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DL_MESO

www.ccp5.ac.uk/DL_Meso
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DL_MESO is a general-purpose simulation package capable of modelling complex fluids, soft matter and transport phenomena using Dissipative Particle Dynamics (DPD) and Lattice Boltzmann Equation (LBE) methods, enabling efficient materials simulations at scales between atomistic and continuum models.

Value for Research

DL_MESO provides researchers with a powerful and computationally efficient way to study systems that are too large or complex for atomistic molecular dynamics, while retaining sufficient physics needed to understand real-world behaviour. With both DPD and LBE methodologies contained in a single framework, DL_MESO enables the investigation of soft matter, complex fluids, biomolecular assemblies, surfactants, polymers, colloids, fluid transport, and multiphase flows across length and time scales that are directly relevant to experiments and industrial processes. Its highly scalable parallelisable DPD and LBE codes allow large simulations to run efficiently on platforms ranging from desktop workstations to high-performance computing systems. As such, it is a valuable tool for fundamental scientific discovery as well as applied research in fields such as energy, healthcare, advanced materials and chemical engineering.

Development

DL_MESO was created in 2003 by the Collaborative Computing Project for Condensed Phase Systems, CCP5, as a flagship project and a complementary package to its molecular dynamics package DL_POLY. It was conceived as a collection of codes for various mesoscale mesoscale modelling methods of interest to CCP5 and other researchers in related fields, with the LBE code first released in 2004 and the DPD code in 2006 and was adopted by the High-End Computing consortium UKCOMES (Mesoscale Engineering Sciences) since 2013. Both codes were designed from the start to run on multiple-processor CPU-based machines, exploiting domain decomposition with MPI for core-to-core communications as a main parallelisation strategy. Subsequent developments on both codes have included adding new features and functionalities to expand the ranges of possible LBE and DPD simulations, optimising for performance on evolving CPUs - including adding OpenMP multithreading – and porting the codes onto other computing architectures with accelerators (e.g. NVIDIA GPUs).

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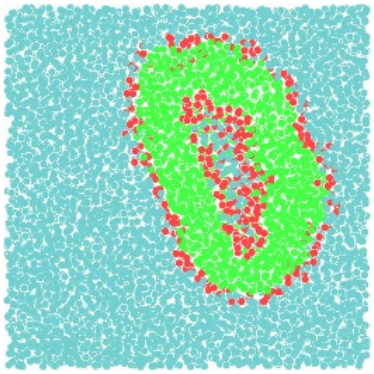
Functionality

The LBE code is capable of modelling multiple fluids with a wide variety of fluid interaction models inside simulation domains that can incorporate complex geometries (e.g. porous media, obstacles). Miscible solutes and/or a temperature field can additionally be coupled to fluid motion to study diffusion and heat transfer problems. The DPD code can model multiple particle species, including those joined together into molecular structures, that interact with a variety of potentials and are coupled to a heat bath with additional pairwise forces ('DPD thermostat'). Interacting hard wall surfaces, frozen particles and linear shear can be included as boundary conditions to study systems with surface interactions or imposed flows.



A cross-section of a vesicle formed from lipid molecules (red beads are hydrophilic head groups, green beads are hydrophobic tails) in water, modelled using the DPD code.

The Future

New functionalities continue to be added to DL_MESO. The next release will add new interaction models for both codes, including fluid-filled vesicles and turbulence models for LBE, and implicit solvents and user-defined interactions for DPD. Developments to improve performance on CPUs and other computing architectures are ongoing, as are efforts to couple the LBE code to other grid-based solvers and adaptive mesh resolution libraries, and to couple the DPD code to the analysis plugin library PLUMED (www.plumed.org). A Python library for easier file reading and writing, simulation set up and analyses is also in preparation.

LICENCE	Programming Language	Repository URL
Available under a dual licence based on academic or commercial use.	C++ (LBE code), Fortran 2008 (DPD code)	Available on STFC GitLab on request