Course content

DL_Software Workshop, Daresbury Laboratory, 19-22 February 2018

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_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.
- Illustration of software capability - use of user-defined force field (udff), customisation and refinement of FF models, etc.
- Introduction to the DL_F Notation, a standardised atom typing expression.
- Multiple potential capabilities including setting up of bio-inorganic models.
- Demonstration of force field models set up, including proteins and complex organic molecules.

ATEN

- Overview of features
- Limitations
- Building molecules, liquids, and crystals
- Calculating properties with dlputils
- Visualisation

ChemShell

The ChemShell session will cover the following aspects of combined quantum mechanical/molecular mechanical (QM/MM) calculations:

- Setting up ChemShell calculations with Tcl scripts
- The principles of QM/MM modelling of biomolecules and materials
- The finite cluster approach for solid state QM/MM calculations
- How to handle the boundary between QM and MM regions
- Case studies for ionic and covalent systems
- Geometry optimisation with DL-FIND
- The redevelopment of ChemShell as a python-based code

DL_MONTE

The DL_MONTE instruction will assume no prior use of the code. We will cover amongst other topics

- Access and installation of the code.
- The structure and input of FIELD, CONTROL and CONFIG files.

- Output file structure
- Free energy methods recently implemented in DL_MONTE-2
- The hands on session will demonstrate NVT, NPT, Grand Canonical Monte Carlo Simulations

If time permits we will demonstrate some more advanced features of the code.

DL_MESO

- Background to DL_MESO software package
- Introductions to Dissipative Particle Dynamics (DPD) and the Lattice Boltzmann Equation (LBE) method, including their capabilities and applicability to complex fluid systems
- Current and future functionalities of DPD and LBE codes
- A brief guide to obtaining and building DL_MESO
- Performance of DL_MESO on various architectures
- Introduction to DL_MESO input and output files
- Hands-on session with tutorial exercises and demonstrations of compiling and running DL_MESO