

A dynamic mesoscale simulation method

Aimed at elucidating industrially important mesoscale structures and kinetics

For complex fluid systems, including polymer melts and blends

MesoDyn

MesoDyn is a dynamic simulation method for studying the long length and time behavior of complex fluid systems, including polymer melts and blends. It has gained wide respect in literature and commercial circles with scientifically astute algorithms aimed at elucidating industrially important mesoscale structure and kinetics. Such structures are found to critically affect the bulk properties of a material and are often frozen in by processing, where timescales may be of the same order as relaxations. The dynamics of the system is described by a set of so-called functional Langevin equations. In simple terms, these are diffusion equations in the component densities which take account of the noise in the system. By means of numerical inversions, the evolution of the component densities is simulated, starting from an initially homogeneous mixture in a cube of typical size 100-1000 nm and with periodic boundary conditions.

What does MesoDyn do?

MesoDyn takes a coarse-grained description of a complex fluid and performs time-evolution dynamics of the density and potential fields of the system. The free energy seeks a minimum which may be achieved by demixing if intermolecular forces are sufficiently disfavored. The coarse-graining of the system involves replacing polymer chains by a Gaussian representation with the same response functions and including non-ideality of the system via effective external potentials, the magnitude of which is determined by the Flory-Huggins interaction parameters of the various binary pairs in the system. Electrostatics may be included via the Flory-Huggins parameter, or may be explicitly included for each bead in the system.

The Materials Studio Advantage

MesoDyn 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 MesoDyn module with two mouse clicks, and run a dynamic simulation of a complex fluid.

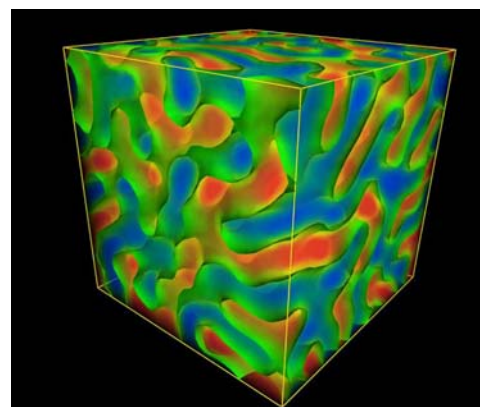


Image from a MesoDyn simulation of the phase separation of diblock copolymer. The surface links point at the dividing surface between the two phases. The entire volume is color-coded by the density of one of the blocks (red at higher density, blue at low density). This image is a state prior to equilibrium, and the system ultimately evolves to a lamellar phase.

A flexible client-server architecture means that calculations can be run on servers located elsewhere on your network. Additionally, MesoDyn uses MPI to run in parallel and is also supported for submission to a server through queuing systems. 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. Structures, graphs, and other data (such as video clips), produced from MesoDyn output can be instantly exchanged with other PC applications.

How does MesoDyn work?

MesoDyn simulates fluid phases that are homogeneous in density, but show compositional fluctuations. The structure and potential energy of the system evolve over time due to chemical potential gradients and Langevin noise. The noise term is important in escaping local minima on the free energy surface of the system. The equilibration of the system can be followed by monitoring the free energy evolution. Order parameters are also calculated to quantify the degree of phase separation.

The inclusion of pseudo-dynamic algorithms makes the simulation much faster, and the direct incorporation of electrostatics greatly increases the number of systems that can be studied with MesoDyn. The ability to create arbitrary confinement scenarios (such as arrays of spheres, planar walls, and wedges) makes studies of confined systems particularly interesting in Materials Studio. For the first time, the user has the ability to visualize the constraint in the absence of the density fields.

Features and capabilities

Calculation tasks

- Define up to 10 chemical species
- Define up to 10 mesoscale molecules (represented by single beads or chains of beads with arbitrary connectivity)
- Define interaction energies for each pair of species in the system, these energies are proportional to the Flory-Huggins interaction parameter χ and lead to the phase separation of various components

References:

1. J. G. E. M. Fraaije, B. A. C. van Vlimmeren, N. M. Maurits, M. Postma, O. A. Evers, C. Hoffman, P. Altevogt, and G. Goldbeck-Wood, "The dynamic mean-field density functional method and its application to the mesoscopic dynamics of quenched block copolymer melts," *Journal of Chemical Physics*, **1997**, *106*, 4260.
2. N. M. Maurits, A. V. Zvelindovsky, G. J. A. Sevink, B. A. C. van Vlimmeren and J. G. E. M. Fraaije, "Hydrodynamic effects in 3d microphase separation of block copolymers: dynamic mean-field density functional approach," *Journal of Chemical Physics*, **1998**, *108*, 500.
3. A. V. Zvelindovsky, G. J. A. Sevink, B. A. C. van Vlimmeren, N. M. Maurits and J. G. E. M. Fraaije, "3D mesoscale dynamics of block copolymers under shear: the dynamic density functional approach," *Phys. Rev. E.*, **1998**, *57*, 4699.

- Define temperature, cell composition, cell size, run length, and output frequencies
- Include walls or other constraints (where preferential adsorption of certain species may be included)
- Define a specific constraint (such as ordered array of spheres and wedge-shaped cell)
- Shear the system
- Perform the free energy integration in potential space only, speeding up the calculation considerably
- Explicitly include charges in the system using a Debye-Huckel approximation for simulation of aqueous systems
- Alter the composition at restart, allowing the study of effects such as titration, solvent evaporation, and shifts in chemical equilibrium
- 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 pH or controlled release of drug)

Properties

- Phase morphology
- Aggregation and coagulation
- Effect of confinement on miscibility
- Effect of shear on morphology
- Concentration profiles
- Density histograms
- Free energy and entropy evolution
- Species potential plots (indicating areas of high and low energy)
- Compositional order parameters, giving a direct measure of phase separation