

## **Programme Details**

### **DL\_SOFTWARE Workshop at Daresbury Laboratory**

**Start date: Monday 19<sup>th</sup> February 2018**

**End date: Thursday 22<sup>nd</sup> February 2018**

### **Summary:**

Day One, Day Two and Day Three are the DL\_POLY, DL\_FIELD, Aten, ChemShell and DL\_MESO lectures including hands-on sessions.

Day Four is the user-driven hands-on sessions or the Hack Day sessions. The whole day is dedicated for users to seek advice and help in various aspects of computational work that make use of DL\_Software. For instance, simulation setup and model development, work flow scriptings such as job submissions, etc. Alternatively, this day can also be used for continuation of the tutorial hands-on sessions.

Concurrently, on Day Three and Day Four, are the DL\_MONTE lectures and training sessions. This is carried out in a separate lecture room nearby.

During Day Three and Day Four, attendees have the freedom to choose what to attend but please state your preferences in the Registration form.

Details of the programme are shown below in the following two pages:

## **Programme**

### ***Day One – Monday 19 February 2018***

#### **Brunner-Mond, A56**

09:30-10:00 Registration  
10:00-10:15 Overview of DL\_SOFTWARE suites  
10:15-11:00 Using DL\_POLY I  
11:00-11:20 *Tea/Coffee break*  
11:20-12:45 Using DL\_POLY II/Hands-on sessions  
12:45-13:45 *Lunch break*  
13:45-15:00 Using ATEN  
15:00-15:30 *Tea/Coffee break*  
15:30-17:00 Hands-on sessions

### ***Day Two – Tuesday 20 February 2018***

#### **Brunner-Mond, A56**

09:15-10:15 Using ChemShell  
10:15-11:00 Hands-on sessions  
11:00-11:15 *Tea/Coffee break*  
11:15-12:15 Hands-on sessions  
12:45-13:45 *Lunch break*  
13:45-15:00 Using DL\_FIELD  
15:00-15:30 *Tea/Coffee break*  
15:30-17:00 Hands-on sessions

#### **Thomson Room, A52**

17:00-18:30 Wine reception and poster presentation

### ***Day Three – Wednesday 21 February 2018***

#### **Brunner-Mond, A56**

09:15-10:15 Using DL\_MESO  
10:15-11:00 Hands-on sessions  
11:00-11:20 *Tea/Coffee break*  
11.20-12:45 Hands-on sessions  
12:45-13:45 *Lunch break*  
13:00-15:00 Hands-on sessions  
15:00-15:30 *Tea/Coffee break*  
15:30-17:00 Hands-on sessions

#### **Thomson Room, A52 : DL\_MONTE training – Day 1**

09:15-10:15 Introduction to Monte Carlo and DL\_MONTE  
10:15-11:00 Hands-on sessions: NVT, NpT, GCMC tutorials  
11:00-11:20 *Tea/Coffee break*  
11.20-12:45 Hands-on sessions: continued  
12:45-13:45 *Lunch break*  
13:00-13:45 Free energy difference (FED) & replica-exchange (REX) in DL\_MONTE-2  
13:45-15:00 Hands-on sessions: FED & REX tutorials  
15:00-15:30 *Tea/Coffee break*  
15:30-16:00 Nano-pore (slit) constraint in DL\_MONTE-2  
16:00-17:00 Hands-on sessions: continued

### ***Day Four – Thursday 22 February 2018***

#### **Brunner-Mond, A56 : Hack days (user-driven hands-on sessions)**

09:15-11:00 Hands-on session  
11:00-11:20 *Tea/Coffee break*  
11.20-12:45 Hands-on sessions  
12:45-13:45 *Lunch break*  
13:00-15:00 Hands-on sessions  
15:00-15:30 *Tea/Coffee break*  
15:30-17:00 Hands-on sessions

#### **Thomson Room, A52 : DL\_MONTE training – Day 2**

09:15-10:15 Phase Switch MC methods in DL\_MONTE-2  
10:15-11:00 Hands-on sessions: PSMC tutorials  
11:00-11:20 *Tea/Coffee break*  
11.20-12:45 Hands-on sessions: continued  
12:45-13:45 *Lunch break*  
13:00-13:45 Histogram re-weighting toolkit (HTK)  
13:45-15:00 Hands-on session: using HTK tutorials  
15:00-15:30 *Tea/Coffee break*  
15:30-17:00 Hands-on sessions: continued

For any query about this Workshop, please contact Dr Chin Yong ([chin.yong@stfc.ac.uk](mailto:chin.yong@stfc.ac.uk))