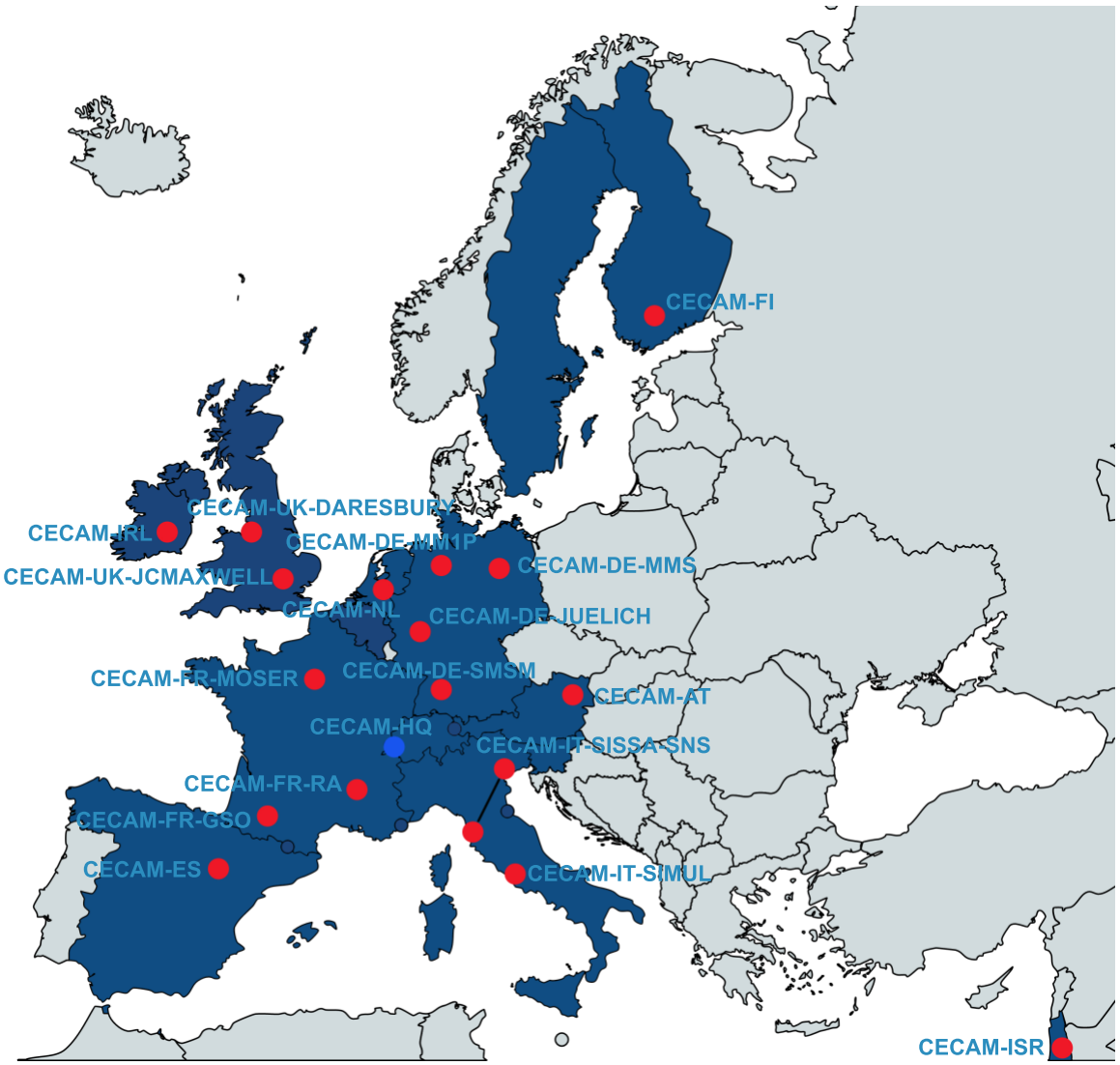
Activities & Scientific Report

2020



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Introduction

2020 was an exceptional year, marked by the onset of the COVID pandemic in late February. The impact of this global crisis on the CECAM Flagship program is clearly visible starting from March 2020. Workshops and schools planned for the three last quarters of the year were canceled, postponed (46 events out of the 60 accepted by the CECAM Council in November 2019) or turned into online events. 14 Flagship events were held (6 onsite, 8 online), with a total of 68 organisers and 852 participants. Due to the exceptional circumstances the CECAM management decided not to enforce strict reporting of the activities that took place, preferring a more informal and interactive monitoring protocol based on exchanges with organizers and node director.

To compensate for the reduction in activities, and to mitigate the effects of sanitary and travel restrictions on scientific networking and collaborations, CECAM developed a set of online initiatives to enable the computational science community to interact, albeit in a different form than usual. These initiatives were articulated in two ways. Firstly, videos of keynote talks recorded in the previous years were published at regular intervals. These are reported in this report under the global label of CECAM Highlights. Secondly, two series of webinars on topical themes were rapidly organized and deployed. An innovative, for the time, format in which on-line participants had ample opportunity to ask questions and interact with the invited speakers was proposed and proved highly successful.

The first webinar series, titled *COVID-19: challenges and responses in modeling, simulation, and beyond*, focused on how the community could contribute to develop a response to the pandemic. Four weekly sessions were held in April-May 2020, with contributions devoted to computational drug design, statistical modeling of epidemics, bioinformatic approaches. Experimental talks were also included. The total number of views (lives or of the recordings uploaded on the CECAM website) for this series was impressive, with around 300 live participants, and with numbers consistently above 1000 views for the recordings posted on the CECAM YouTube channel.

The second webinar series, titled *The importance of being HPC-Earnest*, comprised five sessions that took place in June-July 2020. This series focused on current efforts, in Europe and in the USA, to create scalable and performant community software enabling the community to take advantage of pre-exascale and exascale High Performance Computers. In this case too, attendance was remarkable, with an average of 250+ participants per session, followed by a peak number of visualisations over 2000 and averages around 400 of the videos on YouTube.

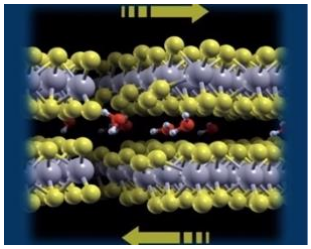
The attendance reported above shows that the response of the community to these activities, and to the Flagship events that were not postponed, was exceptional. These figures, and more broadly the community feedback, indicate that, in spite of very difficult circumstances, CECAM remained a crucial focal point for computational scientists during the crisis, strengthening further the relationship of trust and collaboration with researchers at different stages of their career around the globe.

WORKSHOPS **4**

Molecular Mechanisms of Tribochemistry and Lubrication 4
Frontiers in Computational Methods for Active Matter 12
Digital Event - Open Databases Integration for Materials Design 15
GW goes large-scale 19
(Machine) learning how to coarse-grain 22
Multiscale simulations of soft matter: New method developments and mathematical foundations 29

OTHER ACTIVITIES **35**

CECAM 50th anniversary - Plenary Lectures 35
CECAM Keynote Lectures 39
Mary Ann Mansigh Conversation Series 40
Berni J. Alder CECAM Prize 41
Webinar Series "CoVid-19: challenges and responses in simulation, modeling and beyond" 42
Session 1: Tuesday April 21 2020 ..... *42*
Session 2: Tuesday April 28 2020 ..... *44*
Session 3: Tuesday May 5 2020 ..... *46*
Session 4: Tuesday May 12 2020 ..... *48*
Webinar Series "The importance of being H.P.C. Earnest" 50
Session 1: Thursday June 18 2020 ..... *50*
Session 2: Thursday June 25 2020 ..... *53*
Session 3: Thursday July 2 2020 ..... *55*
Session 4: Thursday July 9 2020 ..... *57*
Session 5: Thursday July 16 2020 ..... *58*



Molecular Mechanisms of Tribochemistry and Lubrication

Location: CECAM-HQ
Webpage: https://www.cecam.org/workshop-details/109
Dates: Jan 27, 2020 - Jan 29, 2020

1 State of the art

Many important tribological phenomena can ultimately be described as chemical reactions occurring in the presence of mechanical forces, i.e., tribochemical reactions. One example is boundary lubrication, where lubricant additives included in motor oils react with the contacting surfaces under sliding conditions to modify their chemical composition with consequent modification of adhesion and resistance to sliding. Another important example is the effect of humidity on solid lubricants; it is well documented that the lubricity of MoS2 is adversely affected by air humidity, while graphite and diamond/diamond-like carbon (DLC) coatings depend on moisture for good lubricating properties. The microscopic origin of these behaviors is still unclear. In order to design new, environmentally friendly, solid and boundary lubricants is necessary to acquire microscopic understanding of tribochemical mechanisms. Our knowledge of the reaction kinetics and thermodynamic driving forces at the open surface is not sufficient to accomplish this goal because the tribological conditions often induce reactions that are not seen in ordinary situations. Tribological conditions include additional effects such as frictional heating, molecular confinement, and high shear stresses and contact pressures. Increases in reaction rates are generally observed at tribological interfaces, a phenomenon that provides a very appealing approach for the synthesis of chemicals without the use of solvents. Addressing these issues will require both novel computational approaches and the use of simplified model systems that nevertheless mimic real tribological systems. This CECAM workshop will, therefore, include both theorists and experimentalists to allow experimental systems to be developed that are sufficiently simple that they are amenable to being simulated under conditions encountered in the experiment to provide a robust comparison between theory and experiment. As a consequence, the workshop will focus on the following themes:

1. Molecular mechanisms and computational strategies in tribochemistry
2. Lubricant Additives
3. Solid Lubrication; Layered Materials
4. Solid Lubrication: Coatings

Each theme will include both invited and contributed talks by both theorists and experimentalists to address the open issues and challenges in each area. Some are listed in the following:

- Which is the best computational strategy to face the complex tribochemistry problem? Can we identify key tribochemical mechanisms to be studied on different time/length scales and a rational way to combine them in a multiscale description?
- Can we define a computational protocol for the in-silico design of lubricant additives? Layered materials represent clean, well-defined interfaces where simulations can combine with experiments to answer fundamental questions such as: what is the effect of load compared to the effect of shear on reaction kinetics? What are the effects of molecular confinement? Is transition-state theory applicable to frictional processes?
- Wear-resistant, low-friction coatings such as diamond and diamond-like carbon (DLC) represent a very efficient way to increase the life of the operating systems and reduce the energy losses by friction. However, the functionality of the carbon-based films is deeply influenced by tribochemistry.

The aim of this workshop is to identify strategies to control the molecular-level mechanisms to facilitate the widespread use of these materials at the macroscale such as automotive and biomedical applications.

2 Major outcomes

The work was organized around themes within the subject area of the conference, staring with a Keynote Lecturer to introduce the state-of-the-art in that particular area, followed by invited and contributed talks that further expounded on the ideas introduced by the Keynote speaker. This was then followed by Round-Table discussions on each of the focus topics. These were organized in various ways for formal panels constituted from expert attendees in that subject area from the conference to informal discussions lead by the moderators. The subject discussed and their moderators are summarized as:

- Real-Time monitoring and surface analysis of tribochemical reactions (Eddy Tysoe and Rob Carpick)
- Molecular dynamics and first principles calculations of tribochemistry: Bridging time and length scales (Clelia Righi and Martin Müser)
- Tribochemistry of coatings (Filippo Mangolini and Michael Moseler)
- Challenges Towards the Scaling Up of Structural Superlubricity (Oded Hod and Oguz Gulseren)
- Real-Time Monitoring and Surface Analysis of Tribochemical Reactions.

The moderators decided to adopt a relatively unstructured format for the round-table discussion by initially making opening summary statements, and then by opening the discussion for all the participants, during which notes were taken on the white boards (see Figure 1). The group discussed how the role of surface analyses to monitor tribochemistry is to establish the composition of an interfacial film that forms, for example to correlate the friction behavior with the film's mechanical or anticorrosive properties, or to monitor the time evolution of the state of the interface in order to develop kinetic models for tribochemical reaction rates. It was pointed out that the study of tribochemical reactions has the advantage over other areas of surface chemistry, for example in the study of catalytic reactions, because the chemistry is induced by the rubbing process. This enables the reaction to be turned on by rubbing, which thus allows the evolution of the surface to be followed in detail. This advantage is offset by the challenges associated with studying the chemistry at a solid-solid interface. This has traditionally been facilitated by arranging for one of the counterfaces to be optically transparent, which then enables optical spectroscopies such as infrared, Raman, UV/visible or fluorescent spectroscopies to be used to interrogate the buried interface. However, while such approaches have yielded many insights, such optical techniques are often not extremely surface sensitive. In addition, engineering interfaces are generally metals or oxides and thus often not optically transparent. There are significant challenges to designing surface analytical tools for tribochemical reactions at the solid-solid interface because of the difficulty with using surface-sensitive probes (namely electrons and photons) at the solid-solid interface. The scant tools that have been used include measure the evolution in topology, the measurement of the friction force and the detection of gas-phase products, where the latter technique requires the use of high- or ultrahigh vacuum. Near-field techniques have been used to provide spatially-resolved images due to the electric-field enhancement at a tip, but this is often challenging to implement, and the results are very sensitive to the tip-surface distance. Recent, an AFM-IR technique has been developed (Dazzi et al, Applied Spectroscopy, 66, 1365-1384 (2012)) by using a high-powered, tunable infrared laser where the interfacial heating, which is proportional to the infrared absorbance, is measured by its influence on an AFM tip. This apparatus is commercially available from ANASYS and claims ~10 nm spatial resolution. Other approaches for obtaining chemically sensitive infrared spectra for buried interfaces is to use Attenuated Total Internal Reflection methods. Another method discussed is the use of in situ contact and sliding experiments in a transmission electron microscope (TEM). Real-time, high resolution (even atomic resolution) contact and sliding can be observed, with forces and displacement measured at the nanonewton and nanometer level respectively (Y. Liao and L.

Marks. International Materials Reviews, 62, 99-115 (2017)). Spectroscopic and structural methods including electron energy loss spectroscopy, energy dispersive spectroscopy, and selected area diffraction can be performed with high spatial resolution. The use of small tips circumvents the need to prepare thin specimens with precise thinning methods as done with conventional TEM. One disadvantage is that the technique is normally confined to the high (but not ultrahigh) vacuum of the TEM environment, but environmental and liquid-cell based techniques are now emerging and being used. Another concern is the possibility of beam damage from the high voltage electrons, which requires careful control of the degree of beam exposure and conducting experiments. Finally, the TEM typically only obtains a quasi-two-dimensional profile of the contact in a transverse view; a fully three-dimensional view, or at least a view of the contact plane, would be beneficial. An alternative approach, rather than directly analyzing the buried interface, it to analyze one or both of the surfaces shortly after carrying out the tribochemical reaction (T. D. B. Jacobs, C. Greiner, K. J. Wahl, and R. W. Carpick. MRS Bulletin, 44, 478-486 (2019); W. G. Sawyer and K. J. Wahl. MRS Bulletin, 33, 1145-1150 (2008)). This can be done periodically, with sliding resumed to build up a progressive set of points of analysis throughout the evolution of the sliding contact. One must be aware that the surface can evolve after rubbing has finished, so that these results should be validated by in-situ methods. These techniques should both be surface sensitive and have reasonable spatial resolution to investigate the composition in the rubbed region. There are examples of electron-based surface techniques being used to analyze tribological interfaces such as X-ray photoelectron, Auger, and near-edge adsorption spectroscopies as well as electron microscopic techniques. These are largely in their infancy, and in many cases necessitate removing the sample from the tribometer to a remote analysis system, with the associated issues with surface contamination and time dependent changes in the nature of the surface. Addressing this issue is an important challenge. The issue of the effect of the reactive substrate was raised, and it was emphasized that the substrate has a profound role on the tribochemistry. Reactivity with the substrate has been shown to be important in the generation of tribofilms, not just in terms of ensuring that the film bonds to the substrate, but in affecting its composition and growth. Tuning the nature of the interface has recently been used to induce chemical reaction to form lubricating films directly from the base oil without the use of lubricant additives, which offers a novel approach by providing a lubricious film that can continually regenerate in situ. Finally, the complexity of the problems was emphasized with a number of the issues that might influence tribochemical activity being highlighted in Fig. 1. This also emphasized the use of model systems, and issue that we addressed by a number of Round Tables arguing that progress will be made when there is overlap between the systems that can be modeled and those on which experiments can be performed. This will require the use of simple model experimental systems and the development of theoretical approaches that can investigate more complex systems. It was also pointed out that issues cut across a large number of disciplines, and this highlights the need to form interdisciplinary teams to address these problems, and to ensure communication and education across disciplines between researchers working on tribology problems. To this end, the gathering of tribologists and non-tribologists with a range of backgrounds and with ample opportunity to discuss, debate, and deliberate through the CECAM Workshop was highly valuable, and more such opportunities should be pursued in the future. Molecular dynamics and first-principles calculations of tribochemistry: Bridging time and length scales. Simulating chemical processes occurring at the buried sliding interface is particularly challenging due to the presence of confinement and non-isotropic, time-dependent mechanical stresses, which alter the kinetics of tribochemical reactions with respect to ordinary reactions, e.g., thermally activated at the open surface or the liquid-phase or gas-phase. On the positive side, tribological conditions typically decrease reaction times to the short time scales accessible to atomistic simulations. However, this advantage is more than annihilated by the problem that thermal and mechanical boundary conditions may be extreme but not very well defined when a reaction occurs.

This entails a series of other problems: It is generally not possible to identify meaningful reaction coordinates whose construction allows a precise analysis of chemical reactions. Demands on total particle numbers are particularly large, because stresses and temperature at the reaction sites may differ substantially from those imposed near the boundaries so that these local conditions cannot simply be imposed but need to evolve (self-consistently) in a

sufficiently large simulation cell. The transferability of classical force fields is reduced because the electronic structure of a system is destabilized quite substantially under severe, tribological conditions. Last but not least, it is virtually impossible to test a force field for the many different atomistic conformations that a tribosystem adopts to. Therefore, both the electronic and ionic degrees of freedom should both be treated explicitly in an accurate simulation of tribochemistry processes. The use of first principles calculations to investigate tribochemical processes has increased significantly in the last decades. Within this approach, the effects of tribochemical modifications on the adhesion and shear strength of many solid interfaces have been identified and quantified by static DFT calculations. However, these studies focused on the effects of the reaction products, and very few studies, based on ab initio Molecular Dynamics (AIMD), have simulated the reaction activation and pathways in real time. The high computational costs of AIMD have limited its application to small systems, constituted of a few hundreds of atoms with simulation times in the range of few tens of picoseconds. Classical MD simulations based on reactive force fields, such as ReaxFF, allows to increase significantly the time and length scales compared to AIMD. However, the current ReaxFF parametrizations and potentially the unavoidable restriction of functional forms of a force field do not necessarily reproduce the changes in the compound reactivity imposed by the tribological conditions. A possible solution, combining the computational advantages of molecular mechanics (MM) with the accuracy of quantum mechanics (QM), is given by the QM/MM approach, first developed by Warshel and Levitt in 1976. In this method only the expected chemical active region is treated at a full quantum level, while the interactions in the remaining part of the simulation box are described by classical force fields. The QM/MM is nowadays widely employed for the simulation of biomolecular systems, less frequently to study mechanical properties in material science. Recently, it has been applied for the first time to simulate tribochemical processes in graphitic materials and at iron interfaces interacting with lubricant additives. The close comparison of the adopted QM/MM scheme with state-of-the-art computational methods used in tribochemistry emphasized the high potential of the hybrid method, which is as accurate as fully QM in describing tribochemical reactions, while offering the possibility to consider much larger systems without the excessive computational costs of QM dynamics. A larger size is often essential for capturing collective atomistic processes, which play a crucial role in tribochemistry. While AIMD or QM/MM simulations provide a reliable description of the chemical interactions at the sliding interface, they cannot be used to obtain quantitative estimates of the energy dissipation by friction. This is because in atomistic simulations the semi-infinite bulks that form an interface are replaced by slabs of finite thickness, which restrict the calculable wave-length of the surface phonons. Indeed, several studies have reported that energy-dissipation properties associated with phonons, such as thermal conductivity and friction, significantly depend on the size of the simulated systems. Another problematic issue is related to the pressure and temperature control in non-equilibrium conditions that are carried out using thermo- and barostat methodologies. Green's functions (GF) constitute an elegant way to overcome these limitations. For surface systems, for example, by considering a semi-infinite solid as a harmonic bath, it is possible to derive the generalized Langevin equation in which all the degrees of freedom of infinitely-large number of the solid atoms are projected onto the surface atoms in the simulation cell. By linking GF to AIMD, it is possible to realize a multiscale AIMD/GF model able to describe the reactive interface with the high accuracy of QM and to obtain at the same time the proper control of temperature, mechanical stresses and energy dissipation in non-equilibrium conditions, as granted by GF. This constitutes an outstanding advancement in the modeling of mechano-chemical systems. The whole tribochemical process that starts from molecular adsorption and leads to the formation of tribofilms occurs on a time scale that cannot be accessed within only one (hybrid) simulation. Therefore, methods such as kinetic Monte Carlo, which allow for the simulation of rare events, could be adopted to link different stages of the tribochemical process. Machine learning is also expected play an important role in the future in designing new materials and investigating tribochemical reactions. This will require key parameters that control the tribochemical reaction to be identified and a set of descriptors for these key parameters to be postulated. It is likely that such approaches will enable new materials and lubricants to be identified and will possibly enable new and unknown correlations to be found that suggest novel areas of investigation. In fact, a first study has appeared, in which different molecular architectures for

base oils were screened at a sufficiently large rate so that new molecules of unusual geometry were obtained with artificial intelligence that has a much-desired, reduced temperature sensitivity of the viscosity than existing base oils. To provide a structured format to the round-table discussion, the moderators decided to invite a group of speakers that included both experimentalists and theoreticians. The roundtable began with the moderators making some opening remarks and listing the current state-of-the-art experimental and theoretical frameworks used to develop a mechanistic understanding of the phenomena occurring in the near-surface region of coatings and thin films upon sliding and controlling their tribological response. Particular emphasis was given to the discussion of the complexity of the phenomena occurring at sliding solid/solid interfaces: the combination of mechanical forces (normal loads, shear forces), temperature fluctuations, and gradients in chemical potentials produce highly non-equilibrium conditions that can lead to phase transformations, plastic deformations, fracture events, surface and interfacial reactions, etc. It was pointed out that to gain insights into the tribological response of coatings and thin films the fundamental physical and chemical processes occurring on them should be elucidated. While significant progress has been made during the last few decades, a holistic picture of effect of interfacial phenomena in the tribology of coatings is still lacking due to their occurrence at different time- and length-scales. It was pointed out that recently several investigations highlighted the major influence of dopants and alloying elements in coatings on the tribological response. While the possibility of tuning surface properties and tribological response through the selection of the nature and contents of the dopants has attracted considerable attention, the origin of the reported improvements in friction and wear behavior has not been established yet. An additional significant challenge that was highlighted during the roundtable and in the presentations was related to the strong environmental dependence of the tribological response of coatings. Even though a number of publications has appeared in the literature on the topic, our understanding of the underpinning surface physical and chemical origin is still limited due to the difficulty of quantitatively characterizing the chemistry and structure of the first few atomic layers of materials. This is particularly true in the case of material systems that exhibit “superlubric” behavior. As pointed out several times during the conference, the advent of novel in situ tribological approaches is paving the way to the evaluation of the surface processes controlling the friction and wear response of materials at the most critical environmental conditions for the system under investigation. However, the number of in situ studies in tribology is still limited due to the difficulties involved in the development of these approaches and the required expertise. Finally, during the roundtable it was discussed the possibility of tuning the surface chemistry of the tribological systems with the aim of controlling their interactions with the environment in an effort to create tribochemical products that can aid in friction and wear reduction. This approach, first demonstrated by Erdemir et al. (Nature, 536, 67, 2016), has opened the possibility of engineering the tribological system (coating structure and chemistry, in particular) depending on the operational space of the application under consideration. While the engineering implications of this approach have been highlighted, during the roundtable it was pointed out that our understanding of the key elementary steps leading to the formation of tribochemical products (as well as the nature of the reaction layers) is very limited. Future developments hinge on shedding light on these aspects. The round-table discussion clearly underlined the fundamental role that computational approaches can have in addressing all open questions related to shear-induced mechanochemical phenomena in coatings and thin films. Significant challenges still remain, however. In particular, quantitative comparisons between modelling and experimental results were pointed out to still be very challenging, which calls for future developments of versatile multiscale tools dedicated to tribology. To this end, the importance of having simple model systems able to be simulated and experimentally investigated effectively was also discussed in detail. The interactions between experts in tribology, surface science, surface physics and chemistry, catalysis offered through conferences such as the CECAM Workshop constitute a pivotal step in tackling all questions that are still open in the evaluation of the friction and wear response of coatings and beyond. Challenges Towards the Scaling Up of Structural Superlubricity Two dimensional (2D) layered materials have become the crown jewel of materials research in recent years, starting with the synthesis of graphene, a single layer form of graphite, by the mechanical exfoliation method in late 2004. Since then, 2D materials are

probably the most studied systems within the condensed matter and materials science communities, due to their unusual properties. To date, the studying and understanding of their exotic properties shed light on fundamental physical phenomena and their remarkable electronic and mechanical properties led to the rising of novel technological applications. Such fundamental physical aspects and potential technological applications of layered materials in general and graphene in particular are found in the field of tribology - the science of friction, wear, and lubrication. Friction is a fundamental phenomenon, which occurs over a very large range of scales ranging from the macroscopic world down to the nanoscale. For example, the frictional forces occurring between the tires of our car and the road surface are very important in order to have a safe drive, but on the other hand, it is necessary to reduce friction between the piston walls inside the engine in order to avoid wear and energy loss. Hence, by controlling friction, we can save energy as well as avoid the wear of machine parts. In fact, it is estimated that ~5% of energy loss in modern times is caused by heat dissipation due to frictional forces between moving parts. Hence, understanding and controlling the friction extremely important. In recent years, tribological properties of homogeneous and heterogeneous nanoscale two-dimensional (2D) material interfaces consisting mainly of graphene, boron-nitride, and 2D transition metal dichalcogenides, have been the subject of numerous studies. At such reduced scales friction does not obey the classical macroscopic Amontons-da Vinci description and new intricate physical phenomena arise due to atomic- and molecular-scale interactions. One of the most intriguing frictional phenomena found at the nanoscale is structural superlubricity. Here, two rigid layers, who's crystal lattices are incommensurate, slide atop each other with negligible friction. Apart from the important fundamental physical aspects of this effect, the vast technological implication that it holds may revolutionize the way we comprehend mechanical friction and wear and have a huge impact on society via the reduction of energy loss and mechanical wear. In the 16 years that have passed from its first demonstration on nanoscale graphitic interfaces, structural superlubricity has been scaled-up to microscale interfaces. While this opens the way for applications in the field of micro-electromechanical systems, broad impact will be achieved only when the effect will be demonstrated in macroscopic interfaces. This, in turn, opens a whole new set of challenges that require careful attention. At the focus of the round-table discussion during the CECAM meeting was the identification of such issues, their grading in terms of urgency and importance to the scaling-up of structural superlubricity, and suggestion of research route to identify ways to overcome them towards the goal of achieving macroscopic superlubric interfaces. The following aspects of structural superlubricity scale-up were mentioned and noted (Fig. 2):

1. Effects of structural defects
2. Chemical contaminants
3. Grain boundaries and edge effects
4. Surface roughness
5. Mechanical failure and layer rupture
6. Adhesion of the 2D stack to the underlying substrate.

It is therefore evident that in order to provide a realistic description of frictional and tribo-chemical properties of 2D systems at the macroscale a multi-scale approach is required. First, an atomic/molecular level understanding is required. This can be achieved by performing quantum mechanical calculations using density functional theory on pristine nanoscopic interfaces. With this respect, for the proper description of 2D materials interfaces, dispersion corrections must be taken into account. The results of such calculations may serve as input for the construction of efficient dedicated force-fields that can simulate the dynamical properties of larger scale material interfaces that include structural defects, grain boundaries, edges, and chemical contaminants. Finally, in order to treat even larger-scale effects, such as surface roughness and rupture, and how external load affects the frictional properties of macroscopic 2D material interfaces, coarse-grained models have to be developed, based on the input from atomistic molecular dynamics simulations. The quest for scaling-up structural superlubricity is, therefore, extremely challenging and requires a joint and coordinated theoretical, computational, and experimental effort. In our round-table discussion we have focused on identifying the main challenges and marking the computational route to attack them. Further discussion is required on how to synergistically connect such investigations to experimental efforts in this field. Achieving the goal of scaling-up superlubricity towards the

macroscopic world is expected to have a huge impact on society. Hence, it is highly desirable that the tribological community in general and the superlubricity sub-community in particular will invest vast efforts in this direction.

3 Community needs

It is clear from the “Major Outcomes” section that there is a need for modern analytical equipment that can investigate buried, sliding interfaces under well-controlled conditions. That invariably means controlled environments in which the nature of the sliding interface is well known so that it is amenable to precise theoretical analyses. This often means an ultrahigh vacuum environment and the most precise tribological experiments are carried out using such apparatus, which is expensive. Indeed, one of the major conclusions from the workshop is the need for overlap between experiment and theory that will require precise results on well-defined model systems that are amenable to analysis using high-level theory.

4 Funding

The availability of funding of the tribology/tribochemistry community depend to some extent on the region. In the United States, the funding for experimental tribology is bleak. The National Science Foundation did have a division in the Engineering directorate that was devoted to the study of tribology and funding from that area made significant advances. This was however subsumed into Advanced manufacturing and no longer specifically funds projects on tribology. In Europe, the picture seems to be somewhat better, where there tends to be more industrial support for tribology from oil, energy and lubricant companies, although funding from national governments still tends to be sparse.

5 Will these developments bring societal benefits?

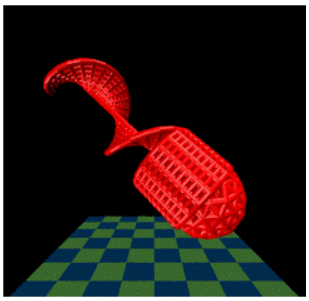
Improvements in the area of tribochemistry and the design of model films can lead to significant saving in energy and a concomitant improvement in the environment. A recent report commission by ARPE-E in the United State indicate that the annual energy consumption in the U.S. has hovered near 100 quads (1 quad = 1015Btu = 1018 J) over the past few years. A substantial amount of this energy is not only not useful but actually lost due to friction and wear. For instance, the transportation sector consumed more than 26 quads of energy in 2014, a third of which is used to overcome frictional losses. Fifty years ago in March 1966, Sir Peter Jost analyzed the state of lubrication research in the UK and estimated potential savings of £515 million per year, equivalent to 1.3% of the UK’s GDP that year and similar conclusions were arrived at in Germany, Canada and China. The consensus was that savings between 1.0 to 1.4 % of a country’s GDP may be achieved through research and development expenditure on the order of 1/50th of the savings (e.g., $1 toward research saves $50 over the course of the following year). The ideas discussed in this CECAM workshop are that the heart of research to achieve such savings.

6 Participant list

Organizers

Lorenz, Chris
King's College London, United Kingdom
Righi, M. Clelia
University of Modena and Reggio Emilia and CNR-Nano, Italy
Tysoe, Eddy
University of Wisconsin-Milwaukee, United States

Bennewitz, Roland - Leibniz Institute of New Materials (INM), Saarbrücken, Germany
Carpick, Robert - University of Pennsylvania, Philadelphia, USA, United States
Chandross, Michael - Sandia National Laboratories, United States
Cobian, Manuel - Laboratoire de Tribologie et Dynamique des Systèmes - LTDS, France
Dini, Daniele - Imperial College London, United Kingdom
Erdemir, Ali - Argonne National Laboratory, Turkey
Ewen, James - Imperial College London, United Kingdom
Ferrario, Mauro - University of Modena and Reggio Emilia, Italy
Frenken, Joost - Advanced Research Center for Nanolithography & University of Amsterdam, Netherlands
Glatzel, Thilo - University of Basel, Switzerland
Gulseren, Oguz - Bilkent University, Turkey
Hod, Oded - Tel Aviv University, Israel
Kajita, Seiji - Toyota Central R&D Labs, Japan
Loehle, Sophie - Total Marketing Services, France
Losi, Gabriele - University of Modena and Reggio Emilia, Italy
Mangolini, Filippo - The University of Texas at Austin, United States
Martin, Jean-Michel - Ecole Centrale de Lyon, France
Mathas, Dimitrios - University of Southampton, United Kingdom
Meuwly, M. - Univ. Basel, Switzerland
Molinari, Jean-François - EPFL, Lausanne, Switzerland
Moseler, Michael - Fraunhofer IWM, Germany
Muser, Martin - Saarland University, Germany
Nicolini, Paolo - Czech Technical University In Prague, Czech Republic
Peeters, Stefan - University of Modena and Reggio Emilia, Italy
Polcar, Tomas - University of Southampton, United Kingdom
Romero, Pedro Antonio - Freudenberg, Germany
Spencer, Nicholas - ETHZ, Switzerland
Stella, Martina - Imperial College London, United Kingdom
Turner, Christoffer - The University of Alabama, United States
Weber, Bart - University of Amsterdam, Netherlands



Frontiers in Computational Methods for Active Matter

Location: CECAM-HQ
Webpage: https://www.cecam.org/workshop-details/87
Dates: Feb 10, 2020 - Feb 12, 2020

1 State of the art

Non-equilibrium dynamics and emergent collective phenomena in active matter have received considerable attention in physics and biology. Active matter systems consume energy, convert it into directed motion, and drive themselves far from equilibrium. Active matter in biology is found on broad scales ranging from molecular motors and swarming bacterial colonies to schooling fish and flocking birds. Formation of dissipative evolving structures in the steady-state, clustering, swarming, phase separation, and giant number fluctuations are examples of emerging collective behavior and self-organization in systems of active particles. To understand the dynamics of active matter one deals with self-moving units, their interactions, and their collective dynamics. While the particle activity is sufficient to explain the underlying mechanisms of self-organization in some cases, hydrodynamic interactions in aqueous (biological) environments and interactions with boundaries play a key role in general. A major current challenge in active matter is to predict the emerging structures or to perform the desired functions, for given components and initial and boundary conditions. The first steps naturally involve developing minimal model systems which are experimentally controllable, to identify the fundamental governing laws. This would then facilitate the design of more complicated systems of components which self-organize themselves towards the desired forms and structures.

2 Major outcomes

In the workshop, a variety of numerical methods that have been used to model active matter systems were presented and recent advances in computational techniques and the most recent ideas and concepts of active matter theory were discussed. Some of the major challenges arising in modeling active systems are: (i) Active matter is a multiscale material similar to other complex fluids such as milk or blood, (ii) Active fluids are intrinsically out of equilibrium due to energy consumption on microscopic scale, (iii) The interactions between active particles can be highly nonlinear and are often of multibody character (e.g. hydrodynamic interactions or interactions due to chemical stimuli), (iv) Active particles are mostly not simple geometrical objects, such as hard spheres, but rather of complex shape due to propulsion and other functional units. So far, a variety of system-specific methods with different levels of resolution, ranging from micro- to macroscale, have been developed and employed. For example, active Brownian dynamics and partial differential equations (PDE) (such as generalized Navier Stokes equations), have been used to model active fluids in a very coarse-grained way. However, coarse gaining of active systems in not trivial and modification of microscopic details can strongly alter the macroscopic behavior. For example, it is unclear how particle-wall and particle-particle interactions translate into proper boundary conditions and transport coefficients of the corresponding macroscale PDE. On the other hand, mesoscale techniques (e.g., lattice Boltzmann method) try to bridge different length and time scales and to model properly the hydrodynamic interaction between active particles. However, these techniques have to compromise strongly between microscopic accuracy and macroscopic system size. Another point is that the existing techniques need to be further developed to cope with real-world applications. For example, the typical environment for micro-organisms is not a simple fluid but rather a suspension of extracellular polymeric

substances (e.g., proteins, lipids and DNA), which can strongly influence the motility and interactions of the moving objects. Another long-term goal for the modeling of biological active matter is to include the adaptive behavior of micro-organisms, i.e., the ability to detect and to respond to different stimuli such as material properties of the surrounding (durotaxis) or chemical concentrations (chemotaxis or quorum sensing), which requires a coupling between intracellular and extracellular models.

3 Community needs

Despite the developments in numerical techniques and improvements in the efficiency of simulation methods, one frequently deals with time consuming simulations of multibody nonlinear interactions on various time and length scales, which necessitates further investment on high-performance computing infrastructure. It would be also helpful to share the methods and techniques that are developed in various research groups to save time and to achieve comprehensive open software solutions. As the field is currently of broad interest and there are continuously new developments in computational techniques, ideas and concepts of active matter theory, follow-up workshops on similar topics should be organized in the near future.

4 Funding

Typically, funding is provided by the home universities of the individual participants and national institutions, such as German Research Foundation (DFG, Germany) or the National Science Foundation (NSF, USA). For example, this workshop was co-financed by the Collaborative Research Center SFB 1027 (“Physical modeling of non-equilibrium processes in biological systems”), which is funded by the DFG. To facilitate international collaborations, supranational or bilateral funding channels are highly desired, and several invited speakers discussed the possibility of joint research proposals.

5 Will these developments bring societal benefits?

The understanding of active matter systems is not only of interest for a broad scientific community, including physics, chemistry, biology, and medicine, but also for the society as a whole due to a possible emergence of promising new technologies. For example, it sounds a bit like science fiction but medical microrobots with potential targeted immunotherapeutic applications have been released recently. Without theoretical investigations and computer simulations of microswimmers a fabrication of such a microrobotic system would not be possible. Also, active transport through microfluidic devices and nanopores is of great interest in various industrial applications. The broad range of emerging collective behavior and self-organization in active biological systems indicates that investigation of such phenomena eventually leads to a fundamental understanding of the behavior of living systems.

6 Participant list

Organizers

Rieger, Heiko
Saarland University, Germany
Shaebani, Reza
Saarland University, Germany
Wysocki , Adam M
Saarland University, Germany

Bardfalvy, Dora - Lund University, Sweden
Chakraborty, Shauri - Saarland University, Germany
Doostmohammadi, Amin - University of Copenhagen, Denmark
Elgeti, Jens - Forschungszentrum Jülich, Germany
Fraden, Seth - Brandeis University, United States
Gompper, Gerhard - Forschungszentrum Jülich, Germany
Hagan, Michael - Brandeis University, Waltham, United States
Kafri, Yariv - Technion - Israel Institute of Technology, Israel
Lewis, Jason - Lund University, Sweden
Liberati, Diego - National Research Council of Italy @ Polytechnic University, Italy
Löwen, Hartmut - University of Duesseldorf, Germany
Mangeat, Matthieu - Saarland University, Germany
Michelin, Sebastien - Ecole Polytechnique, France
Monzon, Gina - Saarland University, Germany
Noh, Jae Dong - University of Seoul, Republic of Korea
Nordanger, Henrik - Lund University, Sweden
Pagonabarraga, Ignacio - CECAM HQ, Switzerland
Peruani, Fernando - Université Nice Sophia Antipolis, France
Pöschel, Thorsten - Universität Erlangen-Nuernberg, Germany
Sadjadi, Zeinab - Saarland University, Germany
Santen, Ludger - Saarland University, Germany
Sesé Sansa, Elena - EPFL, Switzerland
Slomka, Jonasz - ETHZ, Switzerland
Stark, Holger - Technische Universität Berlin, Germany
Stenhammar, Joakim - Lund University, Sweden
Sussman, Daniel - Emory University, United States
Winkler, Roland G. - Forschungszentrum Jülich, Germany
Wittkowski, Raphael - University of Münster, Germany
Yeomans, Julia - Oxford University, United Kingdom
Ziebert, Falko - Ruprecht-Karls-Universität Heidelberg, Germany
Zimmermann, Monika - ETHZ, Switzerland

Digital Event - Open Databases Integration for Materials Design

Location: Online, coordinated by CECAM-HQ
Webpage: https://www.cecam.org/workshop-details/991
Dates: Jun 8, 2020 - Jun 12, 2020

1 State of the art

Materials design has changed quite dramatically in the last few years. Thanks to the increase of computing power, large sets of first-principles calculations can be performed automatically adopting a high-throughput (HT) approach. Large databases (DBs) can then be created with the calculated properties for existing and hypothetical materials. These DBs can further be interrogated, and machine-learning models trained, discovering materials with desired properties. Experimental databases can then provide means for comparing theory and experiment.
In this framework, various DBs have appeared online (such as AFlow, COD, Materials Cloud, Materials Project, NOMAD, and OQMD etc.). In some of those cases, a Representational State Transfer (REST) Application Program Interface (API) is available to interrogate the DB through scripts. However, so far, it is only possible to interrogate one DB at a time and the APIs are very different from one DB to another. The OPTIMADE workshop gathered all the key players involved in these different efforts with the aim to continue to develop a common API.
The present workshop has built upon the achievements of three previous meetings held at the Lorentz Center in Leiden, Netherlands from 2016-10-24 to 2016-10-28, and at the CECAM in Lausanne, Switzerland from 2018-06-11 to 2018-06-15 and from 2019-06-11 to 2019-06-14. This work has been continued at the present CECAM meeting with a special focus on reaching out to new communities (such as molecular dynamics and bio-simulations).

2 Major outcomes

Building on the results achieved in the previous OPTIMADE workshops and subsequent discussions on the OPTIMADE mailing list, the present workshop continued to make the various DBs interoperational through the development of the OPTIMADE API and implementations of it. Furthermore, the workshop was meant to try to increase the extent of the OPTIMADE API by reaching out to other communities.
The digital events comprised two plenary meetings per day (one in the morning and one in the afternoon) in order to gather as many people around the globe as possible (given the time difference), and small-group sessions in between and after the plenary meetings. The first plenary meeting consisted of a series of brief presentations (elevator pitches of 2 minutes) during which the participants to the previous OPTIMADE meetings discussed the state of their implementations. Most of the other plenary meetings consisted of longer presentations by members of other communities. Among others, talks were given by representatives of the new databases, who discussed how the OPTIMADE API could be useful for their databases (focusing on what is currently missing). Finally, some of the plenary meetings were dedicated to general discussions in which one representative of the different small groups would present what had been achieved in their group and gather the opinion of the rest of the attendees. Then, depending on the results of the discussions, new groups would be formed in order either to continue to advance on the topic or to start a new topic.
The small-group sessions were dedicated to focused discussions. One of them was about the OPTIMADE Python tools for which tutorials were first proposed to the newcomers and then further improvements were made. All the talks and the tutorials were recorded and are

available through a dedicated OPTIMADE YouTube channel. Another one focused on the definition of materials and properties. The discussions were so intense that it was decided to continue them after the workshop into a dedicated working group about the definition of an ontology for materials.
In fact, many very fruitful discussions took place (both during the plenary and small-group sessions). Many improvements (this can be measured by the number of pull requests in the OPTIMADE GitHub repository) were adopted for the existing OPTIMADE API. The new specification was finalized a few weeks after the end of the workshop. And, at the beginning of July, version 1.0 was released. During the workshop, the writing of a paper has continued on Overleaf and we hope to be able to submit it within a few months.
The OPTIMADE workshop can definitely be considered a success since very important improvements were achieved for the common API and its actual implementation. A series of implementations are now available (even if some only have a partial implementation of the API) and there is even an online OPTIMADE aggregator. More importantly, very tight connections have been established between the different projects and new projects have been incorporated. The participants really appreciated the workshop and indicated that the chosen online tools had been key to its success.

3 Community needs

The common OPTIMADE API will clearly benefit materials design by making it possible to interrogate all the databases using the same query. The OPTIMADE API will also contribute to making all these data FAIR (Findable, Accessible, Interoperable, and Reusable). The effort that has been started is therefore important and could have really high impact.
The OPTIMADE effort should definitely be continued, trying to involve as many important players as possible. For example, at the present CECAM workshop, we welcomed developers from the Jarvis, OMDB, HybriD3, and OpenKIM databases and some of them have already started implementing the OPTIMADE API to query their database.
It is important to maintain this community with a common target (the OPTIMADE API) that will be beneficial for the community. Furthermore, the links that have been created among the different persons can also serve a different purpose. Indeed, there has already been discussion about the possibility to use the same community to define some standards and an ontology for materials. Moreover, since the meeting gathers an important number of players in the field, this number can be used as leverage to push towards the adoption of a standard.
For all the reasons above, we believe that the OPTIMADE API effort should be continued. We hope that the CECAM will continue to support the organization of this series of workshops.

4 Funding

Since last year, strong links have been established with the European Materials Modeling Council. In particular, they indicated a strong interest about the OPTIMADE API that is clearly in line with their objectives.
Various members of the OPTIMADE community participate to some of the boards of the European Materials Modeling Council. This clearly opens some possible funding schemes at the European level. Indeed, the European Materials Modeling presently benefits from a Coordination and Support Action (CSA) from the EU which started in November 2016. There are plans to submit a new proposal when an appropriate call is made. OPTIMADE could join when this happens.

5 Will these developments bring societal benefits?

Materials design has clearly a great impact on society. Many new applications require specific materials with targeted properties. Furthermore, improving the efficiency of existing technologies (e.g., denser batteries, photovoltaics, faster computers, ...) also benefits from the design of materials with better properties.

The development of the OPTIMADE API can clearly contribute to making materials design easier. Indeed, the users will be able to interrogate many different databases with the same query. This will give them access to such more materials knowledge without the need to learn a different API for each database. Furthermore, machine learning methods can source information from multiple databases. The OPTIMADE API will also avoid the replication of calculations by different databases allowing them to spend resources broadening the bounds of materials knowledge.
The social benefit is thus present, though it is indirect in the sense that the OPTIMADE API is a tool that will clearly contribute to making it easier to design materials that provide benefits to society.

6 Participant list

Organizers

Armiento, Rickard
Linköping University, Sweden
Conduit, Gareth
University of Cambridge, United Kingdom
Gražulis, Saulius
Vilnius University Life Science Center Institute of Biotechnology, Lithuania
Pizzi, Giovanni
EPFL, Switzerland
Rignanese, Gian-Marco
Université Catholique de Louvain, Belgium
Scheidgen, Markus
Humboldt-Universität zu Berlin, Germany
Toher, Cormac
Duke University, United States

Andersen, Casper - EPFL, Switzerland
Bazhirov, Timur - Https://exabyte.io, United States
Bereau, Tristan - University of Amsterdam, Netherlands
Björkman, Torbjörn - Åbo Akademi University, Finland
Blokhin, Evgeny - Tilde Materials Informatics, Germany
Blum, Volker - Duke University, United States
Bonella, Sara - CECAM HQ, Switzerland
Choudhary, Kamal - National Institute of Standards and Technology, United States
Di Stefano, Davide - Ansys UK, United Kingdom
Draxl, Claudia - Humboldt-Universität zu Berlin, Germany
Dwaraknath, Shyam - Lawrence Berkeley Lab, United States
Evans, Matthew - UCLouvain, Belgium
Fekete, Adam - Université Catholique de Louvain, Belgium
Geilhufe, Matthias - Nordita, Sweden
Gopakumar, Abhijith - Northwestern University, United States
Horton, Matthew - Lawrence Berkeley National Laboratory, United States
Huck, Patrick - Lawrence Berkeley National Lab, United States
Katsura, Yukari - The University of Tokyo, Japan
Kumagai, Saori - Starrydata, Japan
Kumagai, Masaya - Kyoto University, Japan
Ladines, Alvin Noe - Humboldt University, Germany
Laio, Alessandro - SISSA, Italy
Lambrix, Patrick - Linköping University, Sweden
Leitherer, Andreas - Fritz Haber Institute of the Max Planck Society, Germany
Lenz-Himmer, Maja-Olivia - Fritz Haber Institute of the MPG, Germany
Li, Huanyu - Linköping University, Sweden

Lysogorskiy, Yury - ICAMS, Ruhr University Bochum, Germany
Marzari, Nicola - EPFL, Switzerland
Merkys, Andrius - Vilnius University Institute of Biotechnology, Lithuania
Minamoto, Satoshi - National Institute for Materials Science (NIMS), Japan
Mostofi, Arash - Imperial College London, United Kingdom
Oses, Corey - Duke University, United States
Parackal, Abhijith S - Linköping University, Sweden
Purcell, Thomas - Fritz Haber Institute, Germany
Tadmor, Ellad - University of Minnesta, United States
Talirz, Leopold - EPFL, Switzerland
Uhrin, Martin - Danish Technical University, Denmark
Van Setten, Michiel - Imec, Belgium

GW goes large-scale

Location: Online, coordinated by CECAM-FI
Webpage: https://www.cecam.org/workshop-details/66
Dates: Jun 8, 2020 - Jun 10, 2020

1 State of the art

Since its proposal by Hedin in 1965, the GW approximation in Green's function theory has become the method of choice to calculate theoretical photoemission spectra for weakly to moderately correlated systems. GW is based on the many-body Green's function formalism, which gives it formal backing to compute excited states. By neglecting a certain class of Feynman diagrams, the GW approximation is computationally tractable for systems with >100 electrons. Computational and algorithmic advances for GW calculations have come rapidly over the past two decades, but some technical issues remain.
GW has been extremely successful as an applied method thanks to efficient computational implementations and large supercomputers. Continued investment in supercomputing shows that this trend will only continue, as the EU's first pre-exascale computing platform Lumi is coming online in 2021 in Finland. The actual properties computed with GW (quasiparticle energies and photoemission spectra, mainly) and its physics are highly relevant for many important applications and research programs including photovoltaics, two-dimensional materials, interfaces, catalysis, and embedding theories for strongly-correlated solids. A common theme of modern GW calculations is application to large systems, whether by numerical brute force on pre-exascale machines or with new algorithms to lower the computational cost.
In this workshop (GW Goes Large-Scale, or GW-XL), we focused on developments for large-scale GW calculations to ensure that GW can continue to be applied to ever larger systems. Developments ***are*** necessary for exascale computing: many exascale machines will be GPU dominated, for example, which is a different programming paradigm altogether than normal GW codes. Other algorithmic improvements based on physical embedding, prefactor reduction, or scaling reduction are also important. We welcomed all types of large-scale GW to the workshop.

Key References

[1] L. Hedin, Phys. Rev. ***139****, A796 (1965)*
[2] D. Golze, M. Dvorak, P. Rinke, Front. Chem., ***7****, (2019)*

2 Major outcomes

We had an excellent set of invited and contributed speakers and poster presenters for our workshop. Our workshop was meant as an in-person workshop in Helsinki but shifted to virtual because of the COVID-19 pandemic, making it one of the first virtual CECAM workshops ever. GW-XL still had excellent enthusiasm, lively discussions, and networking even in its virtual format. We learned a great deal about the organization of virtual workshops that we can pass on to CECAM to help organize future events. The number of technical issues was very low, and participants enjoyed the format overall.
One topic which appeared multiple times during the workshop was the "space-time" method of GW originally developed in 1995 by Rojas, Godby, and Needs (*PRL* **74**, 1827 (1995)). In the space-time method, the polarization is computed in real space and imaginary time. This decouples the occupied and empty states that enter the sum for the polarization and reduces, in combination with sparsity/locality schemes, the scaling from $O(N^4)$ to $O(N^2)$ with respect to system size N. The subsequent steps scale at most with $O(N^3)$ complexity. It has been implemented in VASP (PRB, 94, 165109 (2016)), CP2K (JPCL, 9, 306 (2018)), Fiesta (JCP, 150, 174120 (2019)) and most recently also in ADF (arXiv:2007.01581, 2020). System sizes

with more than 1000 atoms (JPCL, 9, 306 (2018)) have been already computed with low-scaling codes. However, restoring the accuracy of the canonical implementations remains still a challenge and is part of ongoing work, which has been also discussed in the talks (e.g. Jan Wilhelm (CP2K), Arno Förster (ADF)).
We heard about new GPU implementations from the Yambo and BerkeleyGW developers (Andrea Ferretti and Mauro del Ben, respectively). Both of these GW codes already offer substantial support for GPU calculations and their presentations generated a lot of interest. While the number of GPU implementations remains low overall, the interest in these talks and the future of high-performance computing suggest that a GPU specialized event would be valuable.
A couple of speakers discussed new embedding or downfolding methods applied to GW or its extension to optical excitations, the Bethe-Salpeter equation (BSE). In particular, Xavier Blase presented a combined quantum and classical mechanics method to incorporate a surrounding dielectric medium into the GW calculation. This polarizable medium approach substantially increases the feasible system size while maintaining good accuracy. Diana Qiu discussed a downfolding method for calculating optical excitations of amorphous materials in a reduced space. These downfolding methods are similar to each other, in principle, and efficient tools for increasing system size.
A couple of talks and several posters included applications of GW to organic crystals, core levels, and amorphous materials.
We received several talks addressing reducing the computational complexity of GW (lowering the scaling exponent). Contributions from the CP2k package focused on matrix sparsity and tensor contractions to reduce their GW scaling from the N^4 of canonical GW to somewhere between N^2 and N^3. A different approach based on stochastic sampling, discussed by Vojtech Vlcek, reduces the scaling all the way to N.
There were contributions about GW development in solids, the original testbed of the theory, from Xinguo Ren and Georg Kresse. These technical talks focused on the optimization of time and frequency grids for finite temperature calculations and the implementation of periodic GW in a local basis.
Finally, certain presentations showcased impressively large GW calculations on up to 500 000 CPUs, truly putting the XL in GW-XL.

3 Community needs

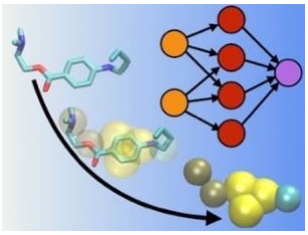
The greatest need for the GW community is developing and sharing expertise in GPU implementations. Many aspects of numerical development covered at the workshop are being carried out successfully and independently by different groups (embedding, scaling reduction, massive parallelization). GPU computing, however, remains the greatest counterexample, with expertise still fairly localized. It is clear that GPU computing is the way of the future, so this expertise must be broadened.
This is certainly a more general issue than for only GW calculations. Scientific computing, in general, apparently needs to move to GPU computing. A general series of workshops about scientific computing on GPUs by CECAM would be beneficial (this may already exist; we do not know). In the GW context, however, it may be possible at this early stage to develop libraries or at least share algorithms that are specific to GW and common to essentially all implementations. A specialized GPU algorithms workshop for GW would be one possibility.
At the same time, increased access to GPUs is necessary for developing these algorithms. The more GPU access code developers can get before the exascale machines arrive, the better. For the purpose of developing code and learning GPU programming, even small development clusters or single nodes within research groups are useful. Single nodes provide the minimal hardware to learn skills that will translate quite directly to exascale machines.

4 Funding

Electronic structure theory is usually well represented in international and national funding calls including ERC grants at all levels, US Department of Energy funding, and national agencies like Academy of Finland or Deutsche Forschungsgemeinschaft (DFG). GW development and applications fit into these calls. A potential new source of funding is the HPC Europa-3 program, which funds research visits for collaboration in high performance computing. HPC europa is excellent source of "small" funding that workshop participants could use to form real collaborations. To our knowledge, no joint research proposals were discussed during the meeting.

5 Will these developments bring societal benefits?

Electronic structure theory is relevant to many technological applications that are major consumers or sources of energy. Improvements in their efficiencies can then reduce the world's energy consumption and create a more sustainable society.
Light emitting diodes (LEDs), photovoltaics, and catalysts are a few examples. The band gap of InN was partly understood with GW calculations (Appl. Phys. Lett. **89**, 161919 (2006)), which helped pave the way for modern LEDs based on InGaN alloys. Currently, hybrid perovskite solar cells are rapidly rising in popularity because of their good efficiency. A large number of theoretical studies based on GW are helping elucidate the electronic structure of these materials, which can ultimately lead to improved device performance and cleaner energy. There is also recent interest in GW applied to aqueous systems. An improved understanding of aqueous chemistry can have far reaching implications in medicine and biochemistry.
There is also the overall benefit of increasing expertise in scientific computing, especially with exascale computers in mind. As we have discussed, exascale computing is largely based on GPUs. Disseminating GPU methods to different research groups can have a broader effect of increasing overall scientific computing competence, which will then spread to all fields as workshop participants share these ideas with their home institutions.



(Machine) learning how to coarse-grain

Location: Online, coordinated by CECAM-DE-SMSM
Webpage: https://www.cecam.org/workshop-details/26
Dates: Sep 28, 2020 - Sep 29, 2020

1 State of the art

Coarse-grained (CG) models aim at a reduced description of a molecular system, offering not only practical benefits, such as significant computational advantages, but also the means to effectively test what subset of degrees of freedom and interactions are sufficient to describe physical processes of interest. While the last few decades have yielded significant advances in the development of coarse-grained models--from foundational considerations to practical force-field parametrization algorithms and methods--a number of strong assumptions the community makes has plagued its further development. For instance, the persistent description of nonbonded interactions in terms of pairwise functions alone puts a severe bound on the quality of these models, ultimately sacrificing accuracy and transferability.
Machine learning (ML) models--a class of statistical models that systematically improve with increased training data--have recently percolated in many areas of science as a novel powerful tool. While significant developments have been made in the context of applying ML in chemistry and materials science as a way to speed-up computationally-expensive quantum-chemistry calculations, the progress for CG models has been much more limited, due in part to a lack of improved computational scaling. While the development of CG force fields, using either kernels or neural networks, have been demonstrated, there is still a need to address more complex systems and computational efficiency.
The purpose of this workshop was to discuss the current state of the art, some of the challenges that the community is facing in furthering the penetration of ML models in CG simulations, and future perspectives. A number of timely topics were addressed during the workshop:

- Computational efficiency and scaling
- Where do we get ahead from traditional force fields? What is the most efficient way of including fundamental symmetries which reduce the amount of data needed? Can we use data-driven methods to build transferable models across chemistry?
- The systematic optimization of mappings from All Atoms (AA) to CG
- Can ML models link scales more systematically by, i.e., bridging ML ideas such as auto-encoders and dimensionality reduction with coarse-grained variables?
- Configurational generators for dense systems

Using ML CG models, can we think of novel ways to generate equilibrium molecular configurations to sample conformational space?
This workshop was established as a satellite meeting of the TRR146 Conference 2020 “Multiscale simulations of soft matter: New method developments and mathematical foundations” taking place from Sept 30 to Oct 2, 2020. Both events have taken place online.
For key references, see our original submission.

2 Major outcomes

On an organizational perspective, the pandemic had initially motivated us to do a hybrid online/in-presence format, but the current situation made it difficult to have any in-presence aspect. It was thus fully online. As such:

- We did not use any funding.
- Instead of having ~30 participants, we opened up the workshop to anyone interested. The excitement around machine learning and multiscale / coarse-grained modeling

has led to the registration of 260+ participants. During the meeting, we had between 140 and 200 participants connected at any time. The lack of in-presence social interactions was offset by the outreach of the workshop to a broad community of scientists, many of whom would not have been able to participate in the in-presence format (e.g., too far, too expensive, or meeting full).

- We relied on a combination of Zoom for talks, using a Zoom webinar paid for by the TRR Consortium (Friederike Schmid, Uni Mainz) to host scientific talks and take questions live. In parallel we set up a (freely available) Discord server to facilitate discussion between the participants and the speakers. You can access the Discord server of our workshop at this address: https://discord.gg/5bHN2rx. The Discord made it easy for speakers to share additional relevant information about their work, and participants to directly interact with them. The Discord server also offered voice channels, for small batches (up to 5 for us) participants to speak with audio/video together, as if they were standing around a coffee table. Overall, we received plenty of feedback telling us that the Discord server helped create some collegial interactions among participants.
- We've generally received very positive feedback on the format, given the circumstances, mostly via private communication. See also this tweet from Michele Ceriotti: https://twitter.com/COSMO_EPFL/status/1311368693356650503?s=20

From a scientific perspective, speakers gave us an update on the state of the art, mostly describing recent publications on the topic. The large audience had 2 implications:

- Speakers were less inclined to disclose unpublished work.
- We did not find easy solutions to conduct intense live discussion, at least within the speakers. Some actually did spontaneously do so in the Discord, even leading to sharing some data sets. The speakers involved seemed very excited about the opportunity to connect and potentially spark new research from that medium.

3 Community needs

We've found the scope of Machine learning in molecular simulations to spark much interest. It is clear that the community at large would like to see more of them. It's also clear that a number of participants were looking for more introductory, tutorial-like formats, which we were not covering. It is clear that more workshops and tutorials on the use of machine learning in multiscale molecular simulations will grow.

4 Funding

No funding was discussed during the meeting.

5 Will these developments bring societal benefits?

Clearly yes, machine learning is having significant impact in all fields, including boosting the use of molecular simulations in industry.

6 Participant list

Organizers

Andrienko, Denis
Max Planck Institute for Polymer Research, Germany
Bereau, Tristan
University of Amsterdam, Netherlands

Addicoat, Matthew - Nottingham Trent University, United Kingdom
Afshar Ghahremani, Fatemeh - University of Tehran, Iran
Akkermans, Reinier - Dassault Systèmes, United Kingdom
Alessandri, Riccardo - University of Chicago, United States
Alibakhshi, Amin - Ruhr University of Bochum, Germany
Amando De Barros, Júlio - University of Sao Paulo, Brazil
Antonini Bertolazzo, Andressa - University of Utah, United States
Arya, Gaurav - Duke University, United States
Avula, Nikhil - Jawaharlal Nehru Centre for Advanced Scientific Research, India
Badin, Matej - SISSA; Comenius University, Italy
Banerjee, Atreyee - Max Planck Institute for Polymer Research, Germany
Baptista Dos Santos, Luis Andre - Max Plank Institute for Polymer Research, Germany
Barcaro, Giovanni - CNR-IPCF, Italy
Barilone, Jessica - Institute of Photonics and Electronics, Czech Republic
Behera, Sudarshan - Jawaharlal Nehru Centre for Advanced Scietific Research, India
Behler, Jörg - Universität Göttingen, Germany
Bendandi, Artemi - University of Zurich, Switzerland
Bernhardt, Marvin - Technical University of Darmstadt, Germany
Boehm, Belinda - The University of Adelaide, Australia
Bolhuis, Peter - University of Amsterdam, Netherlands
Bombarelli, Rafa Gomez - MIT, United States
Bozkurt Varolgunes, Yasemin - Max Planck Institute for Polymer Research, Germany
Brancolini, Giorgia - CNR NANO, Italy
Brennan, John - U.S. Army Research Laboratory, United States
Brotzakis, Faidon - University of Cambridge, United Kingdom
Brunk, Aaron - Johannes Gutenberg University, Germany
Caceres-Delpiano, Javier - Protera Biosciences, Chile
Campomanes, Pablo - University of Fribourg, Switzerland
Campos-Villalobos, Gerardo - Utrecht University, Netherlands
Caylak, Onur - Eindhoven University of Technology, Netherlands
Ceriotti, Michele - Swiss Federal Institutes of Technology Lausanne (EPFL), Switzerland
Chandrasekaran, Suryanarayanan - National Institute of Technology, India
Chavez Rojas, Daniel - Max Planck Institute for Polymer Research, Germany
Chen, Yaoyi - FU Berlin, Germany
Chirila, Adina - Transilvania University of Brasov, Romania
Choudhary, Nilesh - KAUST, India
Clementi, Cecilia - Freie Universität Berlin, United States
Correa, Simon - Protera, Chile
Cortes-Huerto, Robin - Max Planck Institute for Polymer Research, Germany
Csanyi, Gabor - University of Cambridge, United Kingdom
D. Davari, Mehdi - RWTH Aachen University, Germany
Del Mazo Sevillano, Pablo - Universidad Autónoma de Madrid, Spain
Delemotte, Lucie - KTH, Sweden
Demir, Baris - The University of Queensland, Australia
Dettmann, Lorenz - Institute of Physics, Germany
Dhabal, Debdas - University of Utah, United States
Dhar, Aishwatya - University of Rome Tor Vergata, Italy

Diaz Carral, Angel - Universitaet Stuttgart, Germany
Diez, Georg - University of Freiburg, Germany
Dijkstra, Marjolein - Utrecht University, Netherlands
Domene, Carmen - University of Bath, United Kingdom
Domingo, Javier Heras Domingo - Carnegie Mellon University, United States
Duggisetty, Satya Chaithanya - IISc Banglore, India
Duignan, Timothy - University of Queensland, Australia
Durumeric, Aleksander - University of Chicago, United States
Duschatko, Blake - Harvard University, United States
Dutta, Arghya - Max Planck Institute for Polymer Research, Germany
Dutta, Suman - ICTS-TIFR, India
Dutta, Ravi Chandra - Max Plank Institute for Polymer Research, Germany
Dwarkanath, Nimish - Jawaharlal Nehru Centre For Advanced Scientific Research, India
Elahi, Arash Elahi - Ph.D Student, United States
Ellenbroek, Brecht - University of Amsterdam, Netherlands
Empereur, Charly - SUPSI, Switzerland
Especial, João - Faculdade de Ciências Da Universidade de Lisboa, Portugal
Evangelisti, Luca - University of Bologna, Italy
Fan, Zhaochuan - Curtin University, Australia
Ferguson, Andrew - University of Chicago, United States
Finkbeiner, Jan - University of Stuttgart, Germany
Flachmüller, Alexander - University of Konstanz, Germany
Flores Canales, Jose - Aarhus University, Denmark
Franke, Leon - University of Konstanz, Germany
Frommer, Fabio - Johannes Gutenberg-Universität, Germany
Gadewal, Nikhil - ACTREC, Tata Memorial Centre, India
Gallo, Marco - TecNM, Mexico
Gamez, Jose - Covestro Deutschland AG, Germany
Gandhi, Heta A Gandhi - University of Rochester, United States
Garay, Pablo - Insitut Pasteur Montevideo, Uruguay
García Chamorro, Moisés - Universidad de Extremadura, Spain
Gardin, Andrea - Polytechnic University of Turin, Italy
Gatsiou, Christina Anna - NCSR Demokritos, Greece
Ghorai, Sagar Ghorai - Indian Institute of Science, India
Gimenez-Santamarina, Silvia - ICMOL - UV, Spain
Girard, Martin - Max-Planck-Institut für Polymerforschung, Germany
Goswami, Rohit - University of Iceland, Iceland
Goswami, Amrita - Indian Institute of Technology Kanpur, India
Goumans, Fedor - Software for Chemistry & Materials, Netherlands
Grillo, Fabio Grillo - ETH Zurich, Switzerland
Gupta, Abhishek Kumar - Pandit Deendayal Petroleum University, India
Guzman, Horacio V. - Jozef Stefan Institute, Slovenia
Habrich, Oliver - Technische Universität Darmstadt, Germany
Han, Yanxiao Han - University of Illinois at Chicago, United States
Harmon, Rebecca - Northwestern University, United States
Harris, Cooro - Brown University, United States
Henkel, Pascal - Justus Liebig University Giessen, Germany
Heydari Beni, Ali - McMaster University, Canada
Hofberger, Marius - Technical University Munich, Germany
Hooft, Ferry - University of Amsterdam, Netherlands
Hruska, Eugen - Emory University, United States
Huang, David - The University of Adelaide, Australia
Huang, Chao-Min - Duke University, United States
Ilie, Ioana - University of Amsterdam, Netherlands
Isayev, Olexandr - Carnegie Mellon University, United States
Iyer, Sahithya - Indian Insitute of Science, India
Jackson, Nick - University of Illinois, Urbana-Champaign, United States

Jayaram, Ashreya - Johannes Gutenberg University of Mainz, Germany
Jung, Maike - University of Mainz, Germany
Jung, Hyunwook - Yonsei University, Republic of Korea
Jung, Gerhard - CNRS Montpellier, France
Kamath, Roshni - Juelich Supercomputing Center, Germany
Kanekal, Kiran - Max Planck Institute for Polymer Research, Germany
Karagjozov, Ilin - Johannes Gutenberg Universität, Germany
Kesselheim, Stefan - FZ Jülich, Germany
Kidder, Katherine - The Pennsylvania State University, United States
Kimms, Len - University of Münster, Germany
King, Toby - University of Nottingham, United Kingdom
Kjølbye, Lisbeth Ravnkilde - Aarhus University, Denmark
Klippenstein, Viktor - Technische Universität Darmstadt, Germany
Klos, Kyra - JGU Mainz, Germany
Knijff, Lisanne - Uppsala University, Sweden
Ko, Tsz Wai - University of Goettingen, Germany
Kotsis, Konstantinos - University College Dublin, Ireland
Kroon, Peter - Rijskuniversiteit Groningen, Netherlands
Kukharenko, Oleksandra - Max Planck Institute for Polymer Research, Germany
Kulkarni, Mandar - Lund University, Sweden
Lam, Julien - CEMES, CNRS and Université de Toulouse, France
Larentzos, James - US ARMY RESEARCH LABORATORY, United States
Lee, Eunsang - Technische Universität Darmstadt, Germany
Lemcke, Simon - Johannes Gutenberg University Mainz, Germany
Li, Bing - Johannes Gutenberg University Mainz, Germany
Liberati, Diego - National Research Council of Italy @ Polytechnic University, Italy
Loison, Claire - Université Claude Bernard Lyon 1, CNRS, France
Lopez, Jon - University of the Basque Country UPV/EHU, Spain
Loverde, Sharon - CUNY, United States
Lukacova, Maria - Institute of Mathematics, Germany
Luo, Siwei - UBC, Canada
Müller, Klaus-Robert - Technical University of Berlin, Germany, Germany
Markina, Anastasia - Max Planck Institute for Polymer Research, Germany
Martina, Riccardo - University of Padova, Italy
Martonak, Roman - Comenius University In Bratislava, Slovakia
Materzok, Tobias - Technische Universität Darmstadt, Germany
Matta, Micaela - University of Liverpool, United Kingdom
Mayagoitia, Alvaro - Argonne National Laboratory, United States
Meijer, Evert Jan - University of Amsterdam, Netherlands
Méndez Aretxabaleta, Xabier - UPV/EHU, Spain
Mercuri, Francesco - Consiglio Nazionale Delle Ricerche, Italy
Metya, Atanu - University of Utah, United States
Meyer, Jan - Covestrop Deutschland AG, Germany
Miceli, Marcello - Politecnico di Torino, Italy
Miller, Mark - Durham University, United Kingdom
Miszkiewicz, Joanna - University of Warsaw, Poland
Mittal, Sumit - VIT Bhopal University, India
Möckel, Michael - University of Applied Sciences Aschaffenburg, Germany
Modee, Rohit - IIIT, India
Mohamed, Saad Aldin - KAIST, Republic of Korea
Mohr, Bernadette - University of Amsterdam, Netherlands
Mollenhauer, Doreen - Justus-Liebig-University Giessen, Germany
Mosaddeghi Amini, Parinaz - University College Dublin, Ireland
Muthusivarajan, Rajarajeswari - University of Texas MDAnderson Cancer Center, USA
Nagel, Daniel - Albert-Ludwigs-Universität Freiburg, Germany
Nguyen, Tuan - The University of Queensland, Australia
Nguyen, Huong - The University of Adelaide, Australia

Nie, Yihan - Queensland University of Techonology, Australia
Noe, Frank - Free University of Berlin, Germany
Ntim, Samuel - Johannes Gutenberg Universität Mainz, Germany
Nyman, Gunnar - University of Gothenburg, Sweden
Ozmaeian, Masoumeh - University of Texas at Asutin, United States
Pallante, Lorenzo - Politecnico di Torino, Italy
Pampel, Benjamin - Max Planck Institute for Polymer Research, Germany
Panou, Matrona - NCSR DEMOKRITOS, Greece
Pantelopulos, George - Boston University, United States
Papajak, Eve - NASA Ames, United States
Pattni, Viren - Arizona State University, United States
Pedersen, Kasper Busk - Aarhus University, Denmark
Pérez De Alba Ortíz, Alberto - Utrecht University, Netherlands
Peristeras, Loukas – National Centre for Scientific Research "DEMOKRITOS", Greece
Peter, Christine - University of Konstanz, Germany
Petersen, Nanning - Max-Planck-Institute for Polymer Research, Germany
Piskorz, Tomasz - University of Oxford, United Kingdom
Pontes, Frederico - Federal University of Pernambuco, Brazil
Potter, Thomas - Durham University, United Kingdom
Prabhu, Janak - University of Fribourg, Switzerland
Qiao, Le - University of Ottawa, Canada
Ramirez, Carlos - University of Groningen, Netherlands
Ray, Dhiman - University of California Irvine, United States
Razizadeh, Meghdad - Lehigh University, United States
Reiter, Sebastian - LMU Munich, Germany
Rems, Lea - KTH Royal Institute of Technology, Sweden
Riccardi, Enrico - NTNU, Norway
Ricci, Eleonora - NCSR Demokritos, Greece
Rinderle, Michael - Technical University of Munich, Germany
Rodriguez Mendoza, Esteban De Jesus - Santander Industrial University, Colombia
Rosaleny, Lorena E. - Universitat de València, Spain
Rotskoff, Grant - Stanford University, United States
Rouse, Ian - University College Dublin, Ireland
Rudzinski, Joseph - Humboldt University, Germany
Rydzewski, Jakub - Nicolaus Copernicus University, Poland
Rynik, Marián Rynik - Comenius University In Bratislava, Slovakia
Safaei, Nehzat - Max-planck Institute of Polymer Research, Germany
Salgado, Ignacio - Universitat de Barcelona, Spain
Salimi Parvaneh, Leila - University of Mainz, Germany
Sankaranarayanan, Subramanian K. R. - Argonne NAtional Laboratory, United States
Scherer, Christoph - Max Planck Institute for Polymer Research, Germany
Schmid, Friederike - Johannes Gutenberg University Mainz, Germany
Schneider, Simon - Johannes Gutenberg University, Germany
Schwan, Sebastian - Justus-Liebig University, Germany
Seal, Aniruddha - National Institute of Science Education and Research, India
Settanni, Giovanni - Johannes Gutenberg University Mainz, Germany
Sevilla, Mauricio - Max Planck Institute for Polymer Research, Germany
Shajan, Akhil - Central University of Punjab, India
Shao, Yunqi - Uppsala University, Sweden
Shapeev, Alexander - Skolokovo Institute of Science and Technology, Moscow, Russia, Russian Federation
Shea, Jeanine - Johannes Gutenberg University Mainz, Germany
Shen, Kevin - University of California, Santa Barbara, United States
Shen, Kuan-Hsuan - Georgia Institute of Technology, United States
Silveira, Ana - Sloan-Kettering Institute for Cancer Research, United States
Singh, Manjesh K. - IIT Kanpur, India
Singhal, Ankush - Leiden University, Netherlands

Sivak, Jacob - Penn State, United States
Son, Chang Yun - Pohang University of Science and Technology, Republic of Korea
Song, Bin - Max Planck Institute for Polymer Research, Germany
Sourpis, Tasos - Johannes Gutenberg University, Germany
Stieffenhofer, Marc - Max Planck Institute for Polymer Research, Germany
Stuehn, Torsten - Max Planck Institute for Polymer Research, Germany
Subbotina, Julia - UCD School of Physics, Ireland
Sulpizi, Marialore - Ruhr University Bochum, Germany
Sundaram, Vivek - Eindhoven University of Technology, Netherlands
Szukalo, Ryan - Pennsylvania State University, United States
Terao, Takamichi - Gifu University, Japan
Tirimbo', Gianluca - Eindhoven University of Technology, Netherlands
Tkatchenko, Alexandre - University of Luxembourg, Luxembourg
Tolufashe, Gideon Femi - University of Porto, Portugal
Tormet Gonzalez, Sinkler - UNICAMP, Brazil
Toth, Ondrej - Comenius University, Slovakia
Tovey, Samuel Tovey - University of Stuttgart, Germany
Uba, Abdullahi Ibrahim - Rowan University, United States
Uhliarik, Andrej - Comenius University, Slovakia
Molinero, Valeria - University of Utah, United States
Valsson, Omar - Max Planck Institute for Polymer Research, Germany
Van Damme, Robin - Utrecht University, Netherlands
Van Heesch, Thor - Universiteit Van Amsterdam, Netherlands
Vanni, Stefano - University of Fribourg, Switzerland
Vergadou, Niki - National Center of Scientific Research "Demokritos", Greece
Vishnu, Jude Ann - Johannes Gutenberg University, Mainz, Germany
Von Lilienfeld, Anatole - University of Basel, Switzerland
Voth, Gregory - University of Chicago, United States
Vreede, Jocelyne - University of Amsterdam, Netherlands
Wagner, Tobias - Johannes Gutenberg–Universität Mainz, Germany
Wani, Yashraj - Institute of Physics JGU Mainz, Germany
Webb, Michael - Princeton University, United States
Wei, Wenya - UQ, Australia
Wells, Brad - Synopsys, Denmark
White, Andrew - University of Rochester, United States
Wilson, Marltan - The University of Adelaide, Australia
Wu, Zhenghao - Technische Universität Darmstadt, Germany
Yadav, Pankaj - IIT Kanpur, India
Yazaydin, Ozgur - University College London, United Kingdom
Yelash, Leonid - Johannes Gutenberg University, Germany
Zaverkin, Viktor - University of Stuttgart, Germany
Zhang, Chao - Uppsala University, Sweden
Zillmer, Hanne - Max-Planck-Institut für Polymerforschung, Germany
Zizzi, Eric Adriano - Polytechnic University of Turin, Italy

Multiscale simulations of soft matter: New method developments and mathematical foundations

Location: Online, coordinated by CECAM-DE-SMSM
Webpage: https://www.cecam.org/workshop-details/47
Dates: Sep 30, 2020 - Oct 2, 2020

1 State of the art

Multiscale modeling has become an indispensable tool in computational materials science. The central element of multiscale modeling is coarse graining, i.e., the art to describe complex systems with many degrees of freedom by a reduced set of representative degrees of freedom. Even though this idea has a long history, many fundamental aspects of coarse-graining and scale bridging are still poorly understood. Soft materials present a particular challenge because different scales are not well separated quasi by definition.
For many years, multiscale techniques have evolved in parallel and often independently in different communities, i.e., chemistry, physics, applied mathematics, and engineering. In chemistry and condensed matter physics, the focus has traditionally been on developing particle-based coarse-grained models and coarse-graining methods, often targeting structural properties of equilibrium systems. In recent years, dynamic coarse-graining techniques and multiscale models for nonequilibrium systems are also attracting growing interest. In applied mathematics, t the focus in multiscale modelling has traditionally been on multiscale methods for continuum models. Several techniques to model and approximate multiple scale phenomena have been developed. Nevertheless, bridging the enormous range of dynamically coupled scales as they arisen soft matter systems remains a challenge.
Although rigorous numerical analyses for traditional particle- and or continuum-based multiscale methods are available in many cases, similar analyses for the recently developed multiscale methods for soft matter systems are still at the beginning. Another recent development is a shift from traditional deterministic model-building and coarse-graining schemes to data based and machine learning based schemes which is, in particular, benefitting from recent advances in deep learning algorithms.

2 Major outcomes

The goal of the three-day workshop was to bring together scientists from these different communities to discuss new developments in their respective fields. We had 13 invited lectures and 9 additional talks from selected scientists who had registered to the conference. In addition, we had three poster sessions where a total of 17 posters were presented. Due to the Corona situation, the workshop was run as an online event. We created a zoom webinar for the talks, and a discord server for the coffee breaks and discussions. This combination turned out to be much more effective than we had anticipated. In particular, the discord server was used heavily. The recordings of the talks, the corresponding text chats, and the program booklet can still be accessed on the discord server under the following link: https://discord.gg/shj9XRA
To avoid a segregation of participants into subcommunities and maximize their exposure to other fields, the program was not organized in topical sessions, but heavily mixed. Here, we will nevertheless present the highlights topical order. Mathematical foundations were addressed in the lectures by Rupert Klein, Reinhold Schneider, and Daniel Peterseim. Rupert Klein proposed a mathematical rigorous framework for a Hamiltonian description of the popular adaptive resolution models, which relies on a novel type of open mean-field boundary condition. Reinhold Schneider presented a scheme for a rigorous error analysis of numerical solutions of important partial differential equations (such as Fokker-Planck and Hamilton)

which is based on a variational formalism. Daniel Peterseim showed how to derive macroscopic models from heterogeneous microscopic ones by numerical homogenization. A number of further contributions by mathematicians focused on algorithms. Carsten Hartmann introduced a smart reweighting method in trajectory space for rare event simulations which is based on an additional feedback control. Giacomo de Souza (substitute of Assyr Abdulle who was ill) presented a class of efficient and stable explicit numerical methods for solving stochastic differential equations with an inherent multiscale character. Frank Noe showed, among other, how to use neural networks as reweighting tools for enhanced sampling (Boltzmann generators). A number of lectures and talks covered the rapidly evolving field of machine learning in multiscale modelling. Cecilia Clementi introduced a theoretical framework for incorporating information from experiments in model building using graph neural networks. One particularly innovative development was the simultaneous optimization of static and dynamic properties of the model by a combination of force matching and spectral matching. Andrew Ferguson proposed a method to use machine learning for learning dynamics using a reduced "latent space", which allows to accelerate molecular simulations by several orders of magnitude. Houman Owhadi presented results from kernel based and deep network machine learning techniques for extrapolating time series into the future. Some of his unpublished results were so "hot" that he did not want the recording of his talk to be uploaded on the discord server. Finally, a few talks showed applications of advanced multiscale techniques for real world problems. Andela Saric presented simulations of interactions between filaments and membranes in a real cell environment. Benedetta Menucci develops mixed quantum/classical models for simulation of light sensing processes in cells. Jean-Philip Piquemal showed how his highly optimized Tinker-HP package can be used for accurate simulations of a SARS-Cov 2 component. Finally, Christian Holm gave a nice example of a multiscale analysis of a complex system, DNA translocations, with simulation levels ranging from all-atom to continuum simulations with finite element methods.

3 Community needs

The specific needs in the community are rather diverse. They range from exascale HPC computing to mathematical considerations that can be done on a desktop. The links between the communities of mathematics/numerics and modelling people in chemistry, chemical engineering and physics are still not optimal. In the Q&A sessions, the questions were typically asked by people from the same community. The potential of the ideas developed in the mathematics community is not yet fully explored in the other communities. Fortunately, more and more mathematicians are turning to be modelers themselves, which is beneficial for the community. Overall, the biggest need at this point is still to improve networking, i.e., more workshops and schools need to be organized, and more joint education programs should be set up where students are trained in mathematics along with an applied discipline.
Apart from that, access to HPC resources is of course crucial, and the continued support of successful packages and codes should be ensured. This does not only hold for simulation codes, but also for packages that are used in coarse-graining, such as VOTCA (http://www.votca.org/)

4 Funding

The workshop was organized and supported by the collaborative research center TRR146 "Multiscale Modeling Methods in Soft Matter Systems", which is funded by the German Science foundation. Provided positive evaluations, the funding could continue until 2026. That gives us a long-time perspective to develop and explore new ideas and address difficult problems with approaches that may not immediately result in a publication. Similar centers exist elsewhere, e.g., in Berlin and at different places in the US. We have not discussed new joint research proposals on the workshop, but we did discuss the idea of organizing joint workshops.

5 Will these developments bring societal benefits?

Multiscale modeling remains to be one of the grand challenges in many areas of science. Reliable predictions of the future are only possible with multiscale models. This is true not just for soft matter, but for many areas of science as well, such as energy technology, climate research, medical research etc. Progress in all these areas depends crucially on the ability to develop meaningful predictive models. And in turn, progress in many of these areas will decide upon the future of humanity. On a more practical level, established multiscale methods are already now routinely used in industrial research, and the industry is eager to apply the new methods especially in the area of machine learning. Several participants of the conference were not from academia, but from industry.
To optimize the progress in all fields, it is crucial that the communities interact and learn from each other. The multiscale methods developed in different fields overlap to a large extent, and mathematics can provide the link to bring all of them together.

6 Participant list

Organizers

Gauss, Juergen
JGU Mainz, Germany
Hanke-Bourgeois, Martin
University Mainz, Germany
Kremer, Kurt
MPI für Polymerforschung, Germany
Lukacova, Maria
Institute of Mathematics, Germany
Schmid, Friederike
Johannes Gutenberg University Mainz, Germany
Van Der Vegt, Nico
Technische Universität Darmstadt, Germany

Abdulle, Assyr - Max Planck Institute for Polymer Research, Switzerland
Akkermans, Reinier - Dassault Systèmes, United Kingdom
Alberti, Simon - TU Darmstadt, Germany
Arranz-Gibert, Pol - Yale University, United States
Bachmayr, Markus - JGU, Germany
Badr, Rodrique - Johannes Gutenberg University Mainz, Germany
Banerjee, Atreyee - Max Planck Institute for Polymer Research, Germany
Baptista Dos Santos, Luis Andre - Max Plank Institute for Polymer Research, Germany
Barnabas, Shadrack Jabes - TU Darmstadt, Germany
Baul, Upayan - Albert-Ludwigs-Universität Freiburg, Germany
Bendandi, Artemi - University of Zurich, Switzerland
Bereau, Tristan - University of Amsterdam, Netherlands
Bernhardt, Marvin - Technical University of Darmstadt, Germany
Bharadwaj, Swaminath - Technische Universität Darmstadt, Germany
Bley, Michael - University of Freiburg, Germany
Bo, Zonghua - University of Oxford, United Kingdom
Bockius, Niklas - Johannes-Gutenberg-Universität Mainz, Germany
Bozkurt Varolgunes, Yasemin - Max Planck Institute for Polymer Research, Germany
Brinkmann, André - Johannes Gutenberg University Mainz, Germany
Brunk, Aaron - Johannes Gutenberg University, Germany
Cascella, Michele - University of Oslo, Norway
Chandra, Anirban - Rensselaer Polytechnic Institute, United States
Chandrasekaran, Suryanarayanan - National Institute of Technology, India
Chavez Rojas, Daniel - Max Planck Institute for Polymer Research, Germany
Chirila, Adina - Transilvania University of Brasov, Romania

Clementi, Cecilia - Freie Universität Berlin, United States
Cortes-Huerto, Robin - Max Planck Institute for Polymer Research, Germany
Dadhich, Vishal - TU Darmstadt, Germany
Daoulas, Kostas - Max Planck Institute for Polymer Research, Germany
Das, Shubhadip - Technische Universität Darmstadt, Germany
Datta, Ranajay - Johannes Gutenberg Universität Mainz, Germany
Delle Site, Luigi - Institute for Mathematics, FU Berlin, Germany
Deußen, Benjamin - Technische Universität Darmstadt, Germany
Dhabal, Debdas - University of Utah, United States
Diezemann, Gregor - Johannes Gutenberg Universität Mainz, Germany
Donets, Sergii - Covestro, Germany
Duenweg, Burkhard - Max Planck Institute for Polymer Research, Germany
Duggisetty, Satya Chaithanya - IISc Banglore, India
Dutta, Arghya - Max Planck Institute for Polymer Research, Germany
Dutta, Ravi Chandra - Max Plank Institute for Polymer Research, Germany
Dzubiella, Joachim - University of Freiburg, Germany
Egger, Herbert - TU Darmstadt, Germany
Eslami, Hossein - Technische Universität Darmstadt, Germany
Faldum, Manfred - Johannes Gutenberg University Mainz, Germany
Fan, Zhaochuan - Curtin University, Australia
Ferguson, Andrew - University of Chicago, United States
Ferrarini, Alberta - Università di Padova, Italy
Folberth, Angelina - TU Darmstadt, Germany
Frommer, Fabio - Johannes Gutenberg-Universität, Germany
Gamez, Jose - Covestro Deutschland AG, Germany
González, Jorge - Pontificia Universidad Católica de Chile, Chile
Habrich, Oliver - Technische Universität Darmstadt, Germany
Haidar, El-Abed - The University of Sydney, Australia
Hartmann, Carsten - BTU Cottbus - Senftenberg, Germany
Hartung, Lisa - JGU Mainz, Germany
Heydari Beni, Ali - McMaster University, Canada
Holbach, Simon - University Mainz, Germany
Holm, Christian - University of Stuttgart, Germany
Hsu, Hsiao-Ping - Max Planck Institute for Polymer Research, Germany
Ilie, Ioana - University of Amsterdam, Netherlands
Iscen, Aysenur - Max Planck Institute for Polymer Research, Germany
Izvekov, Sergey - U. S. Army Research Laboratory, United States
Jackson, Nick - University of Illinois, Urbana-Champaign, United States
Jain, Yash - Technische Universität Darmstadt, Germany
Jayaram, Ashreya - Johannes Gutenberg University of Mainz, Germany
Jung, Maike - University of Mainz, Germany
Kanekal, Kiran - Max Planck Institute for Polymer Research, Germany
Karagjozov, Ilin - Johannes Gutenberg Universität, Germany
Kirsch, Till - Johannes Gutenberg-Universität Mainz, Germany
Klein, Rupert - Institute for Mathematics, FU Berlin, Germany
Klippenstein, Viktor - Technische Universität Darmstadt, Germany
Kuhnhold, Anja - Albert-Ludwigs-Universitaet, Germany
Kukharenko, Oleksandra - Max Planck Institute for Polymer Research, Germany
Lee, Eunsang - Technische Universität Darmstadt, Germany
Levis, Demian - University of Barcelona, Spain
Li, Zhen - Clemson University, United States
Li, Bing - Johannes Gutenberg University Mainz, Germany
Liberati, Diego - National Research Council of Italy @ Polytechnic University, Italy
Liebchen, Benno - Technische Universität Darmstadt, Germany
Loverde, Sharon - CUNY, United States
Materzok, Tobias - Technische Universität Darmstadt, Germany
Matta, Micaela - University of Liverpool, United Kingdom

Meinel, Melissa - Technische Universität Darmstadt, Germany
Mennucci, Benedetta - University of Pisa, Italy
Meyer, Jan - Covestrop Deutschland AG, Germany
Milano, Giuseppe - Università di Napoli Federico II, Italy
Morozova, Tatiana - Institut Laue-Langevin, France
Mukhopadhyay, Aritra K. - TU Darmstadt, Germany
Müller-Plathe, Florian - Technische Universität Darmstadt, Germany
Nikoubashman, Arash - Johannes Gutenberg University Mainz, Germany
Noe, Frank - Free University of Berlin, Germany
Ntim, Samuel - Johannes Gutenberg Universität Mainz, Germany
Oberlack, Martin - TU Darmstadt, Germany
Oestereich, Marco - Johannes Gutenberg Universität Mainz, Germany
Owhadi, Houman - Caltech, United States
Ozmaeian, Masoumeh - University of Texas at Asutin, United States
Pampel, Benjamin - Max Planck Institute for Polymer Research, Germany
Peterseim, Daniel - University of Augsburg, Germany
Petersen, Nanning - Max-Planck-Institute for Polymer Research, Germany
Pietruschka, Dennis Stefan - Justus-Liebig-University, Germany
Piquemal, Jean-Philip - Sorbonne Université, France
Piskorz, Tomasz - University of Oxford, United Kingdom
Prabhu, Janak - University of Fribourg, Switzerland
Qaisrani, Muhammad Nawaz - Johannes Gutenberg University, Germany
Raos, Guido - Politecnico di Milano, Italy
Rosilho De Souza, Giacomo - EPFL, Switzerland
Rudzinski, Joseph - Humboldt University, Germany
Rydzewski, Jakub - Nicolaus Copernicus University, Poland
Safaei, Nehzat - Max-planck Institute of Polymer Research, Germany
Salgado, Ignacio - Universitat de Barcelona, Spain
Salimi Parvaneh, Leila - University of Mainz, Germany
Saric, Andela - IST Austria, Austria
Sawade, Kevin - Universität Konstanz, Germany
Scherer, Christoph - Max Planck Institute for Polymer Research, Germany
Schneider, Reinhold - Technical University Berlin, Germany
Schwan, Sebastian - Justus-Liebig University, Germany
Settanni, Giovanni - Johannes Gutenberg University Mainz, Germany
Sevilla, Mauricio - Max Planck Institute for Polymer Research, Germany
Shea, Jeanine - Johannes Gutenberg University Mainz, Germany
Shen, Kuan-Hsuan - Georgia Institute of Technology, United States
Shen, Jianxiang - Jiaxing University, China
Singh, Manjesh K. - IIT Kanpur, India
Singhal, Ankush - Leiden University, Netherlands
Son, Chang Yun - Pohang University of Science and Technology, Republic of Korea
Song, Bin - Max Planck Institute for Polymer Research, Germany
Sourpis, Tasos - Johannes Gutenberg University, Germany
Speck, Thomas - Johannes Gutenberg-University Mainz, Germany
Spiller, Dominic - Max-Planck-Institute for Polymer Research, Germany
Stelzl, Lukas - Johannes Gutenberg-University of Mainz, Germany
Stuehn, Torsten - Max Planck Institute for Polymer Research, Germany
Sulpizi, Marialore - Ruhr University Bochum, Germany
Tan, Zihan - Forschungszentrum Jülich, Germany
Terao, Takamichi - Gifu University, Japan
Timr, Stepan - CNRS, France
Tripathy, Madhusmita - Technical University of Darmstadt, Germany
Valsson, Omar - Max Planck Institute for Polymer Research, Germany
Vergadou, Niki - National Center of Scientific Research "Demokritos", Greece
Virnau, Peter - Uni Mainz, Germany
Voulis, Igor - Johannes Gutenberg Universität - Uni Mainz, Germany

Wani, Yashraj - Institute of Physics JGU Mainz, Germany
Webb, Michael - Princeton University, United States
Wesolowski, Tomasz - University of Geneva, Switzerland
Wettermann, Sarah - Department of Physics, Germany
Wu, Zhenghao - Technische Universität Darmstadt, Germany
Xu, Zhen-Hao - JGU Mainz, Germany
Yelash, Leonid - Johannes Gutenberg University, Germany
Zhai, Zack - Covestro, China
Zhang, Jianrui - Max Planck Institute for Polymer Research, Germany
Zhou, Tianhang - Eduard-Zintl-Institute, Germany
Zillmer, Hanne - Max-Planck-Institut für Polymerforschung, Germany
Zimmer, David Noel - Johannes Gutenberg Universität Mainz, Germany

CECAM 50th anniversary - Plenary Lectures

Topology in Biology?

***Julia Yeomans**, University of Oxford*

Julia Yeomans is a professor of Physics at the University of Oxford, UK, and a leading expert in research on active systems. Research in her group addresses a variety of problems in soft matter and biological physics using theoretical and computational tools from statistical mechanics and hydrodynamics. Specific topics include the dynamics of soft-matter, collective behaviour of active systems, mechanobiology, motility at low Reynolds number, and the interactions of fluids with structured surfaces.
On September 9 2019, Prof. Julia Yeomans delivered a plenary lecture at the conference "Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM". We are pleased to present the video of the lecture and renew the opportunity to learn and share exciting science.

TOPOLOGY IN BIOLOGY?
Active materials, such as bacteria, molecular motors and self-propelled colloids continuously transform chemical energy from their environment to mechanical work. Dense active matter shows mesoscale turbulence, the emergence of chaotic flow structures characterised by high vorticity and self-propelled topological defects I shall describe how the ideas of active matter are suggesting new ways of interpreting cell motility and cell division. Recent results indicate that active topological defects may help to regulate turnover in epithelial cell layers and contribute to controlling the structure of bacterial colonies.

View video

Advances in Interatomic Potentials for Materials

***Gabor Csanyi**, University of Cambridge*

Gabor Csanyi is a professor of Molecular Modelling at the University of Cambridge, UK. He is an expert in atomistic simulation, particularly in multi scale modelling that couples quantum mechanics to larger length scales. He is currently engaged in applying machine learning techniques to materials modelling problems e.g., deriving force fields (interatomic potentials) from ab initio *data. He is also interested in statistical problems in molecular dynamics, e.g., in enhanced sampling algorithms that can be used to automate the calculation of phase diagrams from atomistic models.*

ADVANCES IN INTERATOMIC POTENTIALS FOR MATERIALS

Modelling the atomic scale properties of materials is one of the success stories over the past four decades. Increasingly complex functional forms, from pair potentials to embedded atom models and bond order potentials, allowed the quantitative description of different crystal structures, point and line defects, surfaces, shedding light on many elementary processes governing failure, phase stability, etc. The accuracy with which these models describe the potential energy surface corresponding to the electronic ground state has not changed much over the decades and is rather limited. The success is thus largely empirical in nature – and follows from the sophistication of the modeler and the judicious compromises made in order to solve specific problems. The parallel developments in electronic structure theory on the other hand provided exquisite quantitative agreement with experiments. I will report on recent work of a growing community, who have managed to bring these two worlds together, and construct extremely accurate functional representations of the interatomic potential. These developments rely on a very large amount of highly accurate electronic structure data, on nonparametric function fitting, and on sophisticated representation theory that brings with it guarantees of completeness and convergence.

View video

Light-activated matter: from photo-electrochemical cells to optogenetics and quantum information systems

***Giulia Galli**, University of Chicago*

Giulia Galli is the Liew family professor of Molecular Engineering and professor of Chemistry at the University of Chicago, USA. She is also senior scientist at Argonne National Laboratory and the director of the Midwest Integrated Center for Computational Materials. She is a leading expert in first principle molecular dynamics, with a focus on developing and using theoretical and computational methods to understand, predict and engineer materials properties. Method developments include electronic and vibrational spectroscopies, thermal transport, hybrid functionals and constrained density functional theory. Her team develops the WEST code, coupling first principle molecular dynamics with many body perturbation theories and advanced sampling methods. Domains of applications of Prof. Galli's work include nanostructured materials, harvesting of sunlight, materials under extreme conditions, thermal transport, water and solutions and quantum information.

LIGHT-ACTIVATED MATTER: FROM PHOTO-ELECTROCHEMICAL CELLS TO OPTOGENETICS AND QUANTUM INFORMATION SYSTEMS

We discuss first principles, computational methods and strategies to predict light-activated processes in sustainable materials for use in photoelectrochemical cells, optogenetic and quantum information systems.

View video

Molecular dynamics simulations in the age of machine learning

Eric Vanden-Eijnden, *Courant Institute New York University*

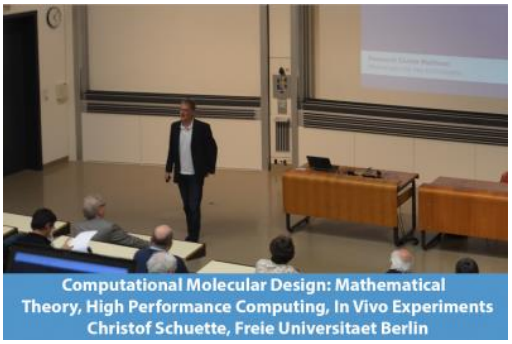
Eric Vanden-Eijnden is professor of mathematics at the Courant Institute, New York University. His research focuses on mathematical tools and numerical methods for stochastic, multiscale dynamical systems with applications in molecular dynamics, chemical and biological networks, materials science, atmosphere-ocean science, and fluid dynamics. He has developed techniques for sampling rare events, multiscale analysis, quantification of the effects of random perturbations of dynamical systems and contributed to modeling turbulence via stochastic partial differential equations. Prof. Vanden-Eijnden's objectives include understating pathways and rate of occurrence of rare events in complex systems and multiscale simulations of random dynamical systems.

MOLECULAR DYNAMICS SIMULATIONS IN THE AGE OF MACHINE LEARNING

The rapid developments in machine learning (ML), leading to its success in the context of complex classification tasks, offer intriguing promises for molecular dynamics simulations. Indeed, ML has already been successfully used for force field parametrization, protein structure prediction, drug design, etc. These tasks rely on processing data obtained by independent means. Here I will discuss how ML could also help in producing long time series data, specifically focusing on free energy calculations and reactive event analysis, two problems that require designing accelerated sampling strategies and can possibly lead to learning low dimensional models.

View video

CECAM Keynote Lectures



Computational Molecular Design: Mathematical Theory, High Performance Computing, In Vivo Experiments

Christof Schuette, *Freie Universitaet Berlin*

Christof Schuette is the President of the Zuse Institute and the Head of the Biocomputing Group at the Freie Universitaet in Berlin. His research interests focus on applied mathematics and scientific computing for complex systems with applications in a broad range of topics such as multiscale modelling and simulation for complex systems, numerical mathematics, data-driven modelling and statistical learning with applications in the natural, materials and life sciences.

COMPUTATIONAL MOLECULAR DESIGN: MATHEMATICAL THEORY, HIGH PERFORMAMCE COMPUTING, IN VIVO EXPERIMENTS

Molecular dynamics and related computational methods enable the description of biological systems with all-atom detail. However, these approaches are limited regarding simulation times and system sizes. A systematic way to bridge the micro-macro scale range between molecular dynamics and experiments is to apply coarse-graining (CG) techniques. We will discuss Markov State Modelling, a CG technique that has attracted a lot of attention in physical chemistry, biophysics, and computational biology in recent years. First, the key ideas of the mathematical theory and its algorithmic realization will be explained, next we will discuss the question of how to apply it to understanding ligand-receptor binding, and last, we will ask whether this may help in designing ligands with prescribed function. All of this will be illustrated by telling the story of the design process of a pain relief drug without concealing the potential pitfalls and obstacles.

View video

Mary Ann Mansigh Conversation Series

Computer modeling for industrial applications

***Massimo Noro**, Daresbury labs,*
***William Curtin**, EPF-Lausanne*

Massimo is the Business Development Director at the Science and Technology Facilities Council (STFC), Daresbury labs, and former science leader of the High Performance Computing division at Unilever. His scientific interests focus on applying atomistic and coarse-grained simulations to study the interaction of nano-objects and surfactants with lipid bilayers for industrial applications (e.g., soaps, detergents, etc.), and he has made considerable contributions to the development and application of the Dissipative Particle Dynamics (DPD) simulation technique to study soft condensed matter systems.

COMPUTER MODELING FOR INDUSTRY

In this conversation, Massimo Noro will discuss with Prof. William Curtin, EPFL, and with the audience, the relevance of simulation for industry and his role as the leader of an important computing facility that interacts directly with industry. This conversation will offer insight on how to promote and facilitate industrial use of simulation and modelling and will allow us to meet a “living example” of a carrier path for simulators outside academia.

View video

Berni J. Alder CECAM Prize

2019 Berni J. Alder CECAM prize award ceremony to Sauro Succi, Italian Institute of Technology and Center for Life Nanosciences at La Sapienza, Rome.

2019 Berni J. Alder CECAM Prize ceremony

***Awardee Sauro Succi**, Italian Institute of Technology and Center for Life Nanosciences at La Sapienza, Rome.*

Prof. Sauro Succi is a leading scientist at the Italian Institute of Technology and the Center for Life Nanosciences at the University of Rome La Sapienza. He is a pioneer of the Lattice-Boltzmann method. In 1989, he was instrumental for the first Lattice-Boltzmann nonlinear flow simulation and, shortly after, for contributing to the highly influential "top-down" interpretation. Following these groundbreaking contributions, he authored a multitude of early fluid-dynamic applications and spearheaded developments which made the approach suitable for modeling flows far from equilibrium, up to inserting the Lattice-Boltzmann method into a multi-scale approach. Over the decades, he has obtained outstanding results. He has continued to lay out and to consolidate the foundations of the Lattice-Boltzmann method, to open it up to new applications and to extend the approach beyond hydrodynamics into new territories of micro- and nano-fluidics, porous media, soft matter, and electronic transport. Over the decades, he has obtained outstanding results. He has continued to lay out and to consolidate the foundations of the Lattice-Boltzmann method, to open it up to new applications and to extend the approach beyond hydrodynamics into new territories of micro- and nano-fluidics, porous media, soft matter, and electronic transport. In addition, he has been pivotal in building and constantly inspiring a community now counting tens of thousands of researchers in academia and industry.

The Berni J. Alder CECAM Prize recognizes exceptional contributions to the field of microscopic simulation of matter. The prize is meant to honour an individual scientist; exceptionally it can be awarded to at most three scientists having equally contributed to the specific topic for which the prize is granted. This is the most prestigious European prize for computer simulations in condensed matter physics/chemistry, statistical physics and physical chemistry. The prize, awarded every three years, was created in 1999. On Sept. 11, 2019, he became the 11th awardee of the Berni J. Alder CECAM prize. The award ceremony was part of a special plenary session at the Conference "Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM", featuring an introductory remote speech by Berni Alder and the awarding by previous prize recipient Hardy Gross.

View video

Webinar Series “CoVid-19: challenges and responses in simulation, modeling and beyond”

Session 1: Tuesday April 21 2020

Erik Lindhal - Stockholm University
The proteins of SARS-CoV-2, joint data repositories, and community collaborations

Francesco Stellacci – EPFL
Supramolecular antivirals

Erik Lindhal - Stockholm University
Professor of Biophysics at the Department of Biochemistry and Biophysics of the Stockholm University, lead scientist of the EU-funded Center of Excellence for Computational Biomolecular Research Bioexcel, and member of the CECAM Council. His team also steers international development of the widely used GROMACS simulation package.
The focus of Professor Lindhal’s research is understanding membrane proteins, with specific focus on ion channels and pumps in the nervous system. His research group uses a number of techniques ranging from bioinformatics to build models of human receptors and channels based on bacterial structures, biomolecular simulations to understand the molecular-level interactions in these complex molecules, and experimental techniques such as electrophysiology or spectroscopy to measure functional effects of conformational transitions, and how these are influenced by mutations in the membrane proteins or small molecules that can work as medical drugs.

THE PROTEINS OF SARS-COV-2, JOINT DATA REPOSITORIES, AND COMMUNITY COLLABORATIONS
The covid-19 pandemic has led to a massive response of computational (and experimental) research groups targeting the viral proteins for drug design or understanding of function and infection properties. We'll briefly bring you up to the latest state in terms of what protein structures are available or in the pipeline, which ones are considered the most important drug targets, and introduce some of the worldwide collaborations that have been established both in US and Europe. I will present a common repository that have been established by BioExcel and MolSSI where you can access both experimental and computational data per target or method, and how you will be able to upload your own early data, get DOIs, and participate in early community review of the data, and how we will try to handle coordination to have groups increasingly collaborate instead of duplicating the same studies on the same structures.

Francesco Stellacci – EPFL
Professor at EPF-Lausanne where he heads the Supramolecular NanoMaterials and Interfaces Laboratory (SuNMiL), principal investigator of the NCCR Bio-Inspired Materials, and has recently been awarded an ERC Advanced Grant to attempt to establish a new paradigm for the recycling of plastics inspired by protein recycling in nature.
Professor Stellacci’s fields of expertise include nanomaterials, nanoparticles, soft materials, supramolecular interactions, solid-liquid interfaces, and notably nanomedicine. His team has developed a line of research on supramolecular approaches to design novel broad-spectrum

non-toxic antivirals based on nanoparticles and other compounds with virucidal inhibition mechanism.

SUPRAMOLECULAR ANTIVIRALS

Viral infections are among the main causes of death in the world. When prevention is not an option, antiviral drugs are the last resort to prevent the spread and the mortality of these infections. There are only a few effective drugs on the market, for the most part they prevent intracellular viral replication. Unfortunately, they are too few when compared to the many viruses that threaten humans.

In this talk, I will show a new design rule to achieve drugs that fight viruses extracellularly by irreversibly inhibiting their infectivity, i.e. I will show how to create virucidal compounds. The design of these macromolecular virucidal agents starts by a bio-mimic approach and is characterized by the limited toxicity towards host cells that one would expect from such compounds. Yet, I will demonstrate that the multivalent binding to the viruses, coupled with a large hydrophobic contact between the compounds and the virus leads to a loss of integrity of the virion that obviously leads to an irreversible loss of infectivity. Results in and ex-vivo will be illustrated especially for the cases of influenza, herpes, and respiratory syncytial virus.

View video

Session 2: Tuesday April 28 2020

Andrea Beccari - DOMPE Farmaceutici SPA
Exscalate4CoV, an introduction

Carmine Talarico - DOMPE Farmaceutici SPA
The computational Task in Exscalate4CoV

Giulia Rossetti - Forschungszentrum Julich and RWTH Aachen
Computational approaches to drug repurposing

Andrea Beccari - DOMPE Farmaceutici SPA
Andrea Beccaris Head is of the R&D Platforms and Services of Dompé Farmaceutici SpA and responsible the Joint Bioinformatics Groups at the IBP institute of the National Research Council of Italy. He led the drug discovery programs and then became responsible for the technological platform R&D, supporting pharmaceutical research activities with computer aided design, advanced modelling and large-scale simulations in Dompé. He was promoter and coordinator of the open innovation initiative: Italian Drug Discovery Network and co-founder and member of the board of the Avicenna Alliance (Brussel), an association of industry and research institutions with the aim to overcome limitations of the pre-digital era, by the development of in silico simulations up to a scale necessary to provide personalized treatments and predictive medicine. He was the originator and chairman of the Computationally Driven Drug Discovery and Italian Drug Discovery Summit series of meetings and has co-organized several initiatives with the European commission and parliament promoting the use of in silico simulation to increase the awareness towards the potentiality of high-performance computing in healthcare. Dr. Beccari is the coordinator of the Exscalate4CoV project.

EXSCALATE4COV, AN INTRODUCTION

Carmine Talarico - DOMPE Farmaceutici SPA
Carmine Talarico is a computational chemistry researcher at Dompé farmaceutici SpA and the leader of the computational Task in Exscalate4CoV. He is also Project Leader of the PRACE granted project called Antarex for Zika, a project that has been recognized as having clear societal impact that will harness the power of HPC to fight diseases that overwhelmingly affect developing countries. He is an expert in modeling of small molecules, structure/ligand-based drug design, pharmacophores development, homology modeling, protein threading, property prediction, high-throughput and single-molecule docking, ab initio and semiempirical quantum chemical calculations, molecular mechanics, molecular dynamics simulation methodologies and conformational analysis.

THE COMPUTATIONAL TASK IN EXSCALATE4COV

The main objective of the Drug Discovery TASK FORCE is the exploitation of the EXSCALATE platform, combined with other Computational tools, to identify the most promising safe in man drugs and de novo small molecules to be active against coronavirus. In the first steps, validated 3D structure models of COVID-19 proteins will be obtained from MD simulations on in-house generated homology models, and the already experimentally obtained 3D structure.

Two sets of simulations will be performed at a different scale, respectively PRACE Tier-0 HPC systems and EuroHPC pre-exascale systems, to virtual screen in a first phase the Safe in Man (SIM) library, containing the commercialized and developing drugs (> 10000), to identify the most promising safe in man drugs ready for immediate treatment of the infected population, and in the second phase the TCS to identify new potential pan Coronavirus inhibitors.

Giulia Rossetti - Forschungszentrum Julich and RWTH Aachen

Giulia Rossetti is professor at the Medical faculty of RWTH University in Aachen, Germany and group leader at the Institute of Neuroscience and Medicine and Jülich Supercomputing. She is scientific manager of the co-design project for drug design and leader of the Molecular Simulation Task in the Human Brain Project. She is also a project leader in the recently approved "Helmholtz Information & Data Science School for Data Science in Life, Earth, and Energy" (HDS-LEE), as well as member of the corresponding steering committee. She was recently awarded of the EU grant 'STIMULATE', a Marie Skłodowska-Curie grant for an Innovative Training Network, which involves several universities across Europe. The aim of STIMULATE is to deliver an innovative interdisciplinary educational and research program in simulation and data science, which educates students to address the challenges posed by exascale computing and intensive data applications.

Prof. Rossetti's group is specialized in modeling structure, dynamics and molecular interactions of key targets in diseases' cause and progression. Virtual screening and drug design exploiting molecular modeling are central activities in her lab. Her research is mostly focused on neuropathologies including but not limited to neurodegenerative diseases, neuropathic pain disorders and Schizophrenia. Her group mostly uses HPC-based molecular simulation, ranging from coarse-grain to classical up to ab initio representation, as well as free-energy calculations, bioinformatics and chemoinformatic.

COMPUTATIONAL APPROACHES TO DRUG REPURPOSING

We have recently created a tailored research team to target viral proteins for drug design. This research activity is mostly within the framework of the project EXSCALATE4CoronaVirus within the EU coronavirus H2020 program. It involves the Jülich, CINECA, Barcelona Supercomputing centers, the Dompè Pharma company, the Fraunhofer Institute, and others, for a total of 18 computational and experimental groups. The aim of the research team is to identify, by virtual screening, effective antiviral drugs against proteins responsible for the virus survival, among the currently commercially available drugs. Preliminary results will be presented here.

Repurposing existing, approved drugs accelerates their transfer into clinical practice remarkably, because their safety has already been proven. In this framework, we plan to establish an effective AI- and HPC-based platform to generate and analyze 3D models, along with protocols for experimental 3D structure resolution (X-Ray, Cryo-EM, ..,) of protein targets from pandemic pathogens. This will lead to a sustainable infrastructure for a fast scientific answer to future pandemic scenarios.

View video

Session 3: Tuesday May 5 2020

Andrea Cavalli - University of Bologna and IIT Genova
Current therapeutic options for CoVid-19: prediction of mechanism of action through atomistic simulations and machine learning

Modesto Orozco - Institute for Research in Biomedicine, Barcelona
HPC and BigData approaches in CoVid-19 research

Andrea Cavalli - University of Bologna and IIT Genova
Andrea Cavalli is Professor of Medicinal Chemistry at the University of Bologna and Director of Computational and Chemical Biology at the Italian Institute of Technology, Genova, where he is also Deputy Director for the Research Domain " Computational Sciences".
Prof. Cavalli's research has combined computational chemistry and physics with biology and drug discovery. He has developed and applied algorithms and protocols to accelerate and enhance the discovery of novel drug candidates in different therapeutic areas, including cancer, Alzheimer's disease, and neglected tropical diseases. He has been a pioneer in the use of molecular dynamics simulations and related methods within drug discovery programs, and in 2014 he founded a high-tech startup company (BiKi Technologies), which develops tools based on statistical mechanics for drug discovery. In 2003, he was awarded the Farmindustria Prize for Pharmaceutical Research.

CURRENT THERAPEUTIC OPTIONS FOR COVID-19: PREDICTION OF MECHANISM OF ACTION THROUGH ATOMISTIC SIMULATIONS AND MACHINE LEARNING
Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2)-associated coronavirus disease 2019 (CoVid-19) has gripped the world in a pandemic, challenging its healthcare infrastructure, economy, and culture. Major efforts are underway to quickly identify therapeutic options to treat and prevent the spread of CoVid-19. A three-stage classification for CoVid-19 has recently been proposed, with increasing severity that corresponds to distinct clinical findings, responses to therapy, and clinical outcomes. The initial stage occurs at the time of the virus inoculation and early establishment of the disease. In the second stage, an established pulmonary disease can be observed with viral multiplication and inflammation usually localized in the lung. The third stage usually shows an extra-pulmonary systemic hyperinflammation syndrome, resulting in a decrease in helper, suppressor, and regulatory T cell counts. Different therapeutic options must be considered for the different stages of the disease, with targets at the virus particles or within the human cells that should be carefully selected and properly modulated. In stage I and IIA, antiviral compounds should be considered, whereas anti-inflammatory drugs and immunomodulators are the best option for stages IIB and III. In this talk, we discuss the current therapeutic options and target selection for the different stages of CoVid-19, with particular focus on computational studies able to in depth rationalize and predict mechanism of actions and point to the most promising drugs from the FDA- (or EMA-) approved medicines. Finally, a study based on machine learning will be presented, which was able to discover promising pathways and targets pointing also to polypharmacology mechanism of action as an innovative way to target current and future coronavirus outbreaks.

Modesto Orozco - Institute for Research in Biomedicine, Barcelona

Modesto Orozco is Director of the Integrative Biology Program at the Institute for Research in Biomedicine, Barcelona, and of the Joint IRB-BSC Research Program in Computational Biology. He acts as a consultant for scientific bodies in Spain and Europe and is the Founder and President of Nostrum Biodiscovery a Biotech Company devoted to rational drug design. Prof. Orozco has been, or is advisor for several biotech and pharmaceutical companies, among others: Lab. Uriach, Lab. Almirall, Lab. Salvat, Pfizer Inc., Boehringer Ing., Kraft Pharm., Lab. Palau Pharma, Amgen Inc., and Nurix Inc. He is the recipient of an advanced ERC grant, and coordinator of H2020 projects in the domain of biosimulations.

His main interest is the understanding of biological systems from first principles. Topics of specific focus include the understanding of the mechanism of flexibility and signal transduction in proteins and the connection between physical properties of nucleic acids and their function, with special emphasis in the study of chromatin. He also contributes to the development of the Self-Consistent Reaction Field method to account for polarization and is a developer of QM/MM approaches for large systems.

HPC AND BIGDATA APPROACHES IN COVID-19 RESEARCH

At a time where we though major threats for human health would never come from infection diseases, CoVid-19 has showed has how fragile we are, both as individuals and as a society to infections originated from viruses that were kept cryptic in exotic animals for centuries. Virus emergences hit us with an expansion rate faster than our ability to find cures and generates a sense of panic in the society. CoVid-19 is being a nightmare, but we cannot neglect a few positive aspects in the current situation, one of them, the impressive multidisciplinary response of the scientific community that is not only focus on finding treatments, but that is sharing all the information. Molecular simulation techniques are become crucial in the multidisciplinary approach to fight CoVid-19 and thousands of groups around the world are running simulations on COVID19 systems, both in local computers and in high performance computer centers which are prioritizing CoVid-19 research. I will comment a couple of initiatives done in Barcelona to: i) optimize the use of HPC resource to CoVid-19 research and ii) optimize the way in which the structural information on COVID19 system is stored, analyzed and shared.

View video

Session 4: Tuesday May 12 2020

Antonietta Mira - Università della Svizzera Italiana and Insubria University
Modeling the pandemic is difficult: hopes and doubts about model building

Andrea De Gaetano - National Council of Research of Italy
Modeling the pandemic is difficult: hopes and doubts about model building

Jean-Philip Piquemal - Sorbonne University
Modeling SARS-CoV-2 Proteins using Molecular Dynamics and Polarizable Force Fields

Antonietta Mira - Università della Svizzera Italiana and Insubria University
Antonietta Mira is professor of Statistics and director of the Data Science Lab, that she founded in 2017, at Università della Svizzera italiana, Lugano, Switzerland. She is also member of the Swiss Federal Statistical Committee, professor at Insubria University, Como, Italy, fellow of the International Society of Bayesian Analysis and of the Istituto Lombardo Academy of Science and Letters, since 2016. Since 2019 she is member of the board of the Harvard Data Science Review, and last year has chaired the Savage Award committee of the International Society for Bayesian Analysis (award of which she was recipient in 1998). She has been a visiting fellowship at Harvard, Cambridge, QUT in Brisbane and holds memberships to several advisory board memberships. She is also PI or co-PI of competitive research grants for approximately 2.000k CHF.
Her main research interests are: Statistical models for complex data, uncertainty quantification, model selection and Monte Carlo efficient simulation algorithms.
In her free time Antonietta is a practitioner magician with specific interest in mathematical magic on which topic she wrote the book in 2012. This is only one of her activities aimed at science popularization which include the creation of an exhibit, Numbed by Numbers! a 3D tour between Digits (math), Dice (probability) and Data (statistics) aimed at kids aged from 6 to 18.

MODELING THE PANDEMIC IS DIFFICULT: HOPES AND DOUBTS ABOUT MODEL BUILDING
We explore the role of both statistical and deterministic models in providing reasonable guidance for extrapolation with data that are insufficient, both in terms of quality and quantity. The concept of what constitutes a good model to support decision makers is also be discussed.

Andrea De Gaetano - National Council of Research of Italy
Andrea De Gaetano is an Italian biomathematician working with the National Council of Research of Italy in Rome. He is an M.D. with a specialty in Emergency Surgery, M.Sc. and Ph.D. in Applied Mathematics, and Juris Doctor admitted to the Italian Bar. He is Director of Research with CNR Institute for Systems Analysis (IASI) and adjunct professor of Mathematical Statistics with the Dept. of Mathematics at Mahidol University Bangkok.
With his colleagues at CNR IASI BioMatLab in Rome he studies mainly deterministic and stochastic dynamical system problems in mathematical physiology (using ordinary, partial, delay, stochastic and fractional differential equations). He is interested in both the modeling of

physiological systems and in the statistical estimation of the model parameters and has published some 160 extended papers on peer-reviewed journals so far. He is the current president of the European Society for Mathematical and Theoretical Biology. Among his non-professional interests are motorbike riding, playing baroque trumpet (very poorly), building rocket stoves, raising donkeys and clearing woodland from thorn bushes.

MODELING THE PANDEMIC IS DIFFICULT: HOPES AND DOUBTS ABOUT MODEL BUILDING

We explore the role of both statistical and deterministic models in providing reasonable guidance for extrapolation with data that are insufficient, both in terms of quality and quantity. The concept of what constitutes a good model to support decision makers is also discussed.

Jean-Philip Piquemal - Sorbonne University

Jean-Philip Piquemal is Professor of Theoretical Chemistry at Sorbonne Université and Director of the Laboratoire de Chimie Théorique (LCT), a joint research center with CNRS. He is also junior member of the Institut Universitaire de France and Adjunct Professor of Biomedical Engineering at the University of Texas in Austin. Since 2019, he is Principal Investigator of the Extreme-Scale Mathematics-based Computational Chemistry ERC Synergy project. His team develops the massively parallel Tinker-HP simulation package dedicated to new generation polarizable force fields molecular dynamics. Professor Piquemal's research is focused on methodological developments for multiscale quantum chemistry methods and new generation force fields. His research group is mainly interested in large scale applications of these techniques to biological systems including metalloproteins with a strong interest for many-body effects, chemical reactivity and drug design. In 2018, he was awarded the Atos Joseph Fourier Prize in High Performance Computing.

MODELING SARS-COV-2 PROTEINS USING MOLECULAR DYNAMICS AND POLARIZABLE FORCE FIELDS

In this talk, I present some aspects of our COVID-HP PRACE project aiming at obtaining a structural and dynamical description of the components of the Sars-Cov-2 virus through extensive new generation polarizable molecular dynamics simulations (AMOEBA force field) using the massively parallel/multi-GPUs Tinker-HP software. To do so, we are currently building large-size models of the various proteins of the virus in link with recently available experimental data in order to produce large, high-resolution, ensembles using polarizable molecular dynamics for post-treatment screening purposes and QM/MM studies. I will focus my talk on the description of our modeling efforts dedicated to the Spike and Main protease (Mpro) proteins. Such computer models will help scientists to design new drugs able to neutralize the coronavirus by preventing it from entering human cells or by blocking its internal machinery.

View video

Webinar Series “The importance of being H.P.C. Earnest”

Session 1: Thursday June 18 2020

Nicola Marzari - EPFL
The great mysteries of computational science, and the marvelous opportunities

Claudia Filippi - University of Twente,
Targeting Real chemical accuracy at the EXascale

Anthony Scemama - University of Toulouse III
Targeting Real chemical accuracy at the EXascale

Giulia Galli - University of Chicago and Argonne National Laboratory
The long and winding road: predicting and designing material and molecular properties through computation

Nicola Marzari - EPFL
Nicola Marzari holds the Chair of Theory and Simulation of Materials at EPFL, where he is also the director of the MARVEL National Centre for Computational Design and Discovery of Novel Materials. He is the current chairperson of the Psi-k Charity and Board of Trustees, and an Excellence Chair at the University of Bremen.

THE GREAT MYSTERIES OF COMPUTATIONAL SCIENCE, AND THE MARVELOUS OPPORTUNITIES
The theoretical, algorithmic and computational prowess of the last decades has brought together a paradigm shift in our scientific approach, especially felicitous for computational condensed matter physics, chemistry, and materials science. I illustrate with a few examples the present strengths, challenges and opportunities in the field, nowadays driven by collective ecosystems of scientists, ideas, and codes that allow to greatly accelerate our capabilities to understand, predict, and design novel or complex materials. I conclude trying to predict or influence the future - what scientific challenges to address, what political and policy ones.

Claudia Filippi - University of Twente,
Claudia Filippi is professor in Computational Chemical Physics at the University of Twente in the Netherlands. She received her PhD from Cornell University, USA, in 1996 and, after a postdoc at the University of Illinois at Urbana-Champaign, USA, she was a lecturer in Physics at University College Cork, Ireland, from 1998 to 2001. She then moved to the Netherlands as assistant professor at the University of Leiden and, since 2008, is professor at the University of Twente. Her research is in the field of electronic structure and multiscale simulations and,

currently, focuses on methodological developments for investigating light-induced phenomena in (bio)molecular systems within the framework of stochastic quantum Monte Carlo methods.

TARGETING REAL CHEMICAL ACCURACY AT THE EXASCALE

Quantum mechanical simulations play an important role in scientific and industrial applications, where understanding at the atomistic and electronic level is needed. In this context, density functional theory is generally the method of choice thanks to its relatively low computational cost and ability to appropriately describe the electronic properties of a variety of systems. Despite the many successes, there are however materials or classes of materials properties (e.g. magnetic systems, photo-induced processes, non-covalent interactions), where the mean-field picture becomes insufficient, and the fully correlated nature of the system must be considered. The computational cost of high-accuracy quantum mechanical approaches is orders of magnitudes larger than the cost of density functional theory, and their implementation must be reconsidered in order to take advantage of the architecture of modern and future supercomputers.

The TREX European Center of Excellence (CoE) will start in October. It aims at developing and promoting an open-source, high-performance software platform in the domain of high-accuracy (stochastic) quantum chemical simulations, designed for the upcoming Exascale architectures. Here, we will present the main aspects of the TREX CoE and, in particular, describe our strategy to design a high-performance library for quantum Monte Carlo simulations.

Anthony Scemama - University of Toulouse III

Anthony Scemama is a research engineer at the Laboratoire de Chimie et Physique Quantiques (CNRS - Université de Toulouse, France), focusing on the development and implementation of computational methods and parallel algorithms for quantum chemistry. His expertise lies at the interface between high-performance computing and computational chemistry, and he is the main author of the massively parallel quantum Monte Carlo code QMC=Chem, and of Quantum Package, a software for making high-accuracy calculations with selected configuration interaction. In the context of the TREX European Center of Excellence, he is coordinating the development of the QMCkl library.

TARGETING REAL CHEMICAL ACCURACY AT THE EXASCALE

Quantum mechanical simulations play an important role in scientific and industrial applications, where understanding at the atomistic and electronic level is needed. In this context, density functional theory is generally the method of choice thanks to its relatively low computational cost and ability to appropriately describe the electronic properties of a variety of systems. Despite the many successes, there are however materials or classes of materials properties (e.g. magnetic systems, photo-induced processes, non-covalent interactions), where the mean-field picture becomes insufficient, and the fully correlated nature of the system must be considered. The computational cost of high-accuracy quantum mechanical approaches is orders of magnitudes larger than the cost of density functional theory, and their implementation must be reconsidered in order to take advantage of the architecture of modern and future supercomputers.

The TREX European Center of Excellence (CoE) will start in October. It aims at developing and promoting an open-source, high-performance software platform in the domain of high-accuracy (stochastic) quantum chemical simulations, designed for the upcoming Exascale architectures. Here, we will present the main aspects of the TREX CoE and, in particular, describe our strategy to design a high-performance library for quantum Monte Carlo simulations.

Giulia Galli - University of Chicago and Argonne National Laboratory

Giulia Galli (https://en.wikipedia.org/wiki/Giulia_Galli) is the Liew Family professor of Electronic Structure and Simulations in the Pritzker School of Molecular Engineering and Professor of Chemistry at the University of Chicago. She also holds a Senior Scientist position at Argonne National Laboratory (ANL) and she is the director of the Midwest Integrated Center

for Computational Materials (MICCoM). Her research activity is focused on the development and use of theoretical and computational methods to understand and predict the properties and behavior of materials (solids, liquids, and nanostructures) from first principles.

THE LONG AND WINDING ROAD: PREDICTING AND DESIGNING MATERIAL AND MOLECULAR PROPERTIES THROUGH COMPUTATION

I briefly describe examples of properties of materials predicted using simulations rooted in first principles theories of matter, and I then discuss some of the open challenges involved in enabling scientific discoveries by computation. Challenges include theoretical and algorithmic advances required to broaden the scope of properties accessible by ab initio simulations, the use of changing computer architectures, including disruptive changes that are brought about by quantum computers, as well as the need for innovative methods to collect, verify and use data generated by simulations.

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Session 2: Thursday June 25 2020

Erik Lindahl - Stockholm University
Simulating the Dynamics of Molecular Biology: Brick Walls, Achievements and Opportunities

Jesus Labarta - Barcelona Supercomputing Center
POP: towards insight on program behavior

Paul Kent - Oak Ridge National Laboratory
Towards Reliable and Accurate Materials Predictions at Exascale

Erik Lindahl - Stockholm University
Professor of Biophysics at the Department of Biochemistry and Biophysics of the Stockholm University, lead scientist of the EU-funded Center of Excellence for Computational Biomolecular Research Bioexcel, and member of the CECAM Council. His team also steers international development of the widely used GROMACS simulation package.
The focus of Professor Lindhal's research is understanding membrane proteins, with specific focus on ion channels and pumps in the nervous system. His research group uses a number of techniques ranging from bioinformatics to build models of human receptors and channels based on bacterial structures, biomolecular simulations to understand the molecular-level interactions in these complex molecules, and experimental techniques such as electrophysiology or spectroscopy to measure functional effects of conformational transitions, and how these are influenced by mutations in the membrane proteins or small molecules that can work as medical drugs.

SIMULATING THE DYNAMICS OF MOLECULAR BIOLOGY: BRICK WALLS, ACHIEVEMENTS AND OPPORTUNITIES
Molecular dynamics simulation of biological systems were born at a CECAM workshop 44 years ago, and what was once a mostly theoretical proof-of-concept has evolved into a widespread technique used even in experimental research labs to make sense of measurements and new structures. The main reason for this is that MD simulations have evolved from spanning a few picoseconds to spanning a few microseconds, not to mention better force fields and algorithms. However, the free ride that has come with faster hardware is about to end - Exascale is bringing many more processors, but they will usually not be faster. I will present some of these challenges, and in particular connect how the scientific results we seek depend on parallelisation, performance, and scaling. I will discuss how the end of Dennard scaling is a brick wall for many traditional algorithms (which we are only beginning to realize), and how we increasingly have been forced to go back and redesign fundamental approaches that dominated fields as molecular simulation for the last 50 years - in particular to be able to move to heterogeneous acceleration. Finally, I will discuss strategies both we and others are using to get around the remaining brick walls and turn Exascale computing resources into biological knowledge by using ensemble techniques, and showcase a few recent examples where computers are actually enabling us to not only simulate chemistry, but increasingly casting light on molecular biology.

Jesus Labarta - Barcelona Supercomputing Center

Prof. Jesús Labarta *received his Ph.D. in Telecommunications Engineering from UPC in 1983, where he has been a full professor of Computer Architecture since 1990. He was Director of European Center of Parallelism at Barcelona from 1996 to the creation of BSC in 2005, where he is the Director of the Computer Sciences Dept. His research team has developed performance analysis and prediction tools and pioneering research on how to increase the intelligence embedded in these performance tools. He has also led the development of OmpSs and influenced the task-based extension in the OpenMP standard. He has led the BSC cooperation with many IT companies. He is now responsible of the POP center of excellence providing performance assessments to parallel code developers throughout the EU and leads the RISC-V vector accelerator within the EPI project. He has pioneered the use of Artificial Intelligence in performance tools and will promote their use in POP, as well as the AI-centric co-designing of architectures and runtime systems. He was awarded the 2017 Ken Kennedy Award for his seminal contributions to programming models and performance analysis tools for high performance computing, being the First Non-US Researcher receiving it.*

POP: TOWARDS INSIGHT ON PROGRAM BEHAVIOR

The talk will describe the activities within the POP Center of Excellence in providing an external assessment to code developers on the behavior of their programs and best practices on how efficiency can be improved. The talk will present a computer science point of view, transversal to application domains, where methodology, models and data analysis techniques constitute the fundamental challenge to provide an external view useful for code owners and users.

Paul Kent - Oak Ridge National Laboratory

Paul Kent is a distinguished R&D staff member at the Center for Nanophase Materials Sciences and at the Computational Sciences and Engineering Divisions of Oak Ridge National Laboratory. He is the Director of the Center for Predictive Simulation of Functional Materials (https://cpsfm.ornl.gov/) and a principal investigator in the Exascale Computing Project (https://www.exascaleproject.org/). His research is in the field of electronic structure and on the development and optimization of quantum mechanics-based methods and their broad application to real materials problems.

TOWARDS RELIABLE AND ACCURATE MATERIALS PREDICTIONS AT EXASCALE

Quantum Monte Carlo (QMC) methods have long held the promise of quantum mechanics-based materials property predictions where all the errors and approximations can be checked and converged. In this talk I will outline the promises and challenges posed at Exascale for these methods, emphasizing the recent developments in the open-source real space and auxiliary field QMC code QMCPACK (https://qmcpack.org/). This is being developed at part of the Center for Predictive Simulation of Functional Materials, which brings together theorists, computational experts and dedicated efforts in experimental validation. QMCPACK is being significantly updated to support Exascale, and I will give some of the broadly applicable lessons learned so far.

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Session 3: Thursday July 2 2020

Cecilia Clementi - Freie Universität Berlin
Enabling software solutions to address outstanding science challenges in molecular sciences

Ignacio Pagonabarraga - CECAM
E-CAM: addressing modelling challenges in multiple scales in the HPC leading edge

Peter Coveney - University College London and University of Amsterdam
Supercomputing, COVID-19 and the transformation of medicine

Cecilia Clementi - Freie Universität Berlin
After 19 years as a Professor of Chemistry at Rice University, in Houston, Texas, since June 2020 Dr. Clementi is a Professor of Physics at Freie Universität Berlin, Germany. Dr. Clementi is also a senior investigator of the Center for Theoretical Biological Physics of Rice University and a co-director of the NSF-funded Molecular Sciences Software Institute (MolSSI). Dr. Clementi's research activities focus on the development and application of theoretical and computational tools to study the long-timescale dynamics of complex macromolecular systems, for the characterization of biological function. Over the years, Clementi's group has proposed coarse-grained and multi-resolution models and analysis tools to study protein dynamics, folding, and function.

ENABLING SOFTWARE SOLUTIONS TO ADDRESS OUTSTANDING SCIENCE CHALLENGES IN MOLECULAR SCIENCES
The field of computational molecular sciences -- quantum chemistry, materials science, and biomolecular simulation -- has made innumerable contributions to the understanding of the molecular phenomena that underlie and control chemical and physical processes. Today, the field stands as a "full partner with experiment" in scientific discovery and is central to solving the next generation of Grand Challenges facing the world's economy, health, and security. Since 2016, the NSF-funded Molecular Sciences Software Institute (MolSSI) is a nexus for science, education, and cooperation serving the worldwide community of computational molecular scientists. MolSSI builds open-source software and data which serves the computational molecular science community. It is designed to serve and enhance the software development efforts of the broad field of computational molecular science, with the goal to enable molecular scientists to tackle problems that are orders of magnitude larger and more complex than those currently within our grasp. I will discuss the ongoing activities of MolSSI in the context of the main scientific challenges faced by computational molecular scientists today.

Ignacio Pagonabarraga - CECAM
Ignacio Pagonabarraga is the CECAM Director since 2017. He is professor in Condensed Matter Physics at the University of Barcelona (Spain) since 2010. His research activity is focused on the development and use of computational and theoretical methods to understand and predict the properties and behavior of soft matter, with special emphasis in non-equilibrium systems and, more recently, active matter.

E-CAM: ADDRESSING MODELLING CHALLENGES IN MULTIPLE SCALES IN THE HPC LEADING EDGE

E-CAM, a Center of Excellence for Computing Applications, supports the development of scientific software with clear industrial and societal interest, in view of exploiting HPC resources. The developed software targets efficient implementation of existing algorithms and optimal first deployment of new methods. Through application co-design for HPC technologies, the provision of libraries and frameworks in domains relevant to exascale computing, such as high throughput computing and load-balancing, and delivery of the respective training, we push the community to exploit the HPC resources available at a European level. These developments open venues to address new scientific challenges across areas including rare events, electronic structure, quantum dynamics, and meso and multiscale modelling. E-CAM benefits from input and coordinated actions within the CECAM network, which includes leaders in each of these areas therefore providing a unique access point to broad simulation expertise. The capabilities of the network are demonstrated by the range of successful pilot project with academic and industrial partners that currently span applications in materials, quantum computing, and biophysics.

Peter Coveney - University College London and University of Amsterdam

Peter V. Coveney holds a chair in Physical Chemistry, is an Honorary Professor in Computer Science at University College London (UCL), a Professor in Applied High Performance Computing at the University of Amsterdam (UvA), and Professor Adjunct at Yale University School of Medicine (USA). He is Director of the Centre for Computational Science (CCS) at UCL. Coveney is active in a broad area of interdisciplinary research including condensed matter physics and chemistry, materials science, as well as life and medical sciences in all of which high performance computing plays a major role. He has published more than 440 scientific papers and co-authored two best-selling books and is lead author of the first textbook on Computational Biomedicine. Coveney is a founding member of the UK Government's E-Infrastructure Leadership Council and a Medical Academy Nominated Expert to the UK Prime Minister's Council for Science and Technology on Data, Algorithms and Modelling which has led to the creation of the London based Turing Institute.

SUPERCOMPUTING, COVID-19 AND THE TRANSFORMATION OF MEDICINE

To deliver a novel drug currently takes on average a decade or longer and costs billions of euros or dollars. As a result of COVID-19, we have no choice but to attempt to deliver treatments at pandemic speed. I believe supercomputers can fix the current broken model of drug development. By placing more emphasis on unravelling the mechanisms underpinning biology, physiology and pathology, using computer models that meet the most rigorous standards of verification, validation and uncertainty quantification, and by running them on the most powerful computers in Europe, America, Japan and globally, I believe we can achieve truly predictive bioscience, marking a paradigm shift in the way we develop new drugs that will transform medicine.

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Session 4: Thursday July 9 2020

Edouard Audit - CEA - Maison de la Simulation
EoCoE : Fostering the energy transition using HPC

Gianluca Palermo - Politecnico di Milano
Exscalate4CoV: Towards an exascale-ready docking platform targeting urgent computing

Edouard Audit - CEA - Maison de la Simulation
Edouard Audit is the coordinator of the EocoE center of excellence. He got a PhD in numerical astrophysics from the university of Paris 7. After 15 years in computational (astro)physics, he became the founding director of Maison de la Simulation.

EOCOE : FOSTERING THE ENERGY TRANSITION USING HPC
At the crossroad of the energy and digital revolutions, EoCoE develops and applies cutting-edge computational methods in its mission to accelerate the transition to the production, storage and management of clean, decarbonized energy. I will present the main technical challenge that EoCoE is addressing on its path to Exascale and show their impact on energy relevant simulations.

Gianluca Palermo - Politecnico di Milano
He is currently an Associate Professor with tenure at Politecnico di Milano, Department of Electronics, Information and Bioengineering. Previously he was consultant engineer in the Low Power Design Group of AST – STMicroelectronics (Agrate, Italy) working on network on-chip and research assistant at the Advanced Learning and Research Institute (ALaRI) of the Universita' della Svizzera Italiana (Lugano, Switzerland). His research interests include design methodologies and architectures for Embedded and High Performance Computing systems, focusing on multi/many-cores architectures, application autotuning, and extreme-scale molecular docking methods. Currently, he is the Principal Scientist for the PoliMi research unit within the Exscalate4CoV project.

EXSCALATE4COV: TOWARDS AN EXASCALE-READY DOCKING PLATFORM TARGETING URGENT COMPUTING
Exscalate4CoV is a public-private consortium supported by the European Commission's Horizon 2020 tender for projects to counter the Coronavirus pandemic and improve the management and care of patients. The aim of the project is twofold, identify molecules capable of targeting the coronavirus (2019-nCoV) and develop a tool effective for countering future pandemics to be consolidated over time. The Excalate4CoV consortium, coordinated by Dompé Farmaceutici, is composed of 18 institutions from seven European countries and can count on the top European Supercomputers.
At the core of the project, there is Exscalate (EXaSCale smArt pLatform Against paThogEns) a drug-discovery platform that includes a "chemical library" of several hundred billions of molecules and a processing capacity in the order of million molecules per second. Exscalate is a Dompè platform, developed thanks to a collaboration between Dompè, Cineca, and Politecnico di Milano. The platform, that has already been used in the study of the Zika virus, has been developed in the context of the Antarex project.

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Session 5: Thursday July 16 2020

Steven G. Louie - University of California at Berkeley and Lawrence Berkeley National Lab
Discovering Nature with Computation: HPC Study of Quantum Interaction Phenomena in Materials

Claudia Draxl - Humboldt-Universität and Fritz Haber Institute, Berlin
Detecting Materials Genes by High-performance Computing and Artificial Intelligence

Modesto Orozco - Institute for Research in Biomedicine, Barcelona
BioExcel Build Blocks and HPC. A test case in CoVID Research

Steven G. Louie - University of California at Berkeley and Lawrence Berkeley National Lab

Professor Louie received his Ph.D. in physics from University of California at Berkeley (UC Berkeley) in 1976. After having worked at the IBM Watson Research Center, Bell Labs, and U of Penn, he joined the UC Berkeley faculty in 1980, where he is professor of physics and concurrently senior faculty scientist at the Lawrence Berkeley National Lab. He is a member of the National Academy of Sciences, the American Academy of Arts & Sciences, and the Academia Sinica (Taiwan), as well as a fellow of the American Physical Society (APS), the American Association for the Advancement of Science, and the Materials Research Society (MRS). Among his honors, he is recipient of the APS Aneesur Rahman Prize for Computational Physics, the APS Davisson-Germer Prize in Surface Physics, the MRS Materials Theory Award, the Foresight Institute Richard P. Feynman Prize in Nanotechnology, the Department of Energy Award for Sustained Outstanding Research in Solid State Physics, as well as Jubilee Professor of the Chalmers University of Technology and H. C. Ørsted Lecturer of the Technical University of Denmark. Professor Louie's research spans a broad spectrum of topics in theoretical condensed matter physics and nanoscience. He is known for his groundbreaking work on the ab initio GW method and for his contributions to surfaces and interfaces, nanostructures, and reduced-dimensional systems.

DISCOVERING NATURE WITH COMPUTATION: HPC STUDY OF QUANTUM INTERACTION PHENOMENA IN MATERIALS

Many fascinating phenomena in nature owe their emergence from the interactions of large number of particles. Traditionally, their discovery and understanding are made through experiment and mathematical theory. Computation has increasingly become equally important as a third pillar in such studies. In this talk, I will discuss recent progress in use of HPC to compute and understand novel quantum phenomena in materials, especially those of excited states that are of importance in energy conversion, transport and storage. Many-electron interactions are dominant in many of these phenomena/properties. The Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) is a DOE funded center with the mission of developing new concepts, methods and software for excited-state phenomena using ab initio quantum many-body perturbation theory. I will present some of our recent accomplishments and future challenges in this effort.

Claudia Draxl - Humboldt-Universität and Fritz Haber Institute, Berlin

Claudia Draxl is Einstein Professor at the Humboldt-Universität zu Berlin, Germany, and Max-Planck Fellow at the Max Planck Graduate Center for Quantum Materials. Her research covers theoretical concepts and methodology of ab initio computational materials science. She is developer of the all-electron full-potential package ***exciting****, implementing density-functional theory and methods beyond, with a focus on theoretical spectroscopy. Actual research projects concern organic/inorganic hybrid structures, wide-gap oxides, thermoelectricity, solar-cell materials, film growth, and more. She is a founder of the NOMAD Laboratory (https://nomad-lab.eu) and the association FAIR-DI (https://fair-di.eu). Based on this open-access data infrastructure, her data-driven research aims at finding structure in Big Data of materials science.*

DETECTING MATERIALS GENES BY HIGH-PERFORMANCE COMPUTING AND ARTIFICIAL INTELLIGENCE

Research data paired with Artificial Intelligence (AI) enable a new level, a new quality of science. The ultimate goal in our research domain is to predict novel candidate materials for a given application, possibly even in regions of the materials space that no-one would think of. A real breakthrough is, however, only possible if a few key prerequisites are brought together: Big Data – the relevant data – reliable data – novel AI tools with predictive power, all combined in a FAIR data sharing platform. In 2014, the Novel Materials Discovery (NOMAD) Laboratory set out to make this happen, and I'll review where we are on this road.

Modesto Orozco - Institute for Research in Biomedicine, Barcelona

Modesto Orozco is Director of the Integrative Biology Program at the Institute for Research in Biomedicine, Barcelona, and of the Joint IRB-BSC Research Program in Computational Biology.

He acts as a consultant for scientific bodies in Spain and Europe and is the Founder and President of Nostrum Biodiscovery a Biotech Company devoted to rational drug design. Prof. Orozco has been, or is advisor for several biotech and pharmaceutical companies, among others: Lab. Uriach, Lab. Almirall, Lab. Salvat, Pfizer Inc., Boehringer Ing., Kraft Pharm., Lab. Palau Pharma, Amgen Inc., and Nurix Inc. He is the recipient of an advanced ERC grant, and coordinator of H2020 projects in the domain of biosimulations.

His main interest is the understanding of biological systems from first principles. Topics of specific focus include the understanding of the mechanism of flexibility and signal transduction in proteins and the connection between physical properties of nucleic acids and their function, with special emphasis in the study of chromatin. He also contributes to the development of the Self-Consistent Reaction Field method to account for polarization and is a developer of QM/MM approaches for large systems.

BIOEXCEL BUILD BLOCKS AND HPC. A TEST CASE IN COVID RESEARCH

We have developed a workflow technology especially developed for HPC which allows an efficient use of supercomputers in real biological problems. The method, developed within the BioExcel center of Excellence has been applied to study interplay between SARS-COV-2 genetic variability and infection and the zoonotic transmission of the virus. I will summarize the main characteristics of our BioBB-Pycommps implementation, and the knowledge gained on the viral genomics

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