BIOVIA MATERIALS STUDIO MESOCITE

DATASHEET

BIOVIA Materials Studio Mesocite is a state-of-the-art coarse-grained simulation module for the study of materials at length scales ranging from nanometers to micrometers and time scale from nanoseconds to microseconds. Such materials pervade industrial research in areas such as composites, coatings, cosmetics and controlled release. BIOVIA Materials Studio Mesocite can provide structural and dynamic properties of fluids in equilibrium, under shear or in confined geometries.

WHAT DOES BIOVIA MATERIALS STUDIO MESOCITE DO?

BIOVIA Materials Studio Mesocite is a method for studying soft materials using either coarse-grained molecular dynamics (CGMD) or dissipative-particle dynamics[1] (BIOVIA Materials Studio DPD). The basic idea of BIOVIA Materials Studio Mesocite is that it should be possible to replace groups of atoms with beads which interact in such a way as to reproduce Newtonian mechanics of the system. The contributions of the atomistic detail of the system, such as bond vibrations, are integrated out, giving much larger time- and length-scales. Capturing the atomistic information in the interaction between the beads means the underlying chemistry of the system is not lost in the coarse-graining. Extending the length and time scales gives the ability to study challenges such as micelle and vesicle formation or phase formation in block copolymers.

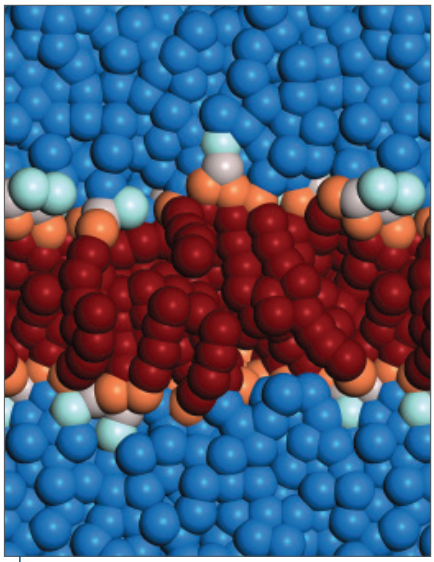

Figure 1: A phospholipid bilayer in a polar solvent such as water simulated using the CGMD method. CGMD is ideally suited to studying such systems as charges can be applied to model the choline and phosphate groups in the hydrophilic head group.

The elementary particle in BIOVIA Materials Studio Mesocite is a bead which represents multiple atoms, or even multiple molecules of a material. The beads can interact with each other using either CGMD or BIOVIA Materials Studio DPD. CGMD uses Newtonian mechanics to represent the interactions in the system and contains valence and non-bonded terms. CGMD allows the simulation of charged systems and retains much more control of the structure compared with BIOVIA Materials Studio DPD models. However, this also means that more parameters need to be generated to describe the system. In BIOVIA Materials Studio Mesocite, BIOVIA Materials Studio DPD is used to reproduce the hydrodynamics of the fluid as a whole. The BIOVIA Materials Studio DPD approach uses the Flory-Huggins interaction parameter to define how the beads interact with each other and a soft potential is used to mimic a fluid. This parameter can be measured experimentally or obtained from modeling with atomistic detail.

KEY USES OF BIOVIA MATERIALS STUDIO MESOCITE

Polymers

The extended time and length scales accessible to BIOVIA Materials Studio Mesocite allow simulation of polymer mesophases. This enables researchers to study the affect of additives, solvents, and monomer ratios, on mesophase formation for homopolymer, block copolymers, random copolymers, and dendrimers. Soft BIOVIA Materials Studio DPD potentials make the equilibration of large polymer systems far faster than using classical techniques. The more detailed CGMD approach enables time dependent properties such as viscosities to be determined more accurately.

Structured materials

Materials which have structure at the mesophase can be studied to evaluate their dynamic properties. For example, the ratio of tail to head or the effect of solvent on lipid bilayer formation can be investigated. The influence of charges makes the CGMD method particularly suited to these calculations.

Nanotechnology

Mesoscale methods offer insight into challenges in nanotechnology where the alignment of carbon nanotubes in a polymer matrix influences electronic properties. Simulating the motion of such nanotubes requires timescales that are not accessible using fully atomistic representations, making mesoscale methods ideal for such property prediction.

THE BIOVIA MATERIALS STUDIO ADVANTAGE

BIOVIA Materials Studio Mesocite is operated from within the BIOVIA Materials Studio® environment. BIOVIA Materials Studio provides an integrated userinterface that is easy to use and quick to learn. BIOVIA Materials Studio Visualizer, the core BIOVIA Materials Studio product, offers a wide range of model building and visualization tools that allow you to rapidly construct models of the system of interest, calculate the necessary molecular level information that is required for the parameterization of mesoscale simulation, select the CGMD or BIOVIA Materials Studio DPD functionality, and run a dynamic simulation of a complex fluid.

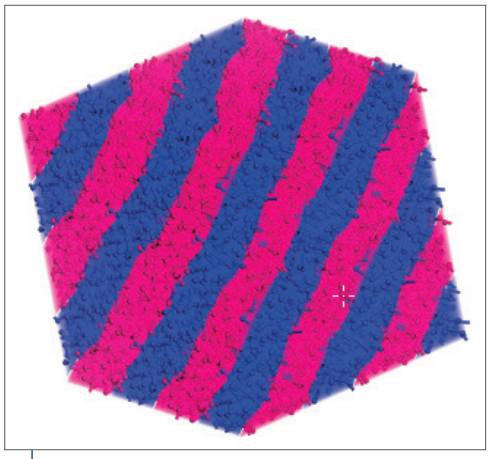

Figure 2: A diblock copolymer with blocks of equal lengths forms a lamellar mesophase from a BIOVIA Materials Studio DPD calculation. The soft potential model of BIOVIA Materials Studio DPD enables fast simulation of the mesophases of large polymer systems.

The bead datamodel and hard-body potential functionality is also exposed through the MaterialsScript API, giving the power to automate workflows and further customize calculations.

A flexible client-server architecture means that calculations can be run on servers located elsewhere on your network. Results are returned to your PC, where they may be displayed and analyzed. You can easily produce high quality graphics of molecular and mesoscopic material structures. These structures, graphs, and other data such as video clips, produced from BIOVIA Materials Studio Mesocite output, can be instantly exchanged with other PC applications.

HOW DOES BIOVIA MATERIALS STUDIO MESOCITE WORK?

BIOVIA Materials Studio Mesocite offers two complementary approaches for coarse grained simulations: CGMD and BIOVIA Materials Studio DPD.

The CGMD approach uses a classical molecular mechanics algorithm with hard particles that cannot penetrate each other. The interactions between each bead are defined by a forcefield which contains parameters for all the different combination of interactions. The interactions are defined by different functional forms which describe valence interactions, such as bond stretches and angle terms, and non-bonded interactions such as van der Waals and electrostatic interactions. The forcefield can contain as many, or few, of the different functional forms as is required to accurately describe the system of interest. As the complexity of the forcefield increases, the number of parameters required also increases. Generating good parameters for the forcefield is key in using the CGMD model of BIOVIA Materials Studio Mesocite to simulate a material. A version of the MARTINI[2] forcefield, developed by Marrink et al[3] for biomolecular systems, is provided. MARTINI has four main forcefield types; apolar, nonpolar, polar, and charged. Each of these types has several subtypes allowing MARTINI to be applied to many different organic molecules.

The BIOVIA Materials Studio DPD approach is based on the concept of fluid droplets that can penetrate each other. In the method this is reflected by soft potentials as well as a thermostat which is related to Brownian motion. BIOVIA Materials Studio DPD simulates fluid phases which are homogeneous in density, but show compositional fluctuations. The composition dependence stems from pair-wise repulsions between the constituent beads. The repulsive force depends upon the nature of the colliding beads. Unlike beads frequently have a stronger repulsion for one another than like beads. This small difference in the bead-bead forces can lead to remarkably complex systems with exotic morphologies. The system reaches equilibrium very rapidly due to the inclusion of thermal noise. Polymeric species are viewed as chains of beads, with harmonic springs connecting successive beads. Chains may contain more than one bead type, e.g. a block copolymer, and chain architecture may comprise branches and complex connectivities. All forces are short-ranged and so the algorithm is rapid allowing calculations on realistic system sizes.

FEATURES AND CAPABILITIES

Specifying input structures

- Build molecule topologies using the Mesoscale Molecule building tools
- Build molecule topologies by coarse graining from an atomistic representation
- Use the Mesotructure templating tools to create initial structures such as micelles, slab, rods, etc
- Use random starting conditions
- Fix the Cartesian positions of beads
- Define charges on beads
- Define rigid walls with different interactions

Calculation Tasks

- Single point energies
- Geometry optimization
- Dynamics
- Dissipative particle dynamics
- Restart all tasks, including optional append to trajectory
- All tasks in BIOVIA Materials Studio Mesocite support MPI parallel execution
- All tasks in BIOVIA Materials Studio Mesocite are exposed through MaterialsScript for automation
- Shearing (Legacy BIOVIA Materials Studio DPD only)

Thermostats and Barostats

- Nose
- Velocity Scale
- Andersen
- Berendsen
- BIOVIA Materials Studio DPD thermostat (accessible through the BIOVIA Materials Studio DPD task)

Ensembles

- NVE
- NVT
- NPT

Forcefields

- MS-MARTINI
- Shinoda2007

Analysis

- Animate trajectories
- Visualize density fields (Legacy BIOVIA Materials Studio DPD only)
- Concentration profiles
- Density profiles
- Dipole autocorrelation function and power spectrum
- Distance, angle, and torsion distributions
- Mean squared displacement of beads
- Pressure profiles
- Radial distribution function and structure factor
- Radius of gyration
- Rotational time correlation
- Space-time correlation function
- Spatial orientation correlation function
- Stress autocorrelation function and shear viscosity
- Stress tensor (available through MaterialsScript)
- Velocity autocorrelation function
- View trajectory data in a study table

To learn more about BIOVIA Materials Studio, go to **accelrys.com/materials-studio**

REFERENCES:

1. Hoogerbrugge, P. J.; Koelman, J. M. V. A. 'Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics', Europhys. Lett., 1992, 19, 155-160. Groot R.D.;Warren, P. B.'Dissipative particle dynamics: bridging the gap between atomistic and mesoscopic simulation', J. Chem. Phys., 1997, 107, 4423-4435.

2. http://md.chem.rug.nl/~marrink/coarsegrain.html

3. S.J. Marrink, H.J. Risselada, S. Yefimov, D.P. Tieleman, A.H. de Vries. "The MARTINI forcefield: coarse grained model for biomolecular simulations." J. Phys. Chem. B, 111:7812-7824, 2007.

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