ESDW4: Meso and Multiscale Methods

Location: CECAM-ES
Webpage: https://www.cecam.org/workshop-1488.html
Dates: July 3, 2017 to July 14, 2017
Organizers: Ignacio Pagonabarraga (CECAM EPFL, Switzerland)

1 State of the art

E-CAM gathers a number of research groups with complementary expertise in the area of meso and multiscale modelling. The aim of the involved groups in this area is to produce the necessary software by combining software modules. It is also interested in developing appropriate software that can bridge different descriptions (quantum, classical, continuum) in a sequential coupling scheme in which input parameters are computed at the higher resolution and then used in the lower resolution model. Many mesoscale methods have been developed, and this is still a highly active field. Of particular importance is the development of systematic “coarse–graining” approaches, where the same physics is being described on two or more differing length and time scales, and relations are established between these in a quantitative fashion.

The goal of this workshop was to discuss currently available software packages for mesoscale simulations in the E-CAM community, the corresponding limitations and potentials, the needs for software development that they have, and the tools that are generically needed. This proper understanding of computational needs and possibilities can naturally lead to an identification of promising software modules to be developed in E-CAM.

The workshop has also addressed the challenge of scalability of software packages for multiscale modelling, and the HPC challenge in E-CAM in general. The ESDW was combined with an E-CAM Extreme-Scale State-of-the-Art Workshop, aimed at providing a forum for fellow E-CAM application end users and developers to a) identify emerging extreme-scale computing requirements across the centre, from both academia and industry partners, b) increase the centre’s awareness of current and emerging HPC hardware and software technologies on the road to exascale computing, c) increase the centre’s awareness of PRACE services (advanced training, software enablement, and industry interactions), d) interface with other members of the European HPC community and e) identify themes of future interest for the centre on the road to exascale computing. The outcome of this extreme-scale workshop has been reported in E-CAM’s deliverable D7.5: Hardware Developments II (https://doi.org/10.5281/zenodo.1207613).

2 Training provided

The primary training component of this ESDW came in the form of the development of software modules for two software packages used by the E-CAM community: DL_MESO_DPD (https://www.scd.stfc.ac.uk/Pages/DL_MESO.aspx) and ESPResSo++ (http://www.espresso-pp.de/). These have been identified as important codes for mesoscale simulations within E-CAM in a recent state-of-the-art workshop in Mesoscale and Multiscale

Modelling that took place in Dublin on the 29th May-1st June 2017 (workshop report available for download at https://www.e-cam2020.eu/scientific-reports/).

The first day of the workshop was dedicated to introducing the two software packages mentioned above, and the work done by E-CAM post-docs in the framework of pilot projects focused on industrially oriented problems and that involve the development of software modules for these codes (https://www.e-cam2020.eu/pilot-projects-with-industry/).

The second day included talks focused on general software development training such as:

- scalable and fast heterogeneous molecular simulation with predictive parallelization schemes;
- software development best practices, introducing software development tools like GitLab and git;
- the E-CAM concept of "module".

The third day was dedicated to Poisson solvers for mesoscale methods and included talks on:

- Poisson solvers and HPC;
- Poisson solvers in DL_MESO;
- Poisson solvers in ESPResSo++;
- Local approaches to electrostatics.

The fourth and fifth days were dedicated to the E-CAM Extreme-Scale State-of-the-Art Workshop (https://www.cecam.org/workshop-0-1512.html) that exposed the workshop participants to current extreme-scale challenges.

The second week of the workshop was dedicated to the “training by doing” component of the event, associated to module contribution within E-CAM. E-CAM programmers assisted the participants on the development of software modules following programming best practices and with an eye on the future of the hardware where they will run such modules.

3 List of software development projects

The following modules were developed at this workshop:

1. Modules based on DL_MESO_DPD:
    a. Using SIONlib (parallel I/O library) to write/read HISTORY files in DL_MESO_DPD
    b. First GPU version of the DL_MESO_DPD code
2. Modules based on ESPResSo++:
    a. Md-Softblob
    b. Minimize Energy

These modules have passed E-CAM's evaluation for quality standard for code, tests, and documentation and are now uploaded into the E-CAM Library at http://e-

cam.readthedocs.io/en/latest/Meso-Multi-Scale-Modelling-Modules/index.html, and included in the following E-CAM Deliverables D4.2 (https://doi.org/10.5281/zenodo.1207372) and D4.3 (https://doi.org/10.5281/zenodo.1210075).

4 Future plans

Modules to be integrated in the two software packages (DL_MESO_DPD and ESPResSo++) have been identified and will be further developed. The GPU implementation of DL_MESO_DPD shall be extended further. In the future, we plan to develop modules for simulating one system by using two different degrees of coarse–graining within two different parts of one simulation box (the so–called AdResS, “adaptive resolution scheme”, method).