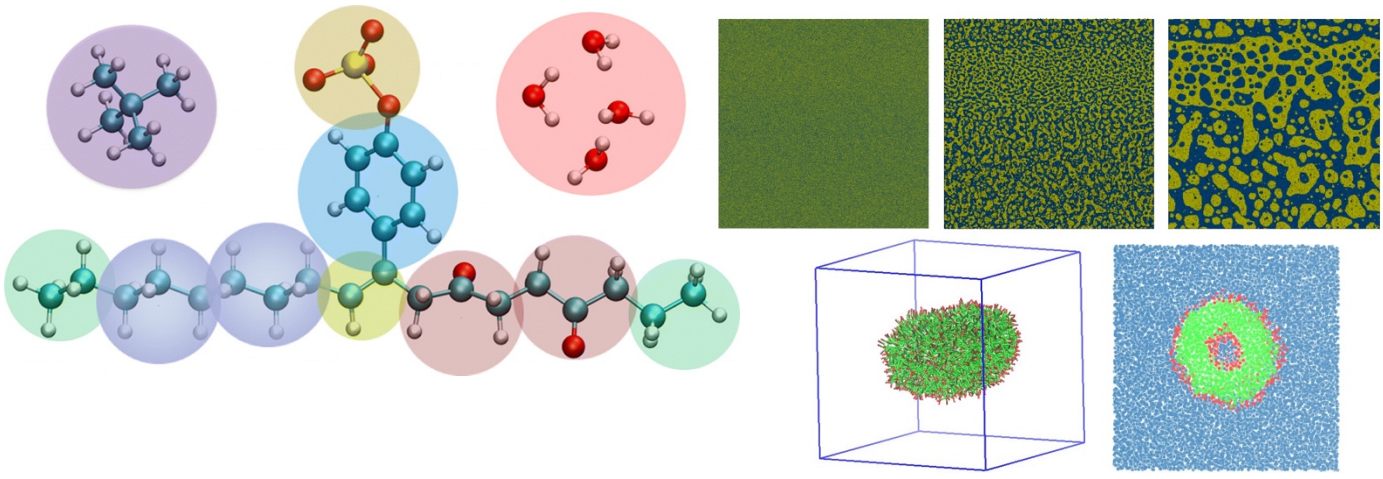

Industry training at the MESOSCALE
22nd – 25th March 2021

DL_MESO_DPD has been used for a wide range of problems of both scientific and industrial interest.

- More than 120 journal articles citations
- Within UKRI STFC, DL_MESO_DPD is involved in projects with Unilever, Syngenta and Infineum – to develop DPD parameterisation strategies and simulation protocols to predict important properties of newly-devised surfactant-based formulations; with IBM Research Europe – to model nanofluidic multiphase flow
- An STFC spinout venture company, Formeric, was formed to help industrial users to study their own formulated projects, primarily by developing a software platform to make it easier for them to access DPD simulations and modelling tools.

Description

In this workshop we will introduce DL_MESO: a software package for mesoscale simulations based on the Dissipative Particle Dynamics (DPD) and Lattice Boltzmann Equation methodologies. The intention is to gradually present the usage of the software, starting with tutorials based on theoretical background and following up with hands-on sessions. We will focus on the DPD methodology, exploring the different capabilities of the DPD code in DL_MESO (DL_MESO_DPD) in order of growing complexity via practical examples that reflect daily industrial challenges: moving from simple soft repulsive (Groot-Warren) interactions to systems with electrostatic potentials. Particular attention will be paid to the problem of parametrization and how to obtain the best results, as well as interpreting simulation outputs.

Following the current growing usage of General-Purpose Graphic Processing Units (GPUs) as computing accelerators, we will introduce the GPU version of DL_MESO to speed up your applications. The participants will be able to run their simulations on the Hartree Centre supercomputer GPU nodes and considerably reduce the computing time as well as increasing the problem system size. This will allow participants to move towards real industrial applications, where the number of particles and computational costs are usually prohibitive on a common laptop.

Don't miss this opportunity. Register now: www.cecam.org/workshop-details/1074/

Participation fee: 150 €. As part of the event, UKRI STFC offers a 6 month one seat free licence of DL_MESO 2.7, to be used soon after the end of the event. A full licence can be purchased at the end of the trial version.

This event falls within the activities of the E-CAM project in connection to industry. E-CAM is funded by the European Union under the grant agreement number 676531.

www.e-cam2020.eu

INDUSTRY TRAINING AT THE MESOSCALE (ONLINE) / 22 – 25 MARCH 2021

Organizers: Jony Castagna[1], Michael Seaton[1], Sara Bonella[2], Formeric[3] ([1] UKRI STFC, [2] CECAM EPFL, [3] https://formeric.co.uk/)

PROGRAMME

MONDAY 22nd MARCH

Introduction to DPD and DL_MESO

09:00 – 11:00 Background and theory

11:00 – 11:30 Break

11:30 – 12:30 Applications

12:30 – 13:30 Break

13:30 – 15:30 Introduction to DL_MESO and DL_MESO_DPD

15:30 – 16:00 Break

16:00 – 17:00 Hands-on session: access/compile DL_MESO_DPD and try running a few test cases

TUESDAY 23rd MARCH

DPD parametrisation strategies

09:00 – 09:30 Background and theory

09:30 – 10:30 Interaction parameters

10:30 – 11:00 Break

11:00 – 12:00 Matching to experimentally-determined properties

12:00 – 12:45 Hands-on session

Electrostatics and surfaces

14:00 – 14:45 Strategies to include charges with DPD particles

14:45 – 15:45 Incorporating charge polarisation effects

15:45 – 16:15 Break

16:15 – 17:15 Surfaces, frozen particle walls and moving boundaries

17:15 – 18:00 Hands-on session

WEDNESDAY 24th MARCH

Accelerating your simulation with DL_MESO on GPU

09:00 – 10:00 Introduction to the GPU version of DL_MESO_DPD

10:00 - 10:30 Break

10:30 - 12:30 Hands-on session: Compile DL_MESO_DPD with CUDA language

12:30 – 13:30 Break

13:30 – 15:30 Hands-on session: try out larger-scale simulations (e.g. parameterisation using partition coefficients)

THURSDAY 25th MARCH

Setting up your own simulations

09:00 – 12:30 Hands-on: getting started on parametrising and running DPD simulations of participants' own systems

All listed times are in GMT

With the support of

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Registration at www.cecam.org/workshop-details/1074/