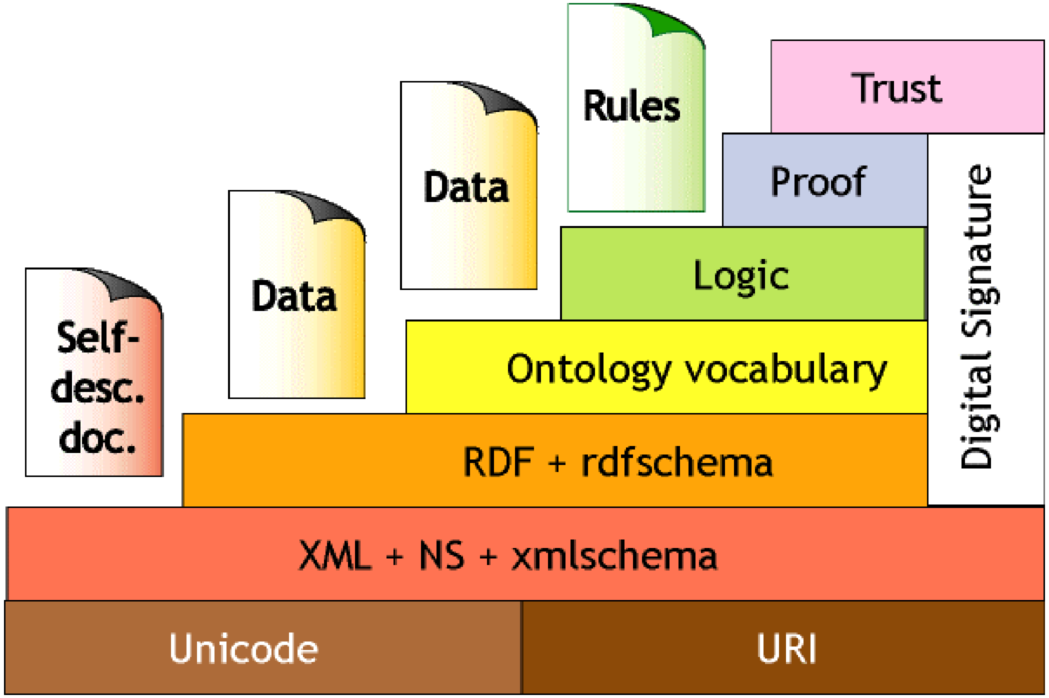
- Background
  - Cyberinfrastructure
  - National Science Digital Library (NSDL)
- Introduction
- Methods
  - Participants
  - Software and Procedure
- Results
- Discussion

Vision of Cyberinfrastructure (CI)

- Blue Ribbon Advisory Panel, *Revolutionizing Science & Engineering Through Cyberinfrastructure*

  http://www.nsf.gov/od/oci/reports/toc.jsp
- "The vision …"
  - ubiquitous, comprehensive digital environments
  - interactive and functionally complete in terms of people, data, information, tools, and instruments
  - unprecedented levels of computational, storage, and data transfer capacity

CI: Social & Technical Layers



Tim Berners-Lee, James Hendler and Ora Lassila. The Semantic Web. *Scientific American*, May 2001.

- Virtual research and education communities
  - complementary needs and expertise
- Structured Information
  - domain and cross domain metadata, markup languages and vocabulary
- Trusted information
  - reuse across research and education

CI: Deliverables & Benefits

- "Raw data and recent results are easily shared, not just within a research group or institution but also between scientific disciplines and locations."
- Individuals, teams, and organizations:
  - revolutionize what they do, how they do it, and who participates
  - over time, geographic, organizational, and disciplinary distance
  - access to more, better information and facilities for discovery and learning (Blue Ribbon Panel, 2003)

NSF, CI & Digital Libraries

NSDL Launch

Fall 2002

NSF NSDL Program 2000

DLs & UG Earth Systems Education initiated FY99, continuing

DLI 2 Special Emphasis in UG Education FY 98-99

DLI 2 - NSF, et al., initiated in FY98, continuing

Digital Libraries Initiative (DLI 1) - NSF/NASA/ARPA, FY 94-97

National Science Digital Library (NSDL)

- An NSF-funded $20 million/year program in Science, Technology, Engineering and Mathematics (STEM) education
- A digital library describing nearly two million carefully selected online STEM resources from well over 100 collections (at http://nsdl.org)
- A core integration team (Columbia, Cornell, UCAR) working with 9 *Pathways Portals* and over 200 NSF grantees
- A large community of researchers, librarians, content providers, developers, students, and teachers

MatDL

Materials Digital Library Pathway

NSF

NSDL

NSDL Materials Digital Library (MatDL) Pathway

- As part of the NSDL
  - Implement an information infrastructure for materials community
  - Provide content and services to support the integration of research and education in materials
  - Disseminate information generated by government-funded efforts in materials
- A collaborative effort …

NIST National Institute of Standards and Technology

Kent State University

MIT Massachusetts Institute of Technology

University of Michigan

Purdue University

Iowa State University

NSDL MatDL Pathway Goals:

- Provide stewardship of significant materials research output & education resources
- Facilitate connections between materials research & education
- Support broad dissemination of materials research & education
- Contribute to increasing impact of NSF initiatives

NSF MS Initiatives
- Nanoscale Interdisciplinary Research Teams
- Materials Research Science & Engineering Centers
- International Materials Institutes

Teaching Resource Development
- MS Teaching Archive

MatDL Repository

Goal: Facilitate interactions between research & education
Audience: Undergraduate and above

Supporting…

Virtual Labs
- Intro to Solid State Chemistry

Collaborative Code Development
- NIST FiPy
- UM

Offering:

- Tools, such as the **MatDL Repository** & **Soft Matter Wiki**, to describe, manage, exchange, archive, and disseminate data from national & international government-funded materials teams & centers
- **MatForge**, for open access development of modeling and simulation codes
- **Teaching Archive**, for collaborative development of core undergrad MS teaching materials
- Services and content for virtual labs in undergrad intro science courses

MatDL

Materials Digital Library Pathway

NSF NSDL

MatForge

FiPy: A Finite Volume PDE Solver Using Python

http://www.ctcms.nist.gov/fipy

Overview

FiPy is an object oriented, partial differential equation (PDE) solver, written in Python, based on a standard finite volume approach. The framework has been developed in the Metallurgy Division and Center for Theoretical and Computational Materials Science (CTCMS), in the Materials Science and Engineering Laboratory (MSEL) at the National Institute of Standards and Technology (NIST).

The solution of coupled sets of PDEs is ubiquitous to the numerical simulation of science problems. Numerous PDE solvers exist, using a variety of languages and numerical approaches. Many are proprietary, expensive and difficult to customize. As a result, scientists spend considerable resources repeatedly developing limited tools for specific problems. Our approach, combining the finite volume method and Python, provides a tool that is extensible, powerful and freely available. A significant advantage to Python is the existing suite of tools for array calculations, sparse matrices and data rendering.

The **FiPy** framework includes terms for transient diffusion, convection and standard sources, enabling the solution of arbitrary combinations of coupled elliptic, hyperbolic and parabolic PDEs. Currently implemented models include phase field treatments of polycrystalline, dendritic, and electrochemical phase transformations as well as a level set treatment of the electrodeposition process .

The primary homepage for **FiPy** is at http://www.ctcms.nist.gov/fipy.

This MatDL Trac site provides:

- a public interface to the Subversion repository holding the **FiPy** source code

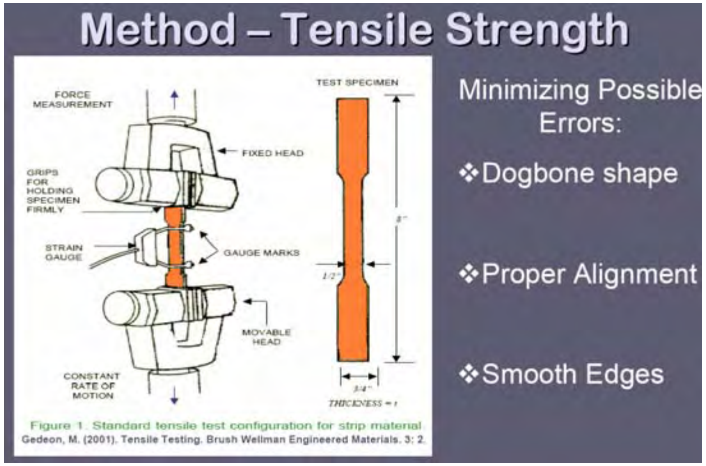
Teaching Archive
(Powell-Veryst/Krane-Purdue)

- Over 100 homework problems, handouts, courseware, readings, pedagogy; 30 authors
- Metadata: title, author(s), description, keywords, time/difficulty
- Version control: modify, keep old versions
- Collaborative development, corrections, etc.
- Editorial Board with 14 members

Virtual Labs
(Sadoway-MIT)

Services and content for:

- Virtual labs in large undergrad intro science courses
- Alternative to traditional labs
- Beginning with MIT *Intro to Solid State Chemistry*



Soft Matter Wiki: An Expanded Example in the MatDL

- Development of
  - Vocabulary on assembly of nanosystems
  - Expert community-driven
  - Bottom-up approach
  - Wiki-based

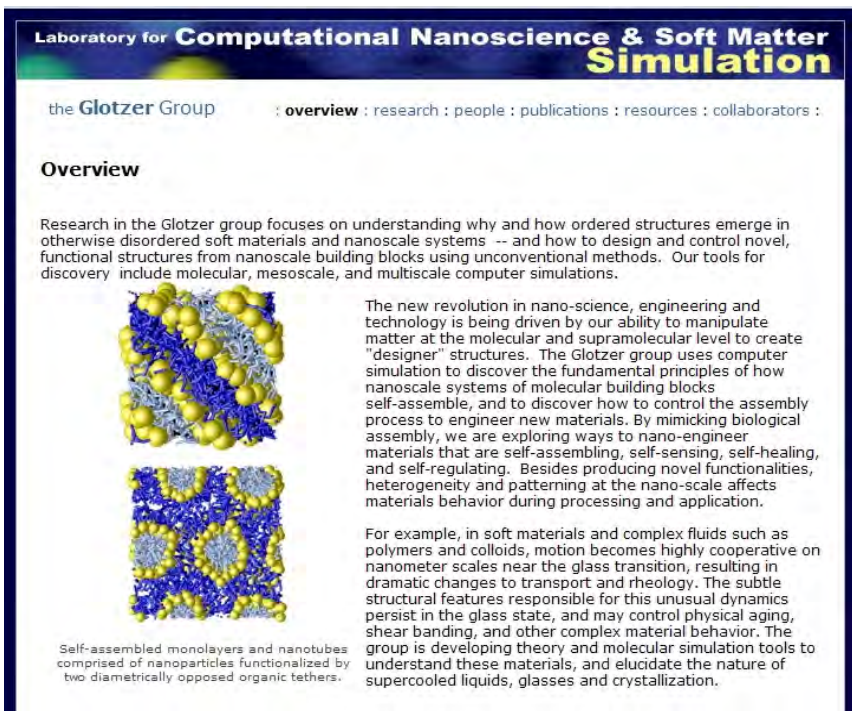
Primary Objectives

- Gather vocabulary, definitions, and relationships
- Collaboration with domain experts
- Low barrier threshold for contributions/working together

Materials Digital Library Pathway

Participants

Research Group


Laboratory for Computational Nanoscience & Soft Matter Simulation

the Glotzer Group : overview : research : people : publications : resources : collaborators :

Overview

Research in the Glotzer group focuses on understanding why and how ordered structures emerge in otherwise disordered soft materials and nanoscale systems -- and how to design and control novel, functional structures from nanoscale building blocks using unconventional methods. Our tools for discovery include molecular, mesoscale, and multiscale computer simulations.

The new revolution in nano-science, engineering and technology is being driven by our ability to manipulate matter at the molecular and supramolecular level to create "designer" structures. The Glotzer group uses computer simulation to discover the fundamental principles of how nanoscale systems of molecular building blocks self-assemble, and to discover how to control the assembly process to engineer new materials. By mimicking biological assembly, we are exploring ways to nano-engineer materials that are self-assembling, self-sensing, self-healing, and self-regulating. Besides producing novel functionalities, heterogeneity and patterning at the nano-scale affects materials behavior during processing and application.

For example, in soft materials and complex fluids such as polymers and colloids, motion becomes highly cooperative on nanometer scales near the glass transition, resulting in dramatic changes to transport and rheology. The subtle structural features responsible for this unusual dynamics persist in the glass state, and may control physical aging, shear banding, and other complex material behavior. The group is developing theory and molecular simulation tools to understand these materials, and elucidate the nature of supercooled liquids, glasses and crystallization.

Self-assembled monolayers and nanotubes comprised of nanoparticles functionalized by two diametrically opposed organic tethers.

CHE 557

Software & Procedure

- Mediawiki software
  - Latex
- Vocabulary procedure
  - Research group: semi-automatic DC metadata capture
  - Course: supplemental course resource and part of course assignments

Metadata Capture

<dc:title>Brownian Dynamics simulation of a nanoparticle aggregating tethered nanosphere</dc:title>

<dc:creator>Chris Iacovella</dc:creator>

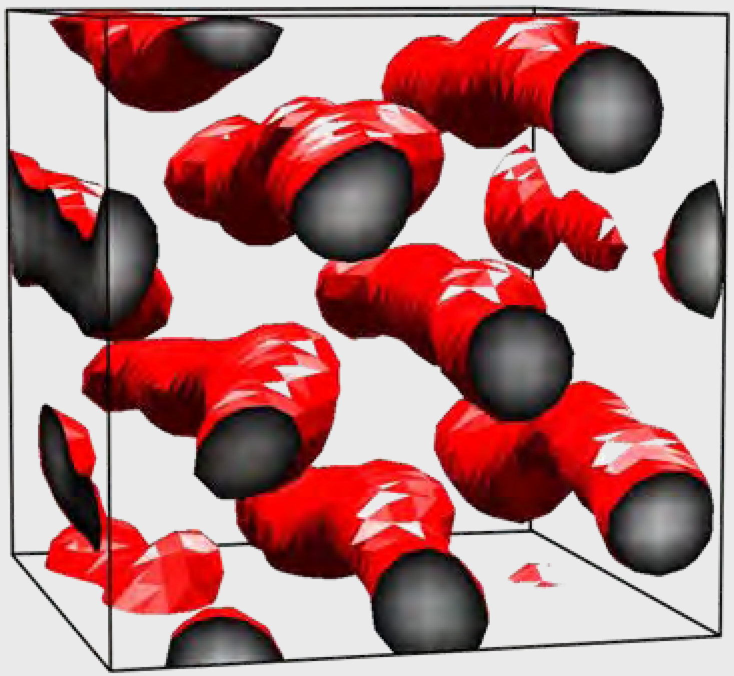
<dc:subject>Tethered Building Block</dc:subject>

<dc:subject>Lennard-Jones</dc:subject>

<dc:subject>Brownian Dynamics</dc:subject>

<dc:subject>NVT</dc:subject>

<dc:subject>FENE</dc:subject>



<dc:description>

Number of tethered building blocks = 800;

Number of beads = 7200;

Length of tether = 8;

Diameter of the nanopshere = 2.0;

System temperature = 0.2667;

System volume fraction = 0.25;

Integration scheme to use = Brownian Dynamics, NVT;

Number of Dimensions = 3;

United Atom Bead Spring with Lennard-Jones and FENE;

Phase: Hexagonally packed cylindrical micelles</dc:description>

<dc:publisher>Glotzer group. Depts of Chemical Engineering, Materials Science & Engineering, Macromolecular Science, and Physics,University of Michigan</dc:publisher>

<dc:date>2006-9-19</dc:date>

Results

- Public view (launched September 2006)
  - Number & range of terms
    - Currently 71 terms under 12 different categories
    - Approximately 70% of terms have definitions
  - Range of entry detail
    - Varies from briefly to considerably detailed
  - Adding context
    - Images, references
    - Related items in MatDL (e.g., preprints, images)

navigation
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Soft Matter Wiki-Overview of Contents

Soft Matter Wiki

[edit]

Soft materials are materials such as polymers, biomolecules, liquid crystals, surfactants, and proteins that are typically organic and can be melted and processed at moderate temperatures as compared with inorganic materials like metals and ceramics. Typically, soft materials have weak interactions among molecular or supramolecular components and are often either amorphous or can self-assemble from the liquid state. There are often many levels of complexity with heirarchical, supramolecular structures that can be cooperative and far from equilibrium. We are most often concerned with the structural arrangments, viscoelastic rheology, and/or mechanical behavior of these materials. Within these pages, you will find information pertinent to soft matter and nanomaterials, with a specific focus on computational methods and modeling.

Course Materials

[edit]

- Computational Nanoscience of Soft Matter, ChE/MSE 557 University of Michigan

Overview of Contents

[edit]

Interaction Potentials:

- The Lennard-Jones Potential
- Weeks-Chandler-Andersen Potential
- Hard Sphere Potential
- Dzugutov Potential
- Yukawa Potential
- Harmonic Spring
- FENE Spring

Simulation Methods:

- Brownian Dynamics Simulation (BD)
- Molecular Dynamics Simulation (MD)
- Dissipative Particle Dynamics Simulation (DPD)
- Monte Carlo Simulation (MC)
- Time-Dependent Ginzburg-Landau (TDGL)
- Car-Parinello Dynamics
- Basic Dynamical Simulation Methodology

Analysis Methods:

- Radial Distribution Function
- Mean Squared Displacement
- Velocity Autocorrelation Function
- Intermediate Scattering Function
- Structure Factor
- Nematic Order Parameter

System Classifications:

- Polymer
- Block Copolymer
- Liquid Crystal
- Surfactant
- Colloid
- Tethered Building Block ←
- Patchy Particle

Interaction Potentials:
The Lennard-Jones Potential
Weeks-Chandler-Andersen Potential
Hard Sphere Potential
Dzugutov Potential
Yukawa Potential
Harmonic Spring
FENE Spring
Simulation Methods:
Brownian Dynamics Simulation (BD)
…
System Classifications:
Polymer
Block Copolymer
Liquid Crystal
Surfactant
Colloid
Tethered Building Block ←

http://matdl.org/matdlwiki/index.php/Tethered_Building_Block

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- Permanent link

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Tethered Building Block

Tethered building blocks constitute a class of "shape-amphiphiles" where microphase separation occurs due to the immiscibility between the tether and building block, similar to Block copolymers and Surfactants. Building blocks can vary greatly, from metallic nanoparticles to molecular nanomaterials such as POSS or Porphyrin. Temperature, solvent quality, concentration, tether placement, number of tethers, building block geometry and composition, are only a few of the many parameters that can have a large impact on the resulting structures and phase behavior.

Cartoon of a tethered nanosphere

Contents [hide]

Experiment [edit]

Examples [edit]

- Tethered Spheres
  - *Bucky Balls*
    - Song T, Dai S, Tam KC, Lee SY, Goh SH, *Aggregation behavior of C-60-end-capped poly(ethylene oxide)s*, LANGMUIR 19 : 4798 2003
    - Lu XM, Hanrath T, Johnston KP, Korgel BA, *Growth of single crystal nanowires in supercritical silicon solution from tethered gold particles on a silicon substrate*, NANO LETTERS 3 : 93 2003

- C.R. Iacovella, A.S. Keys, M.A. Horsch, S.C. Glotzer *Icosahedral packing of polymer-tethered nanospheres and stabilization of the gyroid phase* Submitted, (2006)
  - **Record on MATDL Repository**

Simulation [edit]

Examples [edit]

- *Tethered Spheres*
  - Z-L Zhang, M.A. Horsch, M.H. Lamm, S.C. Glotzer. *Tethered nano building blocks: Towards a conceptual framework for nanoparticle self-assembly*, Nano Letters, 3 (10): 1341-1346, (2003)
  - C.R. Iacovella, M.A. Horsch, Z-L Zhang, S.C. Glotzer. *Phase diagrams of self-assembled mono-tethered nanospheres from molecular simulation and comparison to surfactants* Langmuir, 21 (21), 9488-9494, (2005)
  - C.R. Iacovella, A.S. Keys, M.A. Horsch, S.C. Glotzer *Icosahedral packing of polymer-tethered nanospheres and stabilization of the gyroid phase* Submitted, (2006)
    - Record on MATDL Repository

View Working Paper Details:

Parent Collections: Lab for Computational Nanoscience and Soft Matter Simulation (2006)

Title	Icosahedral packing of polymer-tethered nanospheres and stabilization of the Gyroid Phase
Author(s)	Iacovella, Christopher R. Keys, Aaron S. Horsch, Mark A. Glotzer, Sharon C.
Research Fields, Courses and Disciplines	
Description	We present results of molecular simulations that predict the phases formed by the selfassembly of model nanospheres functionalized with a single polymer "tether". Microphase separation of the immiscible tethers and nanospheres induces the formation of the double gyroid, perforated lamella and crystalline bilayer phases. Confinement effects promote the formation of icosahedral arrangements of nanoparticles that help to stabilize the gyroid and perforated lamella phases. We also present a new metric for determining the local arrangement of particles in liquid and solid configurations.
Keyword(s)	Brownian Dynamics stabilization FENE Lennard-Jones icosahedral nanospheres double gyroid perforated lamella crystalline bilayer
Publisher	
Date	Wednesday, May 17, 2006
Language	
Rights	
School, Department or Centre	Glotzer group. Depts of Chemical Engineering, Materials Science & Engineering, Macromolecular Science, and Physics

MatDL
MATERIALS DIGITAL LIBRARY PATHWAY

NSF NSDL

http://matdl.org/fez/view.php?pid=matdl:151

Attached Files

Name	Description	MIMEType
n2006TNSGyroid.pdf	n2006TNSGyroid.pdf	application/pdf

Related Links

Link	Description
http://testmatdl.lci.kent.edu/fez/view.php?pid=matdl:152	hexagonally packed cylinders
http://testmatdl.lci.kent.edu/fez/view.php?pid=matdl:153	double gyroid
http://testmatdl.lci.kent.edu/fez/view.php?pid=matdl:155	perforated lamellae
http://testmatdl.lci.kent.edu/fez/view.php?pid=matdl:154	lamellar bilayers

Icosahedral packing of polymer-tethered nanospheres and stabilization of the gyroid phase

Christopher R. Iacovella[1], Aaron S. Keys[1], Mark A. Horsch[1], and Sharon C. Glotzer[1,2,*]

[1]Department of Chemical Engineering and [2]Department of Materials Science & Engineering

University of Michigan, Ann Arbor, Michigan 48109-2136

May 17, 2006

*Corresponding author: sglotzer@umich.edu

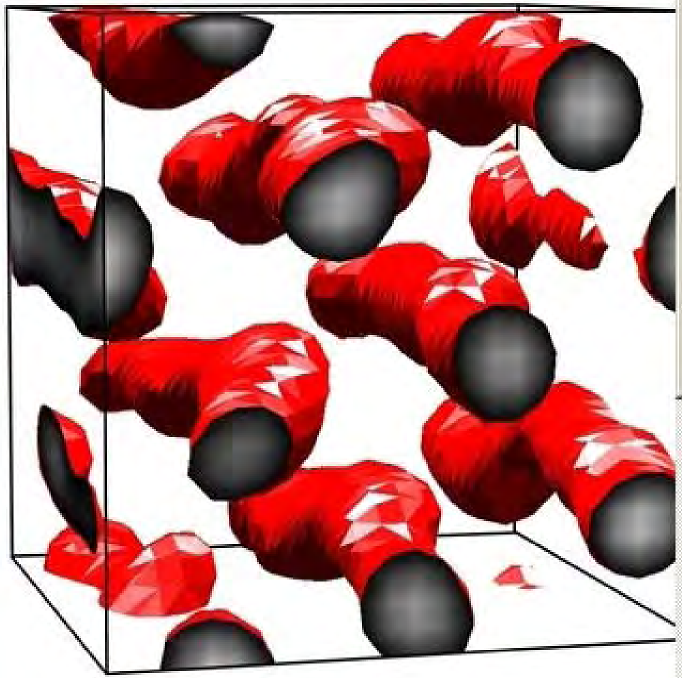
We present results of molecular simulations that predict the phases formed by the self-

View Image Details:

Parent Collections: Lab for Computational Nanoscience and Soft Matter Simulation (2006)

Title	Brownian Dynamics simulation of a nanoparticle-aggregating tethered nanosphere: cylindrical micelles
Creator(s)	Iacovella, Christopher R.
Research Fields, Courses and Disciplines	
Keyword(s)	Tethered Building Block Lennard-Jones Brownian Dynamics NVT FENE Hexagonally packed cylindrical micelles
Description	Number of tethered building blocks = 800; Number of beads = 7200; Length of tether = 8; Diameter of the nanopshere = 2.0; System temperature = 0.2667; System volume fraction = 0.25; Integration scheme to use = Brownian Dynamics, NVT; Number of Dimensions = 3; United Atom Bead Spring with Lennard-Jones and FENE; Phase: Hexagonally packed cylindrical micelles
Publisher	Glotzer group. Depts of Chemical Engineering, Materials Science & Engineering, Macromolecular Science, and Physics,University of Michigan
Contributor	
Date	Tuesday, September 19, 2006
Type	
Format	
Source	
Language	
Relation	

Datastream Preview



7200

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C	4.362575	-5.788690	-2.085299
C	4.652141	-5.706519	-1.085110
C	4.440438	-5.867967	-0.086317
C	5.198133	-6.431645	-0.492979
C	6.170948	-6.122723	-0.331024
C	6.655709	-5.205330	-0.302855
C	6.829866	-4.579781	0.475166
C	6.152726	-4.234416	1.120425
N	-5.335641	1.219896	7.561879
C	-4.141345	1.978315	8.134627
C	-4.846942	2.807071	8.027607
C	-5.361344	3.631443	8.373807
C	-4.795474	4.340785	7.942993
C	-5.007473	3.825229	7.012433
C	-4.319065	3.111145	6.854796
C	-3.856049	3.463092	5.960584
C	-2.992446	3.467759	5.286438
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C	10.771382	1.823140	-1.578372
C	11.682510	1.767767	-2.008284
C	12.357243	1.062552	-1.928116
C	11.997616	0.149579	-2.247943
C	11.004834	0.331229	-2.056996
C	10.048621	0.726084	-2.306973
C	10.721190	0.784067	-3.100297
C	11.303519	-0.037013	-3.279986
N	-9.066666	0.431908	6.194582
C	-9.600149	1.393647	5.137331
C	-9.259403	2.048909	4.476416
C	-9.766872	2.874754	4.386320
C	-10.551077	3.129595	4.938141
C	-11.135406	3.687420	5.581671
C	-12.086658	3.609101	5.850208
C	-11.773656	2.685904	5.575781
C	-12.099995	3.198843	4.734872
N	-6.918579	-7.457943	-6.929947
C	-5.957798	-8.203296	-7.767732
C	-5.054801	-8.127432	-8.181863
C	-5.423317	-9.000019	-8.454616
C	-5.942214	-9.857096	-8.757740
C	-5.154933	-9.746819	-9.446727
C	-5.430925	-9.160188	-10.280985

Course view

- Overview, lectures, assignments, books of interest
- Wiki assignments to be reviewed
- Reviewed assignments are submitted to the public view

Class:Che557

Contents [hide]

Overview [edit]

This class is designed to provide an understanding of the strategies, methods, capabilities, and limitations of computer simulation as it pertains to the modeling and simulation of soft materials at the nanoscale. The course consists of lectures and hands-on, interactive simulation labs using research codes based upon the Glotzilla Simulation Package. The class will hit upon various simulation techniques including Molecular Dynamics, Brownian Dynamics, Collision Dynamics, Dissipative Particle Dynamics, Monte Carlo, and Time-Dependent Ginzburg-Landau.

- **Course Syllabus**
- **Suggested journal and author list**
- Download Glotzilla

Lectures [edit]

1. Lecture 1a
2. Lecture 1b
3. Lecture 2a
4. Lecture 2b

Additional material [edit]

1. Introduction to Soft Materials
2. Force Field Methods

Assignments [edit]

1. Assignment 1
2. Assignment 2

Books of interest [edit]

- The Structure and Rheology of Complex Fluids
- Intermolecular and Surface Forces
- Computer Simulation of Liquids
- Understanding molecular simulation : from algorithms to applications
- Molecular Modelling: Principles and Applications

Surfactant Shear

Contents [hide]

Article

[edit]

G.Arya, A.Z. Panagiotopoulos

"Molecular modeling of shear-induced alignment of cylindrical micelles"

Computer Physics Communications, 169 (2005), 262–266

Summary

[edit]

The shear-induced self-assembly of surfactant into long-ranged cylindrical micelles is studied using nonequilibrium Monte Carlo (NEMC) and Molecular Dynamics (MD) simulations. The effects of shear flow are incorporated into the MC simulations via an additional potential term and modeled in the MD simulations by sliding the boundaries in opposite directions. By analyzing the differences between simulation results obtained from the two methods, the authors show that while the NEMC method is insufficiently reliable, the MD method gives more convincing results for the shear-driven phenomenon.

Nonequilibrium Monte Carlo simulations

[edit]

For equilibrium canonical Monte Carlo Simulation, a trial configuration is accepted with a probability

$$P_{acc} = min[1, exp(-\Delta U_0 / k_B T)]$$

where ΔU_0 is the difference in potential energy between the current state and the trial one. In the presence of shear flow, the acceptance criterion is modified by incorporating a shear-induced potential term into the Boltzmann factor. As proposed by Xu et al [7], this criterion is then given by

$$P_{acc} = min[1, exp(-(\Delta U_0 - \Gamma \sum_{i=1}^{N} \bar{y}_i \Delta x_i)/k_B T)]$$

where the shear rate is controlled by varying Γ; $\bar{y}_i$ is the average position of bead *i* on the velocity gradient axis and Δx_i is its displacement in the shear direction.

A coarse-grained model of liquid n-butane is chosen at T = 300K and ρ = 0.6 g/cm^3. Three modes of trial move are considered: isotropic translations, rotations about the center of mass and regrowth/cutting with the relative frequency of 0.82 : 0.179 : 0.001. The boundary conditions are chosen such that the walls parallel to the shear flow are impenetrable while the others are periodic. The simulation results show that i) for monolayer film, the cylindrical micelles perfectly align with the flow direction and ii) for thicker films, the cylinders tilt with respect to the direction of shear. The tilt angle decreases with the decreasing thickness of the film. Although the results seem to be qualitatively reasonable and the inclusion of shear-induced term into the acceptance equation is straightforward, several drawbacks remain. First, the shear-induced potential part is essentially nonconservative due to its dependence on the average y-coordinate of individual particles. Second, as pointed out by Evans et al [8], the canonical ensemble that this MC scheme samples actually represents a local equilibrium instead of the true nonequilibrium state. Third, the boundary condition effects cannot be reduced with or without Lees Edwards periodic boundary conditions (LEPBCs)[10]. While the former case results in abnormal bond length for molecules located near the center of the simulation box, the latter produces a non-linear velocity profile.

Molecular Dynamics simulations

[edit]

In the MD simulations, a H4T4 surfactant is modeled as a bead chain linked together by finitely extensible nonlinear elastic (FENE) springs. All beads interact with each other via a

Discussion

- Begin with soft matter simulation
  - Expand to: electronic materials, glasses, polymer thin films
- Brings repository into wiki presentation
- Metadata feeds terms into wiki and visa-versa
- Includes experimentalist perspective and data

Questions?

http://matdl.org
http://matdl.org/matdlwiki

The NSDL Materials Digital Library Pathway is supported by the National Science Foundation DUE-0532831. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of NSF.