

Reliable prediction of solubilities, morphologies, and release rates

Rapid access to a range of material properties for structured fluids such as micelles, vesicles, lyotropic liquid crystals, and lamellae

Ideal for research problems in solution, formulation, blend compatibilization, membrane crossing, and processing

## DPD

DPD (Dissipative Particle Dynamics) is a state-of-the-art mesoscale simulation method for the study of complex fluids. Such fluids pervade industrial research from paints to pharmaceuticals and from cosmetics to the controlled release of drugs. DPD can provide structural and dynamic properties of fluids in equilibrium, under shear or confined to narrow cavities, at length- and time-scales beyond the scope of traditional atomistic molecular dynamics simulation methods.

### What does DPD do?

DPD is a robust, coarse-grained, dynamics algorithm for simulating soft matter. The basic idea of DPD is that it should be possible to replace 'blobs' or 'droplets' of fluid with individual particles which interact in such a way as to reproduce Newtonian hydrodynamics of the fluid as a whole. Thus, the contribution of the microscopic details of the system, i.e. the main concern of atomistic simulation methods, is integrated out, allowing access to much larger time- and length-scales. The underlying chemistry of the system is not lost in the coarse-graining. The resulting 'beads' interact with one another via a pair-potential related to the Flory-Huggins interaction parameter. This parameter can be measured experimentally or obtained from modeling with atomistic detail. The particles are subject to pairwise forces which comprise: soft repulsions, stochastic noise, and a dissipation (conceptually similar to a viscous drag). Navier-Stokes behavior is obtained with a suitable choice of functional form of these potentials and so the method captures hydrodynamics.

### The Materials Studio Advantage

DPD is operated from within the Materials Studio® environment. Materials Studio provides an integrated user-interface that is easy to use and quick to learn. Materials Visualizer, the core 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 DPD module with two mouse clicks, and run a dynamic simulation of a complex fluid.

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 DPD output, can be instantly exchanged with other PC applications.

### How does DPD work?

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 in the system. 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. This allows the user to use large systems, 100,000 beads is typical, representing millions of atoms.

## Features and capabilities

### Calculation tasks

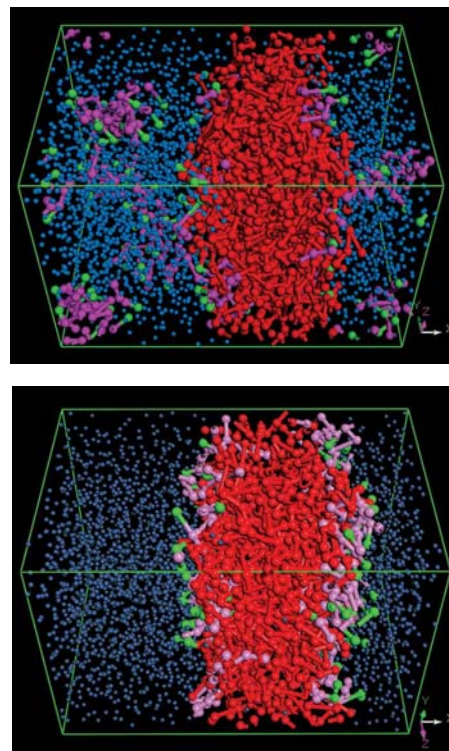
- Define up to 10 bead types (chemical species)
- Define up to 10 mesoscale molecules (connected beads)
- Define interaction energies for each pair of species in the system, these energies are related to the Flory-Huggins interaction parameter and lead to the phase separation of various components
- Define temperature, cell composition, cell size, run length, and output frequencies
- Include walls, where preferential adsorption of certain species may be included
- Shear the system using Lees-Edwards (Sliding Brick) boundary conditions
- Restart a simulation from a previous run, resetting the averages if desired and altering the interactions between beads to create quite complex scenarios, e.g. to model the effect of a change in the drug environment
- Fix the positions of beads
- Create rigid bonds to define particles, such as nanotubes
- Use the mesostructure template builder to specify the initial starting positions of the beads

### Properties

- Phase morphology
- End-to-end distance distribution of any chain molecules
- Bond length distribution of chain molecules
- Stress tensor
- Surface tension
- Critical micellar concentration
- Aggregation and coagulation
- Effect of confinement on miscibility
- Effect of shear on morphology
- Concentration profiles
- Diffusion rates of various species.

### References:

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



The images show a system of oil, water, and detergent. The blue spheres are DPD water molecules, the red chains denote a high molecular weight alkane, and the pink and green are the head and tail of a surfactant. The top image is an initial configuration where an oil droplet has been added to a water/surfactant system. Initially the alkanes remain strongly segregated from the water (with a high interfacial tension) and the surfactant molecules are loosely clustered into micelles in the aqueous phase. The polar head-groups of the detergent (green) point out into the water, with the lipophilic tails (pink) in the interior of the micelles.

The lower image shows the same system at a later time. The surfactant has migrated to the oil-water interface. The system seeks its lowest free energy by reducing the interfacial tension. The hydrophobic tails of the surfactant point into the oil phase and the hydrophilic groups remain preferentially in the aqueous phase. Both the kinetic and thermodynamic properties of such processes are measurable using DPD simulation.