ECAM State of the Art Workshop in Mesoscale and Multiscale Modelling

Date May 29 - June 1, 2017, CECAM-IRL, University College Dublin, Ireland

Organisers: Ignacio Pagonabarraga (CECAM HQ, Switzerland), Vladimir Vladmir Lobaskin (University College Dublin, Ireland), Donal Mackernan (University College Dublin, Ireland)

1. State of the Art

The inclusion of atomistic or electronic detail and the short time-steps required in most quantum and classical MD calculations limit the system size and the total time accessible with these methods. For phenomena of relevance to academia and industry that occur on longer time and distance scales (such as protein folding and docking, polymer and surfactant structuring, lubrication and blood flow) it is useful to integrate out some of the underlying degrees of freedom and to develop coarse-grained models. These mid-scale or meso-scale models can be studied using suitably adapted simulation techniques from classical simulations and by developing new techniques that go beyond the particle-based description. Equally important and challenging is the requirement to work across more than one length or timescale at the same time, using multi-scale simulation techniques targeted at the production of new materials with tailored macroscopic properties (for example, dislocations, grain and phase boundaries, active sites). While considerable theoretical work exists in this domain, there is no generally accepted code in the community that covers a sufficient range of length scales and phenomena.

The use of mesoscale models faces challenges such as

- Do robust parameterization methods exist that enable predictive simulations?
- Can coarse-grained potentials be extended to different families of compounds or are they molecule/system-dependent?
- What is the real computational gain in mesoscale methods? How do they deal with the coexistence of broad variety of time and length scales?
- How can mesoscale methods be parametrized and structured for industrial applications?
- Does the software exist to support predictive simulations?

In order to advance in the understanding, use and exploitation of meso and multi scale computational methods we still need to better identify the (i) current challenges, (ii) the existing software solutions and their limitations, and (iii) need for further development of meso- and multiscale methods and codes. This understanding will allow to identify and propose the kind of software required to bridge different descriptions (quantum, classical, continuum) in a systematic bottom-up scheme, in which input parameters are computed at the higher resolution and then used in the lower resolution model. In particular, existing promising methodologies of systematic static and dynamic coarse-graining, include inverse Monte Carlo, Newton inversion, discretization, Mori-Zwanzig formalism etc.

Significant areas that require special attention in order to be able to advance faster and deeply on the development of meso- and multi-scale methods include: the foundations of mesoscale and multiscale models, the use of particle-based and statistics-based static and kinetic mesoscopic approaches, the understanding of fundamental processes in non-equilibrium and heterogeneous systems, and the use of hybrid and mesoscale approaches to analyze the dynamics of complex materials. These requirements include fundamental topics related to the foundations of these type of models with the objective to

understand the potential of existing approaches and their weaknesses. This is a central aspect in order to identify the major needs in the improvement of the theoretical basis for mesoscale methods.

2. Programme of the workshop

Day 1, May, 29th

10:00 to 11:00 - Didactic Lecture on methodologies of systematic static coarse-graining

11:00 to 11:30 - Coffee Break

11:30 to 12:30 - **Burkhard Duenweg**
Introduction to the Mori-Zwanzig formalism

12:30 to 13:30 - Lunch

13:30 to 14:10 – **Kurt Kremer**
Overview Talk on mesoscale/hybrid approaches

14:10 to 14:30 - **Christian Holm**
Influence of the permittivity gradient on static and dynamic properties of charged macromolecules

14:30 to 14:50 - **Burkhard Duenweg**
Monte Carlo approach to Fluctuating Lattice Boltzmann

14:50 to 15:10 - **Matej Praprotnik**
Adaptive resolution simulations of supramolecular water

15:10 to 15:30 - **Pietro Lio**
Multiscale computational approaches in modelling biological data integration and molecular communication

15:30 to 16:00 - Coffee Break

16:00 to 16:20 - **Pierre Cazade**
Multi-scale modelling of Large Biomolecular Complexes

16:20 to 16:40 - Focused/Question specific talk on mesoscale/hybrid approaches

16:40 to 17:00 - **Jason Reese**
Best of Both Worlds? Hybrid Fluid Simulations for Multiscale Engineering

17:00 to 17:20 - **Gerhard Jung**
Iterative Reconstruction of Memory Kernels

17:20 to 18:20 - Moderated roundtable on current challenges for hybrid approaches, inclusion of ab-initio description

18:20 to 19:50 - Reception-poster session

Day 2, May, 30th

09:30 to 10:10 – **Heiko Rieger**
Overview on non-equilibrium processes and heterogeneous systems

10:10 to 10:30 - **Julija Zavadlav**
Multiscale Simulations of DNA Arrays

10:30 to 10:50 - **Aleksandar Donev**
Coupling a nano-particle with fluctuating hydrodynamics

10:50 to 11:20 - Coffee Break

11:20 to 11:40 - **David Cheung**
Coarse-grain modelling of polymer nanostructures

11:40 to 12:30 - Moderated roundtable on non-equilibrium processes

12:30 to 13:30 - Lunch

13:30 to 14:10 – **Marcus Mueller**

Overview on Coarse Graining
14:10 to 14:30 - **Alexander Lyubartsev**
Multiscale modelling by systematic structure-based coarse-graining
14:30 to 14:50 - **Agur Sevink**
Automated multi-scaling with Stochastic Quasi-Newton (S-QN)
14:50 to 15:10 - **Pep Español**
Non-isothermal coarse-graining of complex molecules
15:10 to 15:30 - **Denis Andrienko**
Many-body effects in systematic coarse graining
15:30 to 15:50 - **Nicolae-Viorel Buchete**
Coarse-Grained Kinetic Models of Protein Folding and Binding Networks
15:50 to 16:20 - Coffee Break
16:20 to 17:00 – **Carlo Massimo Casciola**
Overview on connecting to continuum/engineering level descriptions
17:00 to 17:20 - **Pietro Asinari**
Multi-Scale Modelling of Nanoparticle Suspensions
17:20 to 17:40 - **Serafim Kalliadasis**
From the nano- to the macroscale: bridging scales for the moving contact line problem
17:40 to 18:40 - Moderated Roundtable on connecting to continuum/engineering level descriptions
19:45 to 22:00 - Workshop Dinner on Canal Boat

Day 3, May, 31st
09:30 to 10:10 – Michael Seaton
Overview on Software packages
10:10 to 10:30 - **Kevin Stratford**
Performance portability in coarse-grained mesoscale complex fluids
10:30 to 10:50 - **Danny Perez**
Long-timescale Simulations with Accelerated Molecular Dynamics and the EXAALT package
10:50 to 11:20 - Coffee Break
11:20 to 12:20 - Moderated Roundtable on existing software solutions and their limitations
12:30 to 13:30 - Lunch
13:30 to 14:10 – Discussion session
14:10 to 15:10 - **Denis Andrienko**
Systematic coarse-graining with VOTCA
15:10 to 15:40 - Coffee Break
15:40 to 16:40 - Didactic Lecture on continuum/engineering level descriptions

3. List of Participants

Last Name	**First name**	**Affiliation**
ANDRIENKO	Denis	Max Planck Institute for Polymer Research, Mainz
ASINARI	Pietro	Politecnico di Torino
BUCHETE	Nicolae-Viorel	University College Dublin
CASCIOLA	Carlo Massimo	University of Rome I "La Sapienza"
CAZADE	Pierre	University if Limerick
CHEUNG	David	NUI Galway

CHIACCHIERA	Silvia	STFC
DONEV	Aleksandar	Courant Institute, New York University
DUENWEG	Burkhard	Max Planck Institute for Polymer Research, Mainz
ENGLISH	Niall	University College Dublin
ESPAÑOL	Pep	National University of Distance Education
HARB	Moussab	KAUST University
HOLM	Christian	Institute for Computational Physics, University of Stuttgart
JUNG	Gerhard	Institute of Physics - Johannes Gutenberg Universität Mainz
KABEDEV	Aleksei	University College Dublin
KALLIADASIS	Serafim	Imperial College
KOBAYASHI	Hideki	Max Planck Institute for Polymer Research, Mainz
KREMER	Kurt	Max Planck Institut for Polymer Research, Mainz
LEMMIN	Thomas	UCSF
LIO	Pietro	University of Cambridge
LOPEZ	Hender	University College Dublin
LYUBARTSEV	Alexander	Stockholm University
MAHESHWARI	Nikunj	University College Dublin
MARKINA	Anastasia	Faculty of Physics, Lomonosov Moscow State University
MCCARTAN	Sarah	University College Dublin
MÜLLER	Marcus	Georg-August University, Göttingen
NOLAN	David	Trinity College Dublin
O'REILLY	Eoin	Tyndall National Institute at University College Cork
PEREZ	Danny	Los Alamos National Laboratory
POGGIO	Stefano	University College Dublin
POWER	David	University College Dublin
PRAPROTNIK	Matej	National Institute of Chemistry, Ljubljana
REESE	Jason	University of Edinburgh
RIEGER	Heiko	Saarland University
SAMANTRAY	Suman	National University of Ireland, Galway
SANYAL	Shourjya	CASL, School of Physics, UCD
SCHERER	Christoph	Max Planck Institute for Polymer Research, Mainz
SEATON	Michael	Science & Technology Facilities Council
SEVINK	Agur	Leiden University
SHIELDS	Denis	UCD Conway Institute for Biomolecular and Biomedical Research, Dublin, Ireland
STRATFORD	Kevin	University of Edinburgh
TYWONIUK	Bartlomiej	University College Dublin
XU	Liang	University of Limerick
ZAVADLAV	Julija	ETH Zurich

4. Major outcomes

Given the spirit of the workshop, focused on a survey of the state of the art, the main outcomes of the discussions aim at setting the stage for promoting further development and creating the best research environment. The event recognized the needs to advance in the establishment of mesoscopic models

and their proper calibration to convert them into quantitative predictive tools. The event also serve to agree that the next four years we can expect a consolidation of different mesoscopic methods developed over the last ten years and a more systematic analysis to be able to combine them with molecular methods. Specifically, the main topics explored in the SAW have been,

1. State of the art and challenges in multiscale methods
2. State of the art and challenges in mesoscale methods
3. Software packages of multiscale modelling
4. Engineering problems addressed with materials modelling
5. Kinetic Monte Carlo methods and modelling of non-equilibrium processes

Several debates took place during the meeting which helped provide a focus on key difficulties and challenges for mesoscale/multiscale simulation. Here we highlight a few of the most striking ones:

a) Industrial manufacturing typically involves processing where materials are in far from equilibrium conditions. Yet virtually all simulation methods have been developed for systems that are either in equilibrium or close enough to it that the corresponding force-field parameters and initial conditions are a good estimate of reality, for instance, in regimes where linear response is valid. However, such assumptions are frequently not valid, for example, for complex glassy polymeric systems, or driven systems and so on. An additional complication is that there is no theory on how such systems can be treated, despite their great practical industrial importance;

b) The exascale mission assumes that massive parallelism can resolve the main difficulties in simulation. While it certainly can allow much larger systems to be simulated, it does not directly address the great need to simulate systems over very long time scales, which is a very significant challenge for simulation of complex systems in advanced materials and biology, not to mention the treatment of systems far from equilibrium referred to in the previous bullet point. Were processors capable of running at much higher frequencies, it might help, but even this remains a serious practical challenge. Rare-event based methods can be of significant help, provided the relevant order parameters/reaction co-ordinates can be found. When they are available and appropriate for a given system, they can in principle exploit exascale capabilities. However, that is under the proviso that reliable and relevant order parameters/reaction co-ordinates can be found;

c) There is a schism between the non-expert user community exploiting mesoscale codes for practical problems, and the expert community which tends to focus for instance on questions such as suitable mapping rules develop coarse grained models, frequently using its own in-house simulation engine. As a consequence, the quality of mesoscale/multiscale simulation by the non-expert user community can be quite poor;

d) Many coarse grained methods have been developed by individual groups over the last two decades, but as lead developers leave groups, or group leaders retire, there is a danger that no-one will be left that can maintain those codes in the future;

e) Many particle based coarse grained models need to be used to simulate non-equilibrium behavior of complex and heterogeneous materials. These systems lead to an inhomogeneous distribution of the particles that represent the different components of the materials. These asymmetry poses computational challenges, especially when exploiting mesoscopic models on HPC facilities. The discussions identified load unbalancing as a serious limitation in the scaling of mesoscopic algorithms at the peta-scale and beyond.

The outcomes of the meeting include

1. Overviews of recent advances in systematic coarse-graining and multiscale modelling, inclusion of electrostatic, quantum, and hydrodynamics effects in simulation
2. Identification of remaining challenges in bridging the time and length-scale gaps in soft matter modelling
3. Discussions of the foundations of mesoscale models, hybrid models, and coarse-grained liquid state models
4. Discussions linking ab initio methods with atomistic modelling
5. Identification of bottlenecks in HPC implementation of the multiscale software (AdResS, and computational packages such as ESPRESSO, DLMESO, LAMPPS, PI-GC-AdResS, MP2C, Ludwig, Votca.)
6. Discussions regarding the gaps in dialogue and interaction between academia and industry
7. Discussions regarding the need for further development of meso- and multi-scale methods and soft-ware codes
8. A proposition for a Lorentz workshop in 2018 – still under preparation.

5. Community needs

In the first discussion session, the organisers asked those not giving presentations for their thoughts about the status and prospects on the needs to identify the bottlenecks in the proper foundations of mesoscopic models and the need to identify well defined standards for their calibration to convert them into predictive tools.

There were extensive discussions on the connections between different classes of particle based mesoscopic methods. There was a common agreement on the need to push further a thorough analysis of some of these well established methods (as is the case, e.g. of Dissipative Particle Dynamics (DPD)) in close discussions with industrial partners to address the identified needs from a broader perspective and with an emphasis on ensuring a fast societal impact.

It was recognized the need to procure sufficient human resources is all the more important due to the potential recognized in meso- and multi-scale modelling to cope with complex materials. The meeting also recognized the need of a balance deployment of resources in the foundation of these new methods and in their adaptation to a variety of industrial needs.

A number of the discussion sessions served to recognized that the transition from the early development stage of the different available methods to a stable production activity will drive the evolution of the software towards the creation of community ready package. The existence of the new EINFRA5 CoEs, and in particular of E-CAM, offers a unique opportunity to create an exciting environment for software development, documentation, and maintenance. Identifying the optimal hardware architecture (GPU vs CPU, for example) for the performance of different types of codes is also an interesting question since

the choice is closely related to the performance of the different methods and their performance on complex systems and heterogeneous materials.

The community is eager to promote opportunities for interaction and exchange that bring together different kinds of mesoscopic approaches and to analyze the potential of multi scaling from a wide perspective. These opportunities are clearly key for the development of the field. It was suggested to continue and consolidate the series of workshops hosted by CECAM in the last five years to stabilize this opportunity to exchange on recent developments. CECAM workshops are particularly suitable for this need.

6. Funding and Resources

In terms of funding, the discussions carried out during the workshop have indicated that the development of mesoscale and multiscale methods will increase their potential for direct application to industrially related challenges. In this respect, Horizon 2020 is clearly a potential funding channel, and recent developments, which pave the way to material and energy-related applications, might lead to successful ERC projects. EPSRC, in the UK, is a clear source of funding for the development of new formulation initiatives.
To make progress in the development of new methods and tools for the development of multi-scale methods that build on the solid knowledge of molecular models, the expected advance in our control of mesoscopic methods and finite element approaches, a concerted community effort is needed. To fund such a community-wide effort in a sustainable way, a combined strategy is necessary. While individual PIs can apply for single investigator grants from their national funding agencies, the EU H2020 framework could provide opportunities to set up an international network geared towards method development. More specifically, within the Marie Skłodowska-Curie actions, Innovative Training Networks offer attractive possibilities to train the required human expertise with strong ties to industry. Other opportunities for funding might be available in the Future and Emerging Technologies (FET) Program of H2020.

7. Developments for society and industry

The societal benefits are twofold. On the fundamental level, the model development expected will provide new venues for material modeling and will make it possible to have an impact in the prediction of the properties of new materials, and in general in material science. This will be made possible by the scientific community using the sampling and analysis tools that are being developed.

On an economic level, industry will benefit from software containing efficient and easy to use simulation and analysis tools to extract observables for applications in sectors such as pharma, materials or house-hold products. For example, meso- and multi-scale methods will provide support on

- Drug handling: kinetics of biopolymers, proteins and membrane interactions;
- Food/dairy industry: protein aggregation, chocolate crystallization, grain size in ice cream, food preservation, food stability and texture control;
- Materials science and daily products: surfactant kinetics, material stability, soft matter, self-assembly of nano-materais, colloids, liquid crystal based materials.

Society will benefit from the development of new computational algorithms and the corresponding software that make the development of new materials cheaper and improve food quality and daily products.