NSF NSDL Materials Digital Library
AND MSE Education

2007 TMS Annual Meeting
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Materials Informatics Lab
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Outline

- Cyberinfrastructure for Cyberdiscovery
- NSF NSDL MatDL Pathway: Background
- Collaborative tools for MS community
NSF Report: Cyberinfrastructure to Cyberdiscovery for Materials Science

- 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

Support for Transformational Research & Education
NSF, Cyberinfrastructure & Digital Libraries

National Science Digital Library 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

NSDL Launch Fall 2002
What is NSDL?

- An NSF-funded $20 million/year program in Science, Technology, Engineering and Mathematics (STEM)
- A digital library describing nearly two million carefully selected online STEM resources (at http://nsdl.org)
- A core integration team (Columbia, Cornell, UCAR) working with 10 pathways and services projects
- A community of users: experts and novices
NSF NSDL Materials Digital Library Pathway

- Domain - Materials Science
  - Work with MS community for collaborative information exchange

- Audience – MS education & research community
  - Undergraduate and above

- Goals
  - Implement an opensource information infrastructure
  - Disseminate information generated by government-funded efforts in materials
  - Provide content and services to support the integration of research and education in materials
**Parent Collections:** Lab for Computational Nanoscience and Soft Matter Simulation (2006)

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**Date:** Tuesday, September 19, 2006
Two examples of Collaborative MS Tools

- **Soft Matter Wiki**
  - Authoritative information of expert soft matter community

- **MatForge**
  - Computational methods enabling new/improved predictions of materials behavior
Soft Matter

- What is it?
  - Organic materials -- polymers, biomolecules, liquid crystals, surfactants, and proteins
  - Multidisciplinary & evolving

- Why is it important?
  - Next generation molecular electronic, photonic, drug delivery, and sensing materials and instruments
What is Soft Matter Wiki?

- Website for use by the Soft Matter Community
  - MediaWiki Installation
  - Expert community authored
  - Low-barrier

- Multiple purposes
  - Access: Authoritative scientific information
  - Reference: graduate education
  - Introduction: undergraduate research experience
Soft Matter Wiki-Overview of Contents

Contents [show]

Soft Matter Wiki

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 hierarchical, supramolecular structures that can be cooperative and far from equilibrium. We are most often concerned with the structural arrangements, viscoelasticity, 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


Overview of Contents

Interactions:

Non-bonded Interactions:
- The Lennard-Jones Potential
- Weeks-Chandler-Andersen Potential
- Hard Sphere Potential
- Dzugutov Potential
- Yukawa Potential
- van der Waals Interaction
- Electrostatic Interaction

Bonded Interactions:
- Harmonic Spring
- FENE Spring
- Bond Stretching
- Angle Bending
- Bond Rotation

Simulation:

Simulation Methods:
- Basic Dynamical Simulation Methodology
- Molecular Dynamics Simulation (MD)
- Brownian Dynamics Simulation (BD)
- Dissipative Particle Dynamics Simulation (DPD)
- Monte Carlo Simulation (MC)
- Time-Dependent Ginzburg-Landau (TDGL)
- Car-Parrinello Dynamics
Tethered Building Block

Tethered building blocks constitute a class of "shape amphiphiles" where microphase separation occurs due to the immobility 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 Perphyrins. 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.

Examples

- Tethered Spheres
  - Bucky Balls
    - Song T, Dai S, Tam KC, Lee SY, Goh SH, Aggregation behavior of C-60-ent-capped polyethylene oxide, LANGMUIR 19 : 4798 2003
    - Song T, Dai S, Tam KC, Lee SY, Goh SH, Aggregation behavior of two-arm fullerene-containing polyethylene oxide, POLYMER 44 : 2526 2003


Record on MATDL Repository

Examples

- Tethered Spheres

Record on MATDL Repository
Brownian Dynamics Simulation (BD)

Brownian dynamics (BD) is a mesoscale simulation method commonly used to study solute-solvent systems without explicitly considering the solvent particles. When using BD it is assumed that solvent particles are small as compared to solute particles. To avoid explicitly calculating solvent interactions, the solvent particles are treated as a viscous medium. To account for the Brownian motion and dissipative losses that occur as a result of collisions with large numbers of solvent particles a stochastic force and a drag force are implemented into the simulation. The result is that larger systems and longer time scales are accessible to BD over traditional methods such as Molecular Dynamics Simulation.

Method

Similar to Dissipative Particle Dynamics, BD obeys Newton’s equations of motion. The trajectory of each Brownian particle is governed by the Langevin equation[1, 2]:

\[ m_i \ddot{r}_i(t) = F_i^C(\dot{r}_i(t)) + F_i^R(t) - \gamma v_i(t) \]

where \( m \) is the mass of bead \( i \), \( \dot{r}_i, v_i \), and \( F_i \) are the position, velocity, and force acting on bead \( i \), respectively. \( \gamma \) represents the friction coefficient acting on the beads. The force acting on a particle can again be broken into three components, a conservative, random, and dissipative force respectively. It is assumed that there are no temporal or spatial correlations in the drag force and the random force is assumed to be stationary, Markovian, and Gaussian with zero mean. The variance of the random force obeys the fluctuation dissipation theorem and must satisfy the following conditions[3]:

\[ \langle F_i^R(t) \rangle = 0 \]

\[ \langle F_i^R(t) F_j^R(t') \rangle = 6\gamma k_B T \delta_{ij} \delta(t-t') \]
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Soft Matter Wiki: Next Steps

- New participants
  - MRSECs
  - REUs (undergraduate education)
- 2-way resource integration between Soft Matter Wiki and MatDL Repository
What is MatForge? SourceForge for MS

- Workspace for collaborative code development
- Subversion software repository with Trac web interface
  - Manage changes to program source code
  - Enable teams to work on the same files in a distributed environment
  - Keep track of who has done what and when
Projects hosted on MatForge

- NIST/MSEL FiPy: an extensible object oriented, partial differential equation (PDE) solver
- University of Michigan Computational Nanoscience & Soft Matter Simulation Lab
- Carnegie Mellon Computational Materials Science
- Powell Research Group: Veryst Engineering
- 74495 Computational Materials Science: Chemical Physics Program & Liquid Crystal Institute, KSU
- Computational Materials Science Network: DOE, Consortium of government labs & universities
NIST & Collaborative Code Development

- **Focus:**
  - Computational modeling of materials

- **Issues:**
  - Extensive security inhibits external collaborations
  - Branded, trusted, & neutral site for open source MS code

- **New approaches:**
  - train student to use its tools
  - promote development of its tools
  - develop a pool of next generation users in academe, industry

Using FiPy to model superconformal electrodeposition (superfill) in semiconductors.
Virtual Labs

• Services and content for virtual labs in large undergraduate introductory science courses
• Complement traditional labs
• Beginning with MIT Intro to Solid State Chemistry
Transport Phenomena Archive: Collaborative Development of Teaching Resources

- Online space for collaborative development of educational materials
- Need for high-quality, relevant teaching resources using recent research.
- Problems, Resources, Readings, Pedagogy and Courseware

Encapsulated liposomes for long-term drug delivery
Summary

- Web 2.0 & beyond
  - Exchange & Collaboration
- Materials Science: Heterogeneous data
  - Soft Matter Wiki & MatForge
- Materials Science community
  - New opportunities for working together
Thank you & questions?

lbartolo@kent.edu

MatDL http://matdl.org
Soft Matter Wiki http://matdl.org/matdlwiki
MatForge http://matforge.org

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