Facilitating Wiki/Repository Communication with Metadata

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Outline

- Background Information
  - NSDL & MatDL Pathway
- Rational
  - User Centric
  - Service Centric
- Technical Details
- Concluding Remarks
National Science, Technology, Engineering & Mathematics Education Digital Library

The National Science Foundation’s online library of resources for education and research...

...established to catalyze and support continual improvements in STEM education at all levels (K-12, Higher Education, and Lifelong Learning).
Materials Digital Library Pathway

- **Domain - Materials Science**
  - Study of materials structure & processing-property relations to improve products
- **Audience – MS research & education community**
  - Undergraduate and above
- **Goals**
  - Implement an information infrastructure as part of NSDL
  - Disseminate information generated by government-funded efforts in materials
  - Provide content and services to support the integration of research and education in materials
NSDL Materials Digital Library Pathway

- NSF MS Initiatives (NIRTs, MRSECs, IMIs)
  - Soft Matter Wiki
- Teaching Resource Development
  - MS Teaching Archive
- Stewardship
  - MatDL Repository
- Code Development
  - Matforge
    - NIST FiPy
    - CMU
    - DOE CMSN
- Virtual Labs
  - Intro to Solid State Chem
  - Intro to Bio Physics
  - Modern Chemistry

http://matdl.org/matdlwiki
http://matdl.org/virtuallabs
http://teaching.matdl.org
http://matdl.org
http://matforge.org
Wiki/Repository Communication

Enable 2-way resource integration between Services: Soft Matter Wiki and MatDL Repository

- Developed Wiki2Fedora
- Developing Search Results plug-in
MatDL Repository

- Repository for stewardship of significant content
  - Fedora/Fez Installation
  - Private/public collection space
  - Externally funded resources

- Multiple purposes
  - Disseminate research & education resources
  - Support reuse & repurposing of gov’t funded resources

Collection: Combinatorial Sciences & Materials Informatics
Soft Matter Wiki

- Website for use by the Soft Matter Community
  - MediaWiki Installation
  - Low-barrier collaborative authoring
  - Expert community-driven

- Multiple purposes
  - Reference resource: research lab assistants
  - Education resource: undergrad/graduate students
Soft Matter Wiki-Overview of Contents

Contents [show]

Soft Matter Wiki

Soft matter 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 submolecular 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, 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

- Computational Neuroscience of Soft Matter, ChE/MSE 657, University of Michigan (Authentication Required)

Overview of Contents

Interactions:

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

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

Simulation:

Simulation Methods:
- Basic Dynamical Simulation Methodology
- Molecular Dynamics Simulation (MD)
- Reaxion Dynamics Simulation (RD)
The Lennard-Jones Potential

The Lennard-Jones potential (LJ) is used to model the excluded volume interactions and van der Waals attraction of neutral atoms. The commonly used 6-12 form of the potential is as follows:

$$U_{LJ}(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

Where $\varepsilon$ is the well depth, $\sigma$ is the characteristic diameter (typically the diameter of the smallest particle), and $r$ is the radial separation of the two atoms.

van der Waals Attraction

In theory, the van der Waals interaction for atoms with similar ionization frequencies and where the dispersion (London) interactions are dominant is proportional to $-\left( \frac{\alpha_1 \alpha_2}{r^6} \right)$ where $\alpha_1$ and $\alpha_2$ are the polarizabilities of atom 1 and atom 2 respectively. Again, this assumes that dispersion (London) forces are dominant and that there are no permanent dipoles (Keesom forces) or induced dipoles (Debye forces). In the LJ construction, the term $\left( \frac{1}{r} \right)^6$ is used to describe this attractive van der Waals interaction.

Excluded Volume Interaction

As the separation distance between atoms decreases, the electron clouds will eventually overlap, resulting in a very strong repulsion that rapidly increases as interatomic spacing is further decreased. In the LJ construction, the term $\left( \frac{1}{r} \right)^{12}$ describes this repulsive interaction. The 12th power is used for two main reasons: it is very steep, rapidly becoming dominant as $r$ is small and it is also a multiple of the 6th power allowing for efficient computation.
Tethered Building Block

Tethered building blocks constitute a class of "shape amphiphiles" where micelles 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 nano materials 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.

Experiment

Examples

- Tethered Spheres
  - Bucky Bells
    - Song T, Dai S, Tam KC, Lee SY, Geon SH, Aggregation behavior of C60-end capped polyethylene oxide, LANGMUIR 19: 4706 2003
    - Song T, Dai S, Tam KC, Lee SY, Geon SH, Aggregation behavior of two-arm telechelic-containing polyethylene oxide, POLYMER 44: 2029 2003
  - Quantum Dots
    - Wudloff SF, Kislov NA, Quantum dot on a rope, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 124: 2446 2002
  - Gold nanospheres
    - Park KJ, Pelletier TM, Michael CM, Gerber D, Williams GC, Alberts AF, Conformation of oligopeptides attached to gold nanocrystals probed by gel electrophoresis, NANO LETTERS 3: 33 2003
    - Li Z, Jin RC, Mikin CA, Letting RJ, Multiple thiols anchor capped DNA-gold nanoparticles conjugates, NUCLEIC ACIDS RESEARCH 30: 1662 2002
    - Lu XM, Hanath 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: 29 2003

Simulation

Examples

- Tethered Solutes

[edit]
Rationale: User Centric

User:

- Contributes to service providing most benefit
  - Supports user’s research & teaching
- Incorporates service fitting easily into workflow
  - Easy to do and part of user’s normal work
- Doesn’t duplicate efforts
  - Maximizes user’s time & contributions
Rationale: Service Centric

Services:

- Accommodate user as much as possible
  - Encourages growth
- Support complex digital objects
  - Useful for research & teaching
- Describe individual objects
  - more granular, more routes of discovery
- Establish connections between services
  - Maximizes gains for user & services
Wiki → Repository: Wiki2Fedora

- Wiki (MediaWiki)
- Repository (Fedora/Fez)
- Wiki2Fedora application
  - Runs at scheduled intervals
  - Identifies new/changed Wiki file uploads
  - Extracts available metadata from Wiki
  - Converts to DC metadata
  - Ingests datastream into Fedora
Wiki → Repository: Wiki2Fedora

- Post-processing
  - FEZ Administration function
    - Index new objects into Fez
    - Send items to review area for manual editing
/augmenting
Wiki → Repository: Wiki2Fedora

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Repository Image & Metadata Display

View Image: POSS

Workflows:

Citation: Chris Iacovella (2006). POSS: Gotted group, Depts of Chemical Engineering, Materials Science & Engineering, Macromolecular Science, and Physics, University of Michigan.

Collection: Lab for Computational Nanoscience and Soft Matter Simulation (2006 - Present)

Attached Files

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NOTE: This record is not published.

Title: POSS
Creator(s): Chris Iacovella
Abstract/Summary: Schematic of a POSS cage
Publisher: Gotted group, Depts of Chemical Engineering, Materials Science & Engineering, Macromolecular Science, and Physics, University of Michigan
Date: 2006-06-23
Source: Soft Matter Wiki
Rights: http://creativecommons.org/licenses/by-nc-sa/3.0/

Related Links

Description: referrign wiki page
Repository → Wiki: Search Results Plugin

- Displays Repository search results in Wiki
- MediaWiki markup extended
- Parameters `<fez>`
  - Query terms
  - Display
- Uses existing Fez search function
Repository → Wiki: Search Results Plugin

Brownian Dynamics Simulation (BD)

Brownian dynamics (BD) is a mesoscopic simulation method commonly used to study non-equilibrium systems without explicitly considering the solvent molecules. When using BD, it is assumed that solvent particles are small as compared to solute particles. To avoid explicitly calculating solvent fluctuations, the solute particles are treated as a binary medium. To accomplish this, Brownian motion and collisions, which are a result of collisions with the solvent particles, are treated as a fluctuating noise and are implemented into the simulation. The result is that large systems and long-time scales are accessible by BD, over traditional methods such as Molecular Dynamics Simulations.

**Concrete (p/st)**
1. Method
2. Resolving the equations of motion
3. Examples
4. References

**Method**

Solving the Continuous Particle Dynamics, BD solves Newton's equations of motion. This trajectory of each Brownian particle is governed by the Langevin equation (1, 2):

\[ m_i \ddot{x}_i(t) = F_i^L(t) + F_i(t) - \gamma_i v_i(t) \]

where \( m_i \) is the mass of the Brownian particle, \( \gamma_i \) and \( \dot{x}_i \) are the friction coefficient and velocity respectively, \( v_i(t) \) represents the random component of motion on the Brownian particle. The force acting on the Brownian particle can be broken into three components: a conservative, uniform, and dissipative force respectively. It is assumed that there are no permanent or initial conditions in the dissipation 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 is given by the following:

\[ \langle F_i^R(t) F_j^R(t') \rangle = 6 \pi \eta_i \beta k_B T_d \delta(t - t') \]

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

\[ \langle F_i(t) F_j(t') \rangle = 6 \pi \eta_i \beta k_B T_d \delta(t - t') \]

**MatDL Repository Matches for Brownian**

- Brownian Dynamics simulation of a nanoparticle-aggregating tethered nanosphere: cylindrical micelles
- Brownian Dynamics simulation of a nanoparticle-aggregating tethered nanosphere: double gyroid
- Brownian Dynamics simulation of a nanoparticle-aggregating tethered nanosphere: lamellar bilayers
- Brownian Dynamics simulation of a nanoparticle-aggregating tethered nanosphere: lamellar bilayers
Concluding Remarks

- Provide services to support collaboration & to hold authoritative scientific content
- Better integrate services
  - Avoid duplication of effort
  - Increase discovery
  - Capitalize on strengths of individual services
- Extend wiki/repository communication to other wiki software
Thank you & Questions?

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MatDL Repository     http://matdl.org
Soft Matter Wiki     http://matdl.org/matdlwiki

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