Course content

DL_Software Workshop, the University of Manchester, 14-16 May 2025

DL_POLY

- Brief introduction to the MD method for practitioners, including simple physical and numerical concepts and statistical relevance.
- Brief history and relevance of the project.
- Basics and algorithms within the program.
- I/O infrastructure and its relation to chemistry, physics and statistics.
- Performance, do and don't.
- Obtaining and building including demonstration.
- Additional tools and hands on exercises.

DL_POLY (DPD)

- Brief introduction to Dissipative Particle Dynamics (DPD), including capabilities and differences from MD
- Current DPD functionalities in DL_POLY (comparison with DL_MESO_DPD)
- Simulation setup (optional: side-by-side comparison with DL_MESO_DPD)
- Additional tools and hands on exercises

DL_MESO (LBE)

- Brief introduction to Lattice Boltzmann Equation (LBE), including capabilities and applications to complex fluid systems
- Current and future LBE functionalities in DL_MESO_LBE
- A brief guide to obtaining and building DL_MESO
- Simulation setup and input/output files
- Additional tools and hands on exercises

DL_FIELD

- Brief introduction to force fields in molecular dynamics, the challenges of setting it up and migration of one force field (FF) to the other.
- Illustrations of software capability - use of user-defined force field (udff), customisation and modification of FF models, etc.
- Multiple potential capabilities including setting up of bio-inorganic models.
- FF model setup for DL_POLY, Lammps and Gromacs.
- Demonstration of force field models set up, including proteins and complex organic molecules.

D_ATA/DL_ANALYSER

- DL_F Notation/DANAI: A chemistry-sensitive atomic annotations for use in force field models and atomic interaction analysis.
- Example illustrations for use in post-analysis of molecular dynamics trajectories.

SHAPESPYER

- Overview of the general approach to molecular structure generation, workflows and post-simulation analyses.
- Example use cases: spherical micelles, cylindrical rods, vesicles/liposomes, placement of preexisting structures on a lattice.
- Tutorials for simulation workflows: Gromacs, NAMD, DL_MESO/DL_POLY based on Jupyter/iPython notebooks for interactive self-studying and practicing.