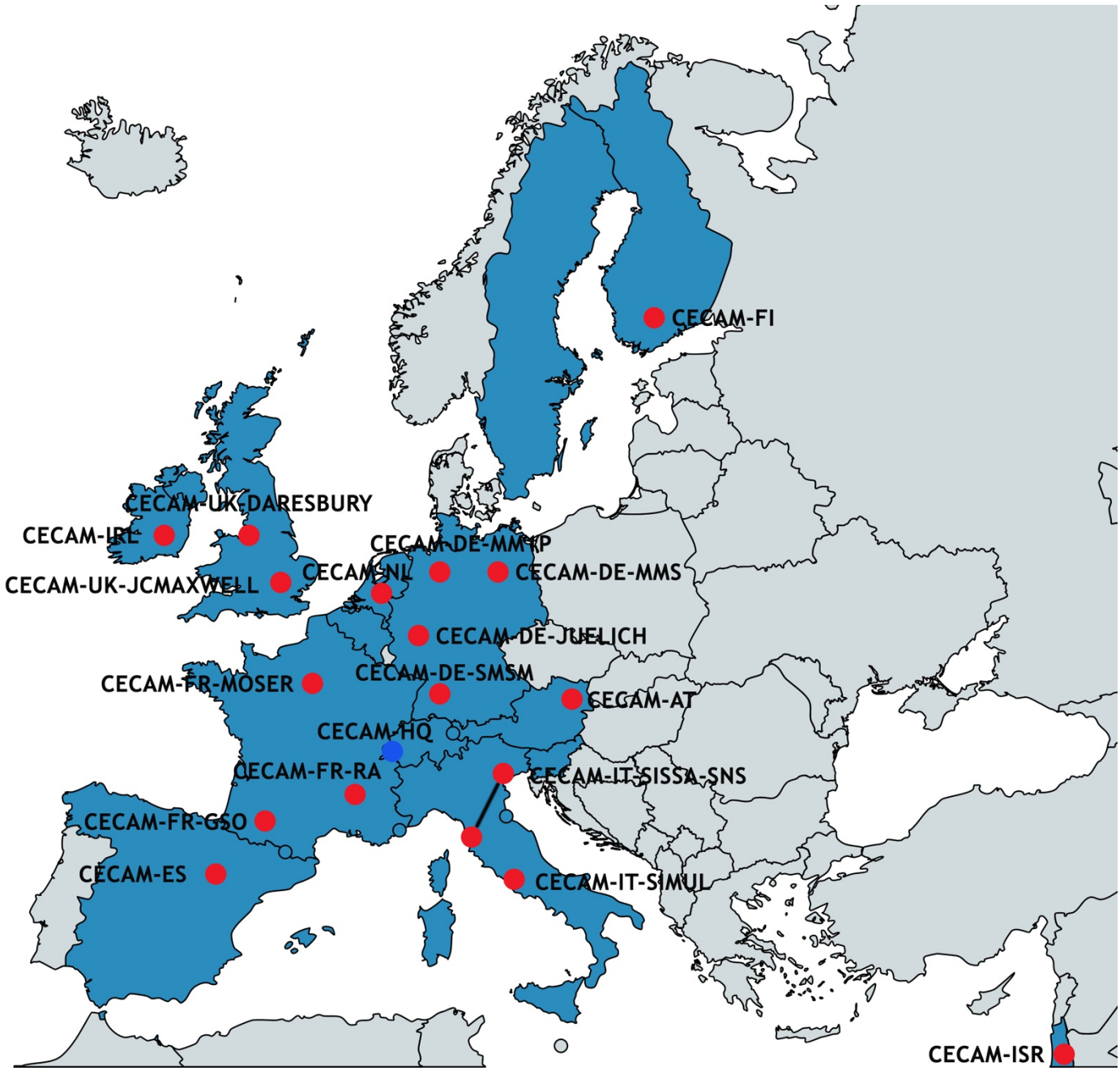
Workshops Scientific Reports

2017



cecam
Centre Européen de Calcul Atomique et Moléculaire

Table of Contents

Introduction

This publication collects the scientific reports summarizing the key outcomes of the workshops held at CECAM in 2017. These workshops were selected, following a well-established and rigorous peer review based solely on scientific excellence, from proposals received from the community of researchers. The events were funded via the contributions of our Member Institutions and carried out with the logistic and technical support of personnel at Headquarters (HQ EPF-Lausanne) and in the nodes. The acceptance proposal rate for the 2017 call was 73%, reflecting a good balance between strong and fair competition between the proposed workshops, in particular for events at CECAM HQ, and the excellent quality of most of the submitted proposals.

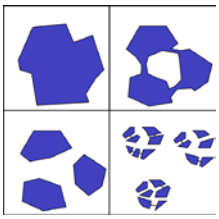
The contents of the 46 workshops in the 2017 CECAM Flagship program reflect the broad, interdisciplinary and intersectorial, interests of our community, while maintaining the traditional focus on methods and algorithm developments. 15 workshops were hosted in Switzerland (12 at EPF-Lausanne, 1 at ETH Zürich, 2 at USI Lugano) and 31 in the 17 CECAM nodes in Europe and Israel. Overall, the activities described here reflect the growing impact of simulation and modelling in topics ranging from physics to chemistry, from biology to engineering and highlight the continued relevance of fostering collaborations, development of new ideas, and efforts to transfer consolidated techniques to a broader audience. The series of workshops related to E-CAM (www.e-cam2020.eu), a project funded by the E-INFRA5 Horizon2020 action to create Centers for Computing Applications and coordinated by CECAM, continued with growing success. The reports for the State-of-the-Art, Scoping (interactions with industry), and Software Development workshops of this initiative are presented in a specific section of this publication.

In addition to the workshops documented here, 19 schools dedicated to advanced and basic training of the next generation of simulators were held in the CECAM network in 2017.

The number of participants to our events, 2530 scientists at different stages of their carrier, registered a noteworthy increase compared to last year (2080 participants). Female participation also increased slightly, passing from 20 to 23% an encouraging, though still not satisfactory, result. Junior scientists were encouraged to play an active role as participants and organizers.

CECAM continues to play a central, internationally recognized, role in simulation and modelling. The scientific excellence of the meetings hosted in our network, the informal, open and careful discussions focused on new ideas and unsolved questions, and the commitment to training in schools where young practitioners can meet and interact with leading experts in the field are the CECAM trademarks upon which our service to the community is founded. We hope that this journal of activities for 2017 will document our efforts and indicate current directions in the field, inspire new activities and stimulate suggestions from the community to continue and enhance our work.

Recent Advances on the Glass and Jamming Transitions



Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1284.html
Dates: January 9, 2017 to January 11, 2017

1 State of the art

This workshop considered various perspectives on the “glass problem”, building on recent theoretical and computational advances. The workshop touches upon various facets of the glass problem that have for a long time been relatively disconnected, including:

- Glass formation: Liquids, when rapidly cooled, solidify in an amorphous state in which the disorder is self-generated.
- Low-temperature glasses: Glasses that are further cooled display unexpected transport and thermal properties. The importance of the recently proposed Gardner transition in this regime is of particular interest.
- Jamming: Collections of frictionless soft spheres can exhibit a jamming transition (the onset of mechanical rigidity) at zero temperature as a function of packing fraction.
- Granular physics: Macroscopic collections of objects, such as rice in a silo or coal in a hopper, can jam, which makes their dynamics and statics similar to that of the ground states of other disordered systems. In addition, recent evidence suggests that these systems can also exhibit a Gardner transition.
- Colloidal glasses: Colloidal suspensions, when raised to high density, can behave become solids although their structure remains disordered, and thus can undergo a glass transition.
- Active matter: a high-density, strongly out-of-equilibrium active matter displays marked changes of behavior reminiscent of glass formation and jamming. Recent progress has revealed deep and somewhat unexpected links between these subfields, and some of these findings are only starting to be understood or more simply consolidated by an important theoretical and experimental research effort. We believe that further progress on the glass problem requires a sustained, interdisciplinary effort taking all these different directions carefully into account, which represented a central goal of the workshop.

2 Major outcomes

Although mostly theoretical, several contributions made very interesting connections between theory and experiments. In particular, a novel method to detect relevant length scales using nonlinear dielectric responses was presented, as well as a theoretical analysis of aging and glassy dynamics in a variety of systems, from crumpled sheets to disordered electronic systems and active materials. A new Monte Carlo-based approach for enhancing the sampling rate in computer simulations of supercooled liquids were presented, which appears to bypass any other known algorithm, and several on-going theoretical and computational projects were presented in talks and posters which are made possible by this methodological advance. For instance, it has enabled a study of the merits and properties of the recent experimental discovery that a new type of ultrastable glasses can be produced using a process called chemical vapor deposition. These early results are in sharp contrast with an extended body of literature, which is a surprising yet robust outcome of this analysis. In a parallel numerical study, the kinetic properties of these stable glassy configurations as they melt upon heating were presented during the poster session. An important number of contributions were dedicated to the existence, properties and physical consequences of the recently discovered Gardner phase transition, which is supposed to take place deep inside the glass phase. Specifically, numerical investigations of the existence of such a phase transitions were presented for various model systems, and for one experimental set-up dealing with granular materials. Theoretical investigations of the phase transition in finite dimensions were discussed, as well as a mean-field treatment of the physical consequences of the existence of a Gardner phase on elastic properties of amorphous solids, which received good support from a set of unpublished computers simulations in finite dimensions. Two novel directions that appear at opposite ends of the spectrum of disordered physical systems were also discussed. First, several contributors discussed the physics of “active glasses”, mostly drawing inspiration and ideas from the physical behavior of biophysical systems such as dense epithelial tissues or allosteric materials. Second, ideas inspired by the physics of glassy materials were shown to have deep connections with exciting quantum problems, such as the physics of black holes and the field of many-body localization.

3 Community needs

The main goal of the workshop was to connect and unify various subfields of the glass problem, in order to enhance and foster collaborations between people having different perspectives on glassy materials. It appears clear that similar models and ideas can be used on different systems, but also that ideas that appear different at first sight may finally have more in common when properly compared. This type of “unification” has been particularly clear during this workshop between the jamming and glass communities, that have long lived a parallel life but are now part of the same research effort. One conclusion of the meeting is that more unifying efforts in this direction should be made, and that meetings such as the present ones should continue to be organized towards this major goal. We had left a great deal of common discussion after each group of talks, in order for the different communities to appreciate better similarities and differences in the methods that are being used. We believe that the research will benefit from such format, and this should help the community to buildnew connections and collaborations in the future. As organizers we had also made an effort so that a large proportion of the audience was composed of PhD students and young postdocs, giving some of them the opportunity to present their own work. We feel that the community will benefit from having young minds coming together and enjoying and also enriching the physics we do in our field.

4 Funding

This workshop actually coincided with the recent grant allocation for a large collaborative effort on the topic of the workshop. This workshop has thus allowed the various members of this collaboration as well as the broader community to sharpen the intellectual and scientific goals that will ensure the proper spending of these resources and their potential renewal. In the future, the “unification” of the various themes mentioned above should presumably give rise to novel opportunities for further funding’s. We expect that novel ideas and projects will emerge soon from our efforts, allowing both young and senior members of our community to apply to various grants, such as ERC grants within the Horizon 2020 European funding scheme.

5 Will these developments bring societal benefits?

Disordered and frustrated systems comprise a vibrant research area in condensed matter physics with applications in fields ranging from mathematics to biology. At their core, these systems share universal features such as rough free energy landscapes and rich sets of phase transitions that can be understood and unified with ideas from physics. This understanding largely arises from the study of glassy systems, which since the 1980s has led to a rich array of concepts, methods and tools that describe systems as diverse as piles of grains, biological tissues and computer algorithms. Although for now these topics are mostly theoretical, there are some potential applications to concrete problems. First of all, the development of new protocols to produce deeply equilibrated glasses, in particular vapor deposition, allows one to produce materials with particularly interesting properties: enhanced rigidity, lower concentration of defects, lower specific heat, etc. During the workshop, computer simulations of such systems have been discussed, which will be very useful to understand their properties. Moreover, the physics of plasticity in amorphous solids can be applied to living tissues, with potentially interesting biological applications, and to other technologically relevant materials. Finally, ideas from the physics of glasses are currently being applied to the vibrant field of machine learning, that nowadays has applications in almost all relevant fields of technology.

6 Participant list

Organizers

Berthier, Ludovic
Laboratoire Charles Coulomb UMR 5221 CNRS - Université de Montpellier, France

Charbonneau, Patrick
Department of Chemistry, Duke University, USA

Zamponi, Francesco
LPT, ENS Paris, France

Agoritsas, Elisabeth - LPT-ENES, France

Altan, Irem - Duke University, USA

Altieri, Ada - Università degli Studi di Roma Sapienza & Université Paris-Saclay, Italy

Amir, Ariel - Harvard, USA

Baity Jesi, Marco - CEA Saclay, France

Banerjee, Atreyee - Post doctoral research associate, United Kingdom

Barrat, Jean Louis - Université Grenoble Alpes, France

Bartolomé, Beatriz Seoane - CEA, France

Biroli, Giulio - CEA Saclay, France

BOMONT, Jean-Marc - Université de Lorraine, France

Byron, Guy - CECAM, Switzerland

Cammarota, Chiara - INFN, La Sapienza, Rome, Italy, Italy

Corwin, Eric - University of Oregon, USA

Coslovich, Daniele - Université de Montpellier, France

Dauchot, Olivier - ESPCI, France

DeGiuli, Eric - NYU, USA

Flenner, Elijah - Colorado State University, USA

Franz, Silvio - Paris-Orsay, France

Fullerton, Christopher - Laboratoire Charles Coulomb, Université de Montpellier, France

Hexner, Daniel - University of Chicago, James Franck Institute, USA

IKEDA, Atsushi - Graduate School of Arts and Sciences, The University of Tokyo, Japan

Ikeda, Harukuni - Department Physics, Nagoya University, Japan

Janssen, Liesbeth - Eindhoven University of Technology, Germany

Jin, Yuliang - Osaka University, Japan

Kallus, Yoav - Santa Fe Institute, USA

Kob, Walter - University of Montpellier, France

Kurchan, Jorge - ESPCI, France

Landes, François - UPenn, USA

Liu, Andrea - U Penn, USA

Manning, Lisa - Syracuse, USA

Marruzzo, Alessia - LPTMS-CNRS, CNR Nanotec Unit of Rome, Italy

Martiniani, Stefano - Cambridge University, United Kingdom

Morse, Peter - Syracuse University, USA

Ninarello, Andrea Saverio - University of Montpellier, France

Nussinov, Zohar - Washington University in Saint Louis, USA

Ozawa, Misaki - University of Montpellier, France

Parisi, Giorgio - Roma I "la sapienza" University, Italy

Pereira da Cruz Benetti, Fernanda - Universidade Federal do Rio Grande do Sul, Brazil

Rainone, Corrado - Weizmann Institute of Science, Israel

Reichman, David - Columbia University, USA

Ridout, Sean - University of Pennsylvania, USA

Ros, Valentina - SISSA- International School for Advanced Studies, Italy

Royall, Paddy - University of Bristol, United Kingdom

Ruscher, Céline - Institut Charles Sadron, France

Scalliet, Camille - Laboratoire Charles Coulomb UMR 5221 CNRS - Université de Montpellier, France, France

Spigler, Stefano - Universite" Paris Sud, France

Szamel, Grzegorz - Colorado State University, USA

Tarjus, Gilles - LPTMC, Université Pierre et Marie Curie, France

Tsekenis, Georgios - University of Oregon, USA

Urbani, Pierfrancesco - CEA, France

Wyart, Matthieu - Swiss Federal Institute of Technology Lausanne, Switzerland

Yaida, Sho - Duke University, USA

Yoshino, Hajime - Osaka University, Japan

2nd NOMAD (Novel Materials Discovery) Industry Workshop

Location: Hamburg
Webpage: https://www.cecam.org/workshop-0-1377.html
Dates: February 6, 2017 to February 7, 2017

1 State of the art

The objective of the NOMAD Laboratory European Center of Excellence include the creation of a materials encyclopedia, and the development of big-data analytics and advanced graphics tools for materials science and engineering. The NOMAD Researchers are currently creating a large, homogenized materials database, as well as the analytical tools and code developments necessary to extract information from it. An essential corner stone of the project is the NOMAD Repository, which contains the produced data and records, the input and output files of many high-quality calculations performed by fellow researchers working all over the world. The Repository is unique in the sense that it is not restricted to one or a few simulation programs ("codes") but it accepts output from all important codes. As of early July 2016, it contained results from more than 3 million different calculations, corresponding to billions of CPU-core hours used on several high-performance computers all over the planet. Recently, there has been a very significant growth of industrial interest in computational materials science, motivated by the innovation potential of new materials and improved existing materials. However, the scientific complexity of the topic and the heterogeneous and fragmented nature of the research field make it difficult to translate research leadership into accomplished innovation.

Thus, it is particularly important at this point in time to bring materials modelling closer to industrial/societal exploitation in real terms. We strive to establish among EU-based industries full awareness of the extent to which the wealth of newly available data could boost their competitiveness. To raise industrial interest, the potential of big-data activities to foster industrial business will have to be made an apparent in practical terms.

2 Major outcomes

Industry Networking

NOMAD has been actively gathering feedback from industry during an initial “Listening Phase” and has evaluated this information in order to determine how to make NOMAD useful for industry. Based on feedback from industry representatives and IAC members, several recommendations have been already implemented. For example, an on-site usage of the platform has been provided for industrial users during the development. In order to ensure uptake of NOMAD tools and services by industry, the NOMAD team wants to ensure that there are minimal barriers to use for industry users. Industry representatives have suggested the possibility of facilitating in-house usage of NOMAD to minimize potential intellectual property rights (IPR) issues.

Furthermore, already two case studies have been carried out in collaboration of academia and industry. Aiming to strengthen this collaboration more case studies are planned.

NOMAD Encyclopedia

NOMAD Encyclopedia is accessible to various types of users (engineers, material scientists, non-experts) and provides general reviews and statistics via a WEB interface.

Up until now, around 400,000 materials have been registered. As suggested at the Industry Meeting last year several features have been added to the Encyclopedia. Among others, a user-friendly GUI has been developed, which enables users to perform a property-based search. In the future, the NOMAD team will add more system types and methodologies to the already existing features.

NOMAD Big-Data Analytics Toolkit

The objective of the NOMAD Big-Data Analytics Toolkit is to facilitate the design of new materials with desired properties; many of the tools apply machine-learning methods to data originating from computational high-throughput methods.

The structure of the NOMAD Big-Data Analytics Toolkit is a combination of a software framework and notebook representation of the actual analytic task.

In the future, the NOMAD team will increase the breadth of the analytic tools, in terms of both methodology and example cases.

NOMAD Advance Graphics

The innovative methods developed allow both for local visualization running on researchers’ workstations, as well as remote visualization tools running on HPC clusters.

Local visualization tools also cover immersive virtual reality (VR) environments. Local tools are complemented by remote visualization tools, which allow for visualization of datasets too large for ordinary workstations, but with a lesser degree of interactivity.

In the future, there will be a closer integration between the Advanced Graphics and the NOMAD Encyclopedia. Furthermore, workshops on the visualization tools in general (September 2017) and the VR tools in particular (April 2018) were announced - both will be open to the participation of industry representatives.

3 Community needs

Two of the main concerns within the industry members are IP and Sustainability issues as well as data quality and usability.

Furthermore, dissemination measures and increase visibility of NOMAD were also addressed as worthwhile. In this context, case studies to demonstrate NOMAD value would be welcome, to help internal 'selling' of collaboration with NOMAD.

IP

A top priority is to protect commercial data, which should not leave commercial environments. NOMAD and data should be able to be downloaded behind the industrial firewalls before performing any kind of sensitive data analytics on it. The local installation of data analytics tool also regards the topic of managing sensitive data and IP and this suggestion was received with mixed enthusiasm among our partners.

Data and Usability

The wish for more tutorial services (training material/courses) and a user-friendly GUI interface to reduce the barrier to use the NOMAD tool was expressed. Searches for properties, rather than materials as well the integration of additional data on a wider range of material properties (bulk properties, surfaces, derived qualities) and experimental data etc. are features that would improve the usability of NOMAD. To a lesser degree searches for authors i.e. networking factor, were also mentioned.

One of the challenges of using NOMAD is to combine in-house data with NOMAD data for cross-analysis, the in-house data must be similarly formatted and of a similar quality to NOMAD (archive) data.

Among other request we find the need for NOMAD to be visible (online, conferencces, etc) and more case studies, which are already planned.

4 Funding

The NOMAD initiative is currently formed by a merging of two projects (the NOMAD Laboratory CoE and the NOMAD Repository) and receives funding from the European Union's Horizon 2020 research and innovation program. On the long-run, applying for a second funding phase beyond the Horizon 2020 funding is planned. The Max-Planck Society has already guaranteed to reassurance the lifetime of the NOMAD Repository for 10 years from last data upload.

Concerning more short-term related funding topics it was agreed upon that reaching out to SMEs needs lower-commitment, low-cost activities (e.g. webinars).

5 Will these developments bring societal benefits?

Since one of the main goals of NOMAD is to be useful to the industry and work in close collaboration with them, the success of this project would immediately deliver several societal benefits such as:

- Setting a standard on how to deal with large data sets but also small-sized datasets (quality and consistency)
- Enabling efficient searches for a wide range of materials properties thus enabling the selection of the most promising materials for a given application. This comprises significant saving time and economic ressources which be beneficial for the industry.
- Promoting constructive resources and information exchange between industry and research institutions and among industry itself.
- Encouraging the embedding and student placements in industry
- Contributing in closing the gap between academic and industrial research

6 Participant list

Organizers

De Vita, Alessandro
King's College London and University of Trieste, United Kingdom

Rubio, Angel
Max Planck Institute for the Structure and Dynamics of Matter, Germany

Sanguino, Graciela
Max Planck Institute for the Structure and Dynamics of Matter, Germany

Scheffler, Matthias
Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany

Filip, Sorin - BP Formulate Products Technology, Research & Innovation, United Kingdom

Ghiringhelli, Luca M. - Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Hernández, Rubén García - Leibniz-Rechenzentrum, Munich, Germany

Huhs, Georg - Barcelona Supercomputing Center, Spain

Klinge, Michael - Springer Material, Springer Verlag Heidelberg, Germany

Pankajakshan, Praveen - Shell India Markets Private Limited, Bangalore, India

Spitaler, Juergen - Materials Center Leoben Forschung GmbH, Austria

Wimmer, Erich - Materials Design, USA

Challenges across Large-Scale Biomolecular and Polymer Simulations

Location: CECAM-AT
Webpage: https://www.cecam.org/workshop-0-1295.html
Dates: February 21, 2017 to February 24, 2017

1 State of the art

Molecular modeling is the science of studying molecular structure and function through model building and computation. In the 1960s, the development of molecular mechanics force fields with energy minimization for refinement of crystal structures led to the development of molecular dynamics (MD) approaches now available in simulation packages such as NAMD, Desmond, or GROMACS.

MD simulations have evolved from the first 1-microsecond simulation of a villin-headpiece in 1998 to the current simulations of much larger biomolecular systems (e.g., an entire satellite mosaic virus with one million atoms) as well as longer time frames (e.g. B-DNA dodecamer, ubiquitin, and beta2 AR protein receptor) for over 1 microsecond, and small proteins for 1 millisecond with specialized MD programs and dedicated supercomputers.

For some proteins, fully atomistic folding simulations can be very successful, and similarly for nucleic acids both atomistic and coarse-grained ribosomes and long DNA minicircles and plasmids. At the same time, coarse-grained models and combinations of enhanced sampling methods are emerging as viable alternatives for simulating complex biomolecular systems.

Various scale coarse-graining allowed to address fundamental questions in protein folding with applications to diseases, such as Alzheimer, RNA folding, DNA assemblies and topologies, protein- protein interactions, DNA chromatin structure and condensation, and many others.

The quantitative accuracy reached by all the description levels allows for a flux of information from the atomistic detail up to complex simulations of cellular mechanisms done with event driven algorithms, up to simulations of whole cells.

In parallel, polymer physics, starting from the pioneering work of P.G. de Gennes, has been developing approaches to the study of complex polymer systems both on the size and time scales and o the complexity of the components.

2 Major outcomes

The workshop emphasized the need to continuously develop and integrate three components of simulations, namely model development, sampling algorithms, and infrastructural tools for trajectory simulation, analysis and visualization.

Model building:

This area comprises the development of models at different scales from atomistic to mesoscopic.

The atomistic force fields for proteins appear to have reached a satisfactory level and are indeed used for long simulations of large systems, while nucleic acids force fields are still an active area of development, in particular for the study of systems departing from double helical DNA.

Polarizable force fields are still under active development and are still too expensive computationally to be included in most simulations.

A variety of coarse-grained models of different resolution has been developed for both proteins and nucleic acids, aiming at various purposes, from folding to rational design. One of the main difficulties in developing such models is the parametrization, which requires the integration of many different sources of data (for instance, thermodynamic, structural, and kinetic data). Still, these methods have proven their usefulness to overcome the sampling problems of atomistic simulations.

Mesoscopic models are able to address the dynamics of proteins such as molecular motors as a whole, adopting a continuum description of the system, or study the properties of long stretches of DNA. They often integrate concepts and techniques from polymer physics as well as from the engineering of macroscopic systems.

Winning strategies in model building are integrating different levels of description for the systems into multi-scale simulations.

Sampling:

Simulations of large macromolecular objects require the use and further development of enhanced sampling techniques.

When the initial and final states are known, path sampling and biased dynamics are efficient tools to study the transition and unveil transition pathways, kinetic barriers, and metastable states.

Experimental information, when available, can also be integrated into some simulations, in particular by coarse-grained and mesoscopic models, where this is practically more feasible than in atomistic simulations.

The advantage of simulations is their ability to generate a multitude of possible states for a given system. Simulations now focus on generating ensembles of conformations rather than on obtaining a single structural prediction.

Analysis tools:

All the non-standard models and methods described above require a specific treatment of the data they generate. Most research groups develop their own trajectory descriptors, order parameters, topology and architecture descriptor. It would be useful to have wider communications on these tools (a web repository?) to share these tools with the community.

New technologies open the way to innovative tools to analyse simulation data with the interplay between state-of-the-art visualisation tools (3D, virtual reality,) and embedded analysis.

The participation at the meeting of scientists from the biomolecular and polymer simulation communities further expanded the discussion of the themes mentioned above. Within the biomolecular community, an important result of the meeting was to bring together scientists working on the modelling of both proteins and DNA/RNA. The development of hybrid protein/DNA models is an important future step that the biomolelcular simulation community is investing considerable effort in achieving and was a central discussion point.

3 Community needs

1) Needs for computational infrastructure:

One clear message that was repeated in several contributions was that all the studies require large-scale HPC facilities to be performed. The accurate models on the market at the moment are still very expensive to simulate at the space and time scales needed for the problems addressed. Interesting solutions have been presented during the workshop with innovative minimalistic models that, while maintaining the necessary accuracy, could be a game changer on the computational costs side.

2) Needs for networking:

The networking was one the main objectives of the workshop. In fact, the main motivation was to gather leading scientists, from a wide spectrum of disciplines ranging from biophysics to material sciences. Two aspects were strongly supported during the discussion: the first is the need for strong collaboration between theoretical and experimental research to refine and test the current modelling methods; the second was the necessity of analysis and data resources

shared across the community to uniform the comparison of the results. The meeting provided the ideal opportunity to gather scientists, both with a theoretical as well as experimental background, that are interested and willing to discuss different approaches and issues to make an advance in this relevant field.

3) Needs for event organisation:

The success of the meeting and the feedback from many participants that appreciated the novel wide interdisciplinary program suggests that it would be important to continue such event into a recurrent meeting opportunity either every two years alternated with a similar repeating meeting in the US.

Such frequency and alternation will help tighten the bonds between the scientific communities across the ocean.

4 Funding

During the meeting, several discussions occurred about funding options to support research collaboration within Europe (e.g. Horizon2020 and ETN network grants) and between Europe and USA. For the latter, we found that list option was rather limited and strongly variable from country to country. It became rapidly evident that it was necessary to formulate a strategy to fill such a gap. The funding necessary to keep alive a regular meeting on the subject was found as a crucial initial step to support the collaborations.

5 Will these developments bring societal benefits?

Quoting the Nobel Prize for chemistry 2013

“Today the computer is just as important a tool for chemists as the test tube. Simulations are so realistic that they predict the outcome of traditional experiments” (http://www.nobelprize.org). Such a statement might appear bold but it does describe the growing importance of computer modelling across modern Biochemical research.

For instance, polymers are still a central material in the modern industrial production. The design and development of novel smart materials with environmental response or complex composite material could profit enormously from advanced large-scale computer simulations capable of scanning a wide spectrum of combinations faster and cheaper than what can be done with experiments.

For medical applications, the field of drug design is in desperate need of a better understanding of protein-protein, protein-drug and protein-DNA/RNA interactions. The solution of the latter could open the way to a larger use of computational methods to speed up and the reduce the costs of the search for new drugs.

All the topics above have been extensively discussed during the meeting and there was an opportunity to have a debate on the role of science in the development of sustainable technologies.

From the program of the workshop, it is immediately clear that the topic is highly interdisciplinary and has a wide spectrum of social and industrial impacts.

6 Participant list

Organizers

Capone, Barbara
Università degli Studi Roma Tre, Italy

Coluzza, Ivan
Center for Cooperative Research in Biomaterials, Spain

Dellago, Christoph
University of Vienna, Austria

Pasquali, Samuela
Paris Descartes University, France

Schlick, Tamar
New York University, USA

Baaden, Marc - CNRS-Institute of Physico-Chemical Biology, Paris, France

Bianchi, Emanuela - Institute for Theoretical Physics, TU Wien, Austria, Austria

Bianco, Valentino - University of Vienna, Austria

Bolhuis, Peter - University of Amsterdam, The Netherlands

Boresch, Stefan - University of Vienna, Austria

C. Smith, Jeremy - Oak Ridge National Laboratory, USA

Calligari, Paolo - University of Rome - Tor Vergata, Italy

Cardelli, Chiara - University of Vienna, Austria

Chebaro, Yassmine - CNRS, Institut de Génétique et de Biologie Moléculaire et Cellulaire, Strasbourg, France

D. Davari, Mehdi - RWTH Aachen University , Germany

de Groot, Bert - Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

de Llano, Elisa - Austrian Institute of Technology, Austria

Dharan, Nadiv - Department of Biomedical Engineering, Ben-Gurion University of the Negev, Israel

Doye, Jonathan - University of Oxford, United Kingdom

Elber, Ron - UT Austin, USA

Emperador, Agusti - Institute of Advanced Chemistry of Catalonia, CSIC, Spain

Faccioli, Pietro - Physics Department of Trento University, Italy

Freddolino, Peter - University of Michigan, USA

Frezza, Elisa - Université Paris Descartes, France

Garcia, Angel - Rensselaer Polytechnic Institute, USA

Garon, Arthur - University of Vienna, Austria

Goethe, Martin - University of Barcelona, Spain

Grubmüller, Helmut - Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Güssregen, Stefan - Sanofi-Aventis Deutschland GmbH, Frankfurt am Main, Germany

Harris, Sarah - University of Leeds, United Kingdom

Hummer, Gerhard - Max Planck Institute of Biophysics, Germany

Ibrahim Adam, Yagoub Ali - University of Sao Paulo, Brazil

Im, Wonpil - Lehigh University, USA

Ivanov, Ivaylo - Georgia State University, USA

Jin, Fan - Max Planck Institute for Terrestrial Microbiology, Germany

Kirmizialtin, Serdal - NewYork University Abu Dhabi, United Arab Emirates

Kulczycka-Mierzejewska, Katarzyna - University of Warsaw, Poland

Kuzmanic, Antonija - IRB Barcelona, Spain

Lahiri, Ansuman - University of Calcutta, India

Lattanzi, Gianluca - University of Trento, Italy

Locatelli, Emanuele - University of Vienna, Austria

Lohrasebi, Amir - University of Isfahan, Iran

Melchionna, Simone - IPCF - Consiglio Nazionale delle Ricerche, Italy

Micheletti, Cristian - International School for Advanced Studies (SISSA), Trieste, Italy

Mohammadyarloo, Zahra - Institute for Advance Studies in Basic Science, Iran

Mouhib, Halima - Laboratoire de Modélisation et Simulation Multi Echelle, Université Paris-Est, France

Nerattini, Francesca - Computational Physics Group - University of Vienna, Austria

Nilsson, Lennart - Karolinska Institutet, Sweden

Oostenbrink, Chris - University of Natural Resources and Life Sciences, Austria

Oprzeska-Zingrebe, Ewa Anna - University of Stuttgart, Germany

Orozco, Modesto - University of Barcelona and Institute for Research in Biomedicine, Spain

Piotto, Stefano - University of Salerno, Italy

Potestio, Raffaello - University of Trento - Physics Dept., Italy

Rosa, Angelo - International School for Advanced Studies (SISSA), Trieste, Italy

Rudzinski, Joseph - Max Planck Institute for Polymer Research, Germany

Sanbonmatsu, Karissa - Los Alamos Natl. Lab., USA, USA

Singh, Kuldeep - MLSM College Sundernagar, Himachal Pradesh University Shimla, India

Steinhauser, Othmar - University of Vienna, Austria

Theodorou, Doros - National Technical University of Athens (GR), Greece

Thirumalai, Dave - University of Maryland, MD, USA

Tubiana, Luca - University of Vienna, Austria

Vendruscolo, Michele - University of Cambridge, United Kingdom

Walther, Jürgen - IRB Barcelona, Spain

Walton, Pauline - University of East Anglia, United Kingdom

Wieder, Marcus - University of Vienna, Austria

Zimmermann, Olav - Forschungszentrum Juelich, Germany

Challenges in crystal plasticity: from discrete dislocations to continuum models

Location: CECAM-Lugano, Lugano, Switzerland
Webpage: https://www.cecam.org/workshop-0-1306.html
Dates: February 27, 2017 to March 1, 2017

1 State of the art

Plasticity of crystalline materials is a perfect example of a multi-scale phenomenon: it is affected by the specimen shape, the electronic structure of the constituent atoms and many further features with characteristic scales between these limits. The main goal of the workshop was to initiate progress in linking two particular scales involved, that is, those of discrete dislocations and continuum plasticity.

The corresponding research activities date back to many decades and mainly focused on developing models that properly describe dislocation patterns that form upon plastic deformation. Some of these models were purely phenomenological while others did include some properties of the physics of discrete dislocations. These models were successful in describing pattern formation in different simplified situations, but a general continuum plasticity model applicable for any loading condition is still lacking.

The progress has somewhat slowed down recently, because there are intriguing conceptual questions that have not been answered by the community yet, for example

- What are the minimum ingredients one should include in continuum models?
- How to perform the coarse graining between the scales correctly?
- What is the role of intermittency, and should it be included in continuum models?
- How to represent internal inhomogeneities in continuum descriptions?
- What are the most important conceptual differences between crystal and amorphous plasticity?

The intention of the workshop was to discuss and answer these questions by bringing together top researchers of various sub-fields of plasticity.

2 Major outcomes

As suggested by the title of the workshop, the main discussions focused on the overarching problem of multiscale modeling, and particularly on coarse-graining methodologies/strategies to link small, meso and large scales. This is a classical and ubiquitous problem in material science, but which became particularly sharp in the field of crystal (and amorphous) plasticity modeling in recent years. More specifically, the following problems were discussed:

- From atomistic to nodal representation of dislocations in discrete dislocation dynamics (DDD) modeling
- From DDD to mesoscale modeling
- From mesoscale to continuum, classical and large-scale modeling of plasticity

Note that different mesoscale approaches have been discussed, such as lattice models (particularly in case of amorphous plasticity) or mean-field descriptions.

The discussions during this workshop raised, in a general and classical sense, the problem of coarse-graining small-scale variables (e.g. discrete dislocation dynamics) to meso- (e.g., through the definition/parameterization of dislocation densities) and continuum (e.g., definition of a strain) scales. It was demonstrated that in order to give a kinematically correct description of 3D continuum density fields one has to include the loop density of dislocations in the evolution equations. In addition, a continuum dislocation model was presented in which a cellular dislocation structure develops very similar to experimental findings.

Another overarching topic covered by the workshop was the intermittent, avalanche-like nature of plastic deformation. Indeed, over the last two decades, it became apparent that amorphous and crystal plasticity, at least in pure metals, can proceed through intermittent bursts of activity with scale-free properties. In addition, this intermittency is particularly pronounced in small-sized (sub-micrometer) systems, whereas patterning effects might mitigate the development of fluctuations at larger scales. These challenges numerical modeling of plasticity in two ways: (i) How can we coarse-grain a dynamical process characterized by scale-free avalanches, and (ii) how can we model the emergence of complex dislocation patterns (e.g. dislocations cells) in meso- to large-scale models of plasticity? As it emerged at the workshop a key ingredient in continuum models is to represent local inhomogeneities using a stochastic field variable. By including such a term in the continuum models, they were able to model scale-free avalanches, the main features of microplasticity

and dislocation pattern formation, too. It turned out that this particular aspect is also a hot topic in the amorphous community, where the statistical properties of inhomogeneities seem to be responsible for shear banding, fracture and scale-free events. The different approaches used by the two communities inspired lengthy discussions and promising new ideas.

A significant fraction of the talks focused on applications of crystal plasticity, such as plasticity of colloidal crystals, and nuclear materials as well as interpretation of nanoindentation data. These talks not only provided nice examples of applied materials modeling but also emphasized the technological importance of the main aim of the workshop, that is, linking discrete and continuum dislocation scales.

3 Community needs

Dislocation-based crystal plasticity is a field that exists now for more than half a century. As a topic that is still rather on the fundamental side of things it has, by comparison with more technologically oriented topics, only a relatively small but growing community. The last topical conference "Dislocations" (held every 4 years) attracted about 200 participants but is strongly growing. Since there are also a few other conferences and workshops that are exclusively dedicated to dislocation plasticity we currently do not see the need for a full series of CECAM workshops on this topic. However, having highly specialized and smaller workshops with up to 40 participants might be something that is well appreciated by the community. Generally, the combination of experiments and simulations is well established and highly appreciated. The computational infrastructure of the community is in a very mixed state: there are a number of open source (and probably an even larger number of closed source) software projects for, e.g., molecular dynamics (MD) and discrete dislocation dynamics (DDD). However, less well-developed sub-topic of this community are still behind in terms of code development. In general, our community would most certainly highly benefit from more open source projects that are supported (or at least: somewhat influenced) by software developers.

4 Funding

As is the case for any field of research, further advancing the study of multiscale modeling of crystal plasticity relies on the availability of sufficient funding. In addition to the various and quite scattered national funding schemes, instruments under Horizon 2020 may offer interesting possibilities. In addition to individual grants such as those offered by European

Research Council (ERC), Horizon 2020 encompasses instruments for Europe-wide collaboration, something that would likely be highly beneficial for advancing the topic of the workshop. Out of these, for instance applying for a Marie Curie Innovative Training Network (ITN) with a topic related to multiscale materials modelling in general and/or crystal plasticity in particular could be a viable option in the near future.

5 Will these developments bring societal benefits?

The talks and related discussion during the workshop not only provided nice examples of applied materials modeling but also emphasized the technological importance of the main aim of the workshop, that is, linking discrete and continuum dislocation scales. Indeed, an important part of engineering of various structural applications is based on applying continuum models of plasticity to estimate their strength and other mechanical properties. A key aim of the more applied branch of research on the topic of the workshop is to improve the accuracy of such models, something that could in the longer term allow to more precisely design various engineering applications. Such advances should contribute to more reliable (and thus safer) components and structures in engineering applications, which may be, thanks to the improved accuracy, also designed to be lighter and thus more energy efficient.

A related issue in micro and nanotechnology is given by the constraints on the formability of materials due to the inherently fluctuating nature of small scale crystal plasticity - something that was extensively discussed during the workshop - giving rise to unstable plastic deformation in small enough samples. Advances in understanding and controlling such fluctuations may thus contribute to developments allowing to push the limits of formability of micro and nanoscale crystalline materials, and thus the limits of what is possible in terms the relevant technological applications and their further miniaturization.

6 Participant list

Organizers

Ispanovity, Peter Dusan
Eötvös University, Hungary

Laurson, Lasse
Aalto University, Finland

Sandfeld, Stefan
University of Erlangen-Nuremberg, Germany

Weiss, Jerome
CNRS & University Grenoble Alpes, France

Zaiser, Michael
University of Erlangen-Nuremberg, Germany

Admal, Nikhil Chandra - University of California Los Angeles, USA

Alava, Mikko - Aalto University, Finland

Angheluta, Luiza - University of Oslo, Norway

Derlet, Peter - Paul Scherrer Institute (PSI), Villigen, Switzerland

Devincre, Benoit - LEM, CNRS-ONERA, France

El-Azab, Anter - Purdue University, USA

Greer, Julia - California Institute of Technology, USA

Groma, Istvan - Eötvös Loránd University, Hungary

Hatano, Takahiro - University of Tokyo, Japan

Hochrainer, Thomas - Universität Bremen, Germany

Lehtinen, Arttu - Aalto University, Finland

Marian, Jaime - UCLA, USA

Martens, Kirsten - LIPhy, University Grenoble Alpes & CNRS, France

Mester, David - Budapest University of Technology and Economics, Hungary

Papanikolaou, Stefanos - Johns Hopkins University, USA

Robinson, Marianne - CECAM, Switzerland

Swinburne, Tom - Culham Center for Fusion Energy, United Kingdom

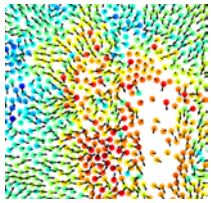
Truskinovsky, Lev - Paristech, France

Tüzes, Daniel - Eötvös University, Budapest, Hungary

Vandembroucq, Damien - ESPCI, CNRS, Paris, France

Zapperi, Stefano - University of Milan, Italy

Microswimmers, Self-Propelled Particles, and Active Matter



Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1323.html
Dates: March 6, 2017 to March 8, 2017

1 State of the art

The investigation of the physical behavior of microswimmers and self-propelled particles has started in the late 60s, early 70s of the last century with the pioneering work of Lord Rothschild about the surface accumulation of spermatozoa, and the insightful paper by Purcell on “Life at Low Reynolds Numbers”. Since then, much physical and mathematical progress in the investigation and understanding of these systems has been achieved.

Recent studies have focused on the various kinds of propulsion mechanisms of biological and artificial microswimmers, on the different types of active noises in the swimming motion, e.g. active Brownian motion versus run-and-tumble dynamics, swimming in confinement and near surfaces, synchronization of several swimmers or motile components, the collective motion of many self-propelled organisms, and the behavior of microswimmers in external (flow) fields. Here, active systems exhibit a remarkable wealth of non-equilibrium phenomena and emergent behaviors like swarming, active turbulence, activity-induced clustering and phase transitions, and a shift of the glass transition temperature.

The field of microswimmers and self-propelled particles is characterized by a very fruitful interplay of experiments, theory, and simulations. Simulations play a particularly important role, because the non-equilibrium behavior of many self-propelled particles, and more generally active matter, is too complex to be analyzed theoretically. At the same time, there is a lack of easily accessible experimental systems, or these systems are by themselves rather complex. Computer simulations have therefore been essential in recent years to drive the field forward.

2 Major outcomes

Self-propulsion, thermal and active noises, hydrodynamic interactions, steric repulsion, and possibly chemical concentration gradients all contribute to the collective dynamics of active matter – to name just the most intensively studied contributions. Due to the complexity of the systems and phenomena, different studies have focused on different aspect. This implies that also many different numerical methods and approaches have to be employed.

Several key topics and important objectives for future studies have emerged from the presentations and discussions during the workshop:

1- Bioswimmers:

The understanding and control of the motion of biological microswimmers has certainly been among the earliest motivations in this field and remains a very important topic today. The study of the mechanisms of propulsion of spermatozoa, bacteria, and algae has brought new insights, which pave the way towards a better control of their motility. For example, simulations and experiments have revealed a novel mechanism for the steering of sperm.

2- Synthetic Microswimmers:

The design and construction of synthetic microswimmers can be based on completely new (non-biological) principles. Theoretical calculations of diffusiophoretic motion show that the behavior is more complex than anticipated previously. Self-assembled microswimmers composed of magnetic particles can be activated and controlled by external magnetic fields. Synthetic microswimmers have an enormous potential for the design and control of complex micro-machines.

3- Continuum Theories versus Particle-Based Modeling:

In equilibrium statistical mechanics, the emergent behavior of critical systems can be understood by considering a phenomenological coarse-grained description. A similar path is now possible for active systems. In particular, both phase-separation and time-reversal symmetry breaking can be analyzed at a macroscopic level, capturing emerging features that may be inaccessible from microscopic analysis due to the overwhelming complexity of the systems.

4- Active Nematics:

A hot topic is the emergent chaotic dynamics of suspension of bacteria (and more generally, active microscopic agents) that can be modeled as self-propelled rods. However, our understanding of both the origin of this ``bacterial turbulence" and its properties remains elusive. Various approaches, including both the derivation of hydrodynamic descriptions of active nematic systems as well as numerical simulations of their emerging properties have been employed.

5- Phase Behavior and Structure Formation:

How active particles self-organize spatially is one of the major questions, instrumental in the design of future active materials whose properties need to be tailored. Self-organization is seen in very different active systems, from bacteria to Janus colloids, from vibrated disks to Quincke rollers. This helps to elucidate the common, universal features shared by these systems as well as how their specificity impacts the emerging behavior.

A hot topic is the role of hydrodynamic interactions in clustering and phase separation. The importance of the hydrodynamic near-field implies that details of the propulsion mechanism are essential to understand collective motion.

6- Rheology of Active Systems:

In the quest for innovative active materials, the understanding of the rheological properties of active systems is key to their control. Important results concern both, explaining the rheological properties of suspensions of bacteria in complex fluids as well as the fundamental problem of defining the pressure and viscosity of active suspensions.

7- Geometric Confinement and Surfaces:

Many, if not most, potential applications of microswimmers concern their motion near surfaces and obstacles. Accumulation at walls implies that near-field hydrodynamics dominates; this opens many possibilities for the design of confining walls to control microswimmer motion.

3 Community needs

The community of active matter strongly relies on numerical simulation to explore the properties of active materials. There is currently no organized network or collective computational infrastructure which means that researchers rely on their local capacity. One of the limitations is that many newcomers thus do not have access to advanced codes or enough computing power. The release of open-source codes to simulate active particles and their hydrodynamic interactions would certainly boost the productivity of the community.

Conference-wise, individual initiatives have also helped structure the community so far, and there are several workshops, conferences, and schools planned for the next two years, which are related to or contain a significant portion of active-matter research, such as the Cargese summer school on “Microswimmers – From Single-Particle Motion to Collective Behavior” (Sept. 2017), the Aspen workshop on “Fundamental Problems in Active Matter” (Jan.-Feb. 2018), the Jülich spring school on “Physics of Life” (Feb.-Mar. 2018), a session on “Living and Active Matter” at the Annual European Rheology Conference (Apr. 2018), the Les Houches summer school on "Active Matter and Non-Equilibrium Statistical Physics” (Aug.-Sept. 2018), and the Erice workshop on “The Statistical Physics of Active Matter”.

However, the active-matter community lacks any kind of structured recurrent workshops and conferences with reasonable funding.

A contribution of CECAM to this outstanding problem would be most welcome.

4 Funding

Apart from Germany, which has developed a priority program on active matter, supported by the German Science Foundation (DFG), there is no structured funding for the study of active systems. It has not been identified as a structural axis of the H2020 programs, and researchers thus compete for resources with much better organized and established communities. This is problematic, even though the level of the candidates has allowed the community to benefit from many prestigious grants such as ERC fellowships. More efforts are needed to secure a structured, longer-term funding for research in active and living matter.

5 Will these developments bring societal benefits?

Active matter consists in the study of materials made of many individual units capable of converting energy stored in the environment to self-propel. A first obvious application lies in biological physics: from the formation of biofilms to the spreading of cancer cells, motility plays a major role in many important biological challenges. While our studies are still mostly dedicated to fundamental problems, societal benefits are probably just around the corner.

On a longer timescale, it is hard to imagine that the development of active matter will not impact industry. When one thinks about the achievements of soft matter in the 20th century, from liquid crystal displays to the control of texture in the food industry, it is quite natural to expect that active soft materials, that have a much richer phenomenology than their passive counterparts, will lead to exciting developments. We are, however, only at the beginning of the development of synthetic active matter and these will take place on a much longer time scale.

6 Participant list

Organizers

Gompper, Gerhard
Research Center Jülich, Germany

Lauga, Eric
Cambridge University, United Kingdom

Tailleur, Julien
CNRS-Université Paris Diderot, Paris, France

Alaimo, Francesco - tu dresden, Germany

Alcanzare, Maria Michiko - Aalto University, Finland

Bartolo, Denis - Ecole Normale Supérieur Lyon, France

Baskaran, Aparna - Brandeis University, USA

Brader, Joseph - University of Fribourg, Switzerland

Brady, John - California University of Technology, (CalTech), USA

Carrara, Francesco - ETH Zurich, Switzerland

Cates, Michael - Edinburgh, United Kingdom

Chate, Hugues - CEA, France

Cottin-Bizonne, Cecile - University Lyon 1, France

Curatolo, Agnese - Laboratoire MSC, Université Paris-Diderot, France

Daerr, Adrian - Université Paris Diderot, France

Dauchot, Olivier - ESPCI, France

de Buyl, Pierre - KU Leuven, Belgium

de Graaf, Joost - Utrecht University, Netherlands Antilles

DiLeonardo, Roberto - University La Sapienza, Italy

Elgeti, Jens - Forschungszentrum Jülich, Germany

Fielding, Suzanne - Durham University, United Kingdom

Geyer, Delphine - ENS Lyon, France

Koss, Xeniya - Joint Institute for High Temperatures of the Russian Academy of Sciences, Russian Federation

Levis, Demian - EPFL, Switzerland

Liverpool, Tannie - University of Bristol, UK, United Kingdom

Löwen, Hartmut - University of Duesseldorf, Germany

Lozano, CELIA - Max Planck Institute Suttgart, Germany

Mazza, Marco - Max Planck Institute for Dynamics and Self-Organization, Germany

Michelin, Sebastien - Ecole Polytechnique, France

Morozov, Alexander - University of Edinburgh, United Kingdom

Nardini, Cesare - CEA - Paris Saclay, France

Navarro Argemí, Eloy - Universitat de Barcelona, Spain

Nie, Pin - Nanyang Technological University, Singapore

Pagonabarraga, Ignacio - CECAM EPFL, Switzerland

Paliwal, Siddharth - Utrecht University, The Netherlands

Poon, Wilson - University of Edinburgh, United Kingdom

Prymidis, Vasileios - Soft Condensed Matter Group, Debye Institute, Utrecht University, The Netherlands

Rafai, Salima - Liphy, University Grenoble, France

Rorai, Cecilia - Queen Mary University of London, United Kingdom

Scholz, Christian - FAU Erlangen, Germany

Seyrich, Maximilian - TU Berlin, Germany

Sharma, Abhinav - University of Fribourg, Switzerland

Speck, Thomas - Institute of Physics, JGU Mainz, Germany

Stark, Holger - Technische Universitaet Berlin, Germany

Uspal, William - Max Planck Institute for Intelligent Systems, Germany

VACHIER, Jérémy - Max-Planck-Institute for Dynamics and Self-Organization, Germany

Valeriani, Chantal - Universidad Complutense de Madrid, Spain

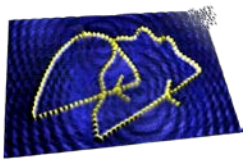
Winkler, Roland G. - Forschungszentrum Jülich, Germany

Wittmann, René - Université de Fribourg, Switzerland

Yeomans, Julia - Oxford University, United Kingdom

Zoettl, Andreas - University of Oxford, United Kingdom

Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond



Location: CECAM-DE-MM1P
Webpage: https://www.cecam.org/workshop-0-1382.html
Dates: March 19, 2017 to March 24, 2017

1 State of the art

Density functional theory (DFT) has made an unmatched contribution by providing first-principles atomistic insights to chemistry, condensed matter physics, materials science, and many other fields. However, most commonly used density functional approximations (DFAs) suffer from some well-known failures, including the incapability to correctly describe charge transfer processes, weak dispersion interactions, and strongly interacting scenarios. Recent effort attempting to cover such intricate many-body effects in DFT has initiated many new concepts at varying theoretical levels and has led to a bunch of new concepts and insights, as well as new DFAs. Some of these developments can be viewed as a merger of wavefunction theories of quantum chemistry and DFT.

2 Major outcomes

The symposium covered the progress in DFT by inviting well-known international experts as well as young researchers who have already significantly contributed to the field. The symposium attracted a diverse audience: those involved in method developments, practical DFT practitioners, as well as theoreticians in wave-function theory, quantum Monte Carlo, GW, and other fields.

This was an official symposium at the DPG spring meeting, which is hosted by the surface science division, but topics were not restricted to surface science. In 8 sessions 9 invited talks and more than 70 contributed talks and posters which cover the general field of computational materials science were presented.

Other divisions of the DPG that supported the symposium were the Chemical and Polymer Physics Division (CPP), the Thin Films Division (DS), the Semiconductor Physics Division (HL), the Magnetism Division (MA), the Metal and Material Physics Division (MM), the Surface Science Division (O), and the Low Temperature Physics Division (TT).

List of invited talks:

- Towards effcient orbital-dependent density functionals for weak and strong correlation | Igor Ying Zhang
- Including spin effects in the strong-coupling limit of DFT | Paola Gori-Giorgi
- Electronic excitations in 2D materials and heterostructures | Kristian Sommer Thygesen
- Spectacular success of DFT in predicting novel topological phases | Arun Bansil
- Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations | Weitao Yang
- Multi-reference density functional theory | Andreas Savin
- Density functionals from machine learning | Kieron Burke
- Taming Memory-Dependence in Time-Dependent Density Functional Theory | Neepa Maitra
- Quantum Embedding Theories | Fred Manby

More information can be found here: https://th.fhi-berlin.mpg.de/meetings/DPGSym2017/

CECAM ENDORSED THIS MEETING BUT DID NOT PROVIDE ANY FINANCIAL SUPPORT.

Workshop on ab initio nonorthogonal Valence Bond and nonorthogonal CI approaches in electronic structure.

Location: CECAM-FR-IDF
Webpage: https://www.cecam.org/workshop-0-1331.html
Dates: March 27, 2017 to March 30, 2017

1 State of the art

VB theory and other approaches based on non-orthogonal orbitals, important in the beginning of electronic-structure calculations, has become much less attractive since the 1970s up to recent years due to the rapid development of very efficient algorithms and programs based on orthogonal molecular orbitals. More recently, the development of computational resources and further improvements in algorithms nowadays make it possible of treating immense linear problems in brute-force manner, by augmenting basis sets for developing orbitals and excitation spaces. Several billions of determinants may be treated this way due to the Slater-Condon rules allowing for a rapid evaluation of matrix elements between determinants in orthogonal orbitals. However, important information is lost and diluted in this massive amount of data generated. Valence-Bond methods, based on a more limited number of configurations, and more importantly using localized or semi-localized orbitals, can provide more easily chemical insight owing to the intimate connection that such wave functions offers with Lewis model and chemical structures. Recent breakthrough in formalism and algorithm make it nowadays feasible to perform Valence Bond calculations on significantly large systems with a moderate effort. Calculations up to an active space of 20 electrons in 20 orbitals are now feasible within the VB framework, with one of the most developed programs in the VB community, i.e. the XVMB program by Pr. Wei Wu and his colleagues, at the VBSCF level which includes the so-called static correlation. However, several challenges remain open. First, the convergence of VBSCF wave functions may still be improved, because of redundancies issues inherent to the use of non-orthogonal orbitals that slow the convergence process and may be prevented. Second, a method able to efficiently include (computationally speaking) the dynamical correlation, while preserving the chemical readability of the VB wave function, is still wanted. Third, very little interest has been given to whole areas such as excited states, and transition metal rich molecules, that may require advances in VB methodology. The meeting managed to gather first-rank scientists all involved in methodological

development of methods, approaches, or formalism connected with methods based on non-orthogonal orbitals, together with mathematician's expert in numerical techniques.

2 Major outcomes

The meeting started with an overview of David Cooper which laid the grounds for the discussions during the whole discussion meeting, as we have the ideal Wigner space-spin product as a N! problem to which tractable approximations are searched for. The recall of the Gallup or the Moffitt method for generating matrix elements were not known to everybody. J Olsen presented an economical way to construct Gelfand states in second quantization, and a first step is his NO-CASSCF, which achieves much more rapid convergence in a smaller configuration space than a conventional CASSCF (example Cr2). Recent developments pose on top of these CAS spaces second-order perturbation theory, in a framework of bi-orthogonal basis functions. Selection of configurations with help of seniority numbers seems a promising tool, and the connection to ionicity has been made clear. Mr. Head-Gordon presented wavefunctions based on recoupling of electron pairs in singlets and triplets, which circumvent some of the major obstacles for small transition-metal complexes, but still fail for extended carbon frameworks. Another strategy may be to pass into complex space making use of theorems for holomorphic functions (A Thom). W Yang discussed possible combinations with density-functional theory, in a general perspective of coupling DFT with multi-reference wavefunctions, Geminals as spin-coupled pairs are closely related to VB wavefunctions (K Pernal), at the example of a He dimer.

R Broer and P Reinhardt presented the use of VB wavefunctions for intermolecular interactions, in the hope of avoiding long expansions to be combined term by term for interacting multi-reference wavefunctions. Debashis Mukherjee pointed out the link of non-orthogonal VB in breathing orbitals to multireference Coupled-Cluster theory when reducing the theory to doubly excited configurations and seeing the ingle excitations as orbital relaxations. This cross-community view was the essential advancements throughout the whole meeting of theory and algorithm-focused discussions.

Still all methods presented aimed at obtaining as good as possible solutions and energies of ground states and excited states as a complete solution of Schrödinger's equation. In particular Nakatsuji's total energy of the He atom. Obtaining by VB methods with less effort equally good energy differences, this point stressed by Hiberty was discussed only by A Shurki, and otherwise neglected.

3 Community needs

The discussion showed clearly that the contact between the two communities, high-level molecular-orbital theory and non-orthogonal valence-bond theory, should publish together, for that efficient algorithms implemented may spread in commonly used codes. This process has started with the implementation of the code of D Cooper in MOLPRO and M Head-Gordon in NWChem. Otherwise codes are still experimental and may be used by specifically trained researchers. The spreading of codes is not hindered by copyright issues. Strategies with respect to automatic code generation for highly complex formulas should be made available to members of the community in research and teaching, and discussions upon these strategies documented. A real need of the community seems to be the chemical understandability of the produced numbers, avoiding the impressing of « you get out what you put into the calculation ».

4 Funding

The discussion meeting was of interest to the LabEx MiChem, the laboratory of Theoretical Chemistry in Paris, and the research federation IP2CT, which all contributed financially to the success of the meeting. Paris, as a central place for international meetings, and the subject of the meeting where interesting enough to motivate researchers even from far away to participate.

5 Will these developments bring societal benefits?

One of the main benefits of the workshop was for leading researchers in these different communities to meet and collectively share recent advances and new ideas in nonorthogonal

orbital-based formalisms, useful approximations to the exact Schrödinger equation, and program/algorithm implementations; and also to have identified and started to address current challenges and limitations of nonorthogonal and/or VB-type approaches. For some of the colleagues present, new contacts were established, in particular with the Chinese community from Xiamen University. Four mathematician's colleagues also participated, and suggested ways of addressing some of the key challenges and difficulties that are identified at the workshop as bottlenecks. It is hoped that this workshop has made very important contacts and advances to electronic structure methods based on non-orthogonal orbitals, and that it will contribute to trigger un the future the availability of even more efficient algorithms/programs for accurate calculations on complex electronic structure problems, and that the legacy will include a significant extension to the range of systems for which the interpretative and conceptual capabilities of nonorthogonal ab initio VB theory can be applied.

6 Participant list

Organizers

Ayers, Paul
McMasters University, Hamilton (Canada), Canada

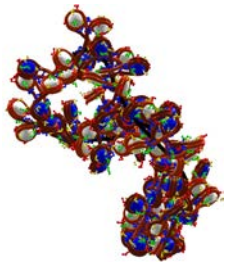
Benoît, Braida
Université of Paris VI, France

Cooper, David L.
The University of Liverpool, United Kingdom

Reinhardt, Peter
Sorbonne Universités, UPMC, France

Wei, Wu
Xiamen University, China

Multiscale Modeling and Experimental Approaches to Genome Organization



Location: Ecole de Physique, Les Houches (F)
Webpage: https://www.cecam.org/workshop-0-1422.html
Dates: April 2, 2017 to April 7, 2017

1 State of the art

Understanding and interpreting the structure and function of the genomic material in the live eukaryotic cell has been an enduring challenge in modern science. As our appreciation for the diversity and flexibility of DNA on the dodecamer level has deepened, its large-scale bending and coiling around histone proteins to form the chromosomal material in higher organisms has posed many structural and mechanistic questions. The genomic information in the DNA is packaged in a hierarchy of levels, from the nucleosome to condensed chromatin fibers to chromosomes and chromosomal territories. Thus, profound questions regarding DNA geometry, topology, and function span from the single nucleosome/base-pair level to condensed chromosomal arrangements on the mega-basepair level in the metaphase cell cycle. Not only do we lack an understanding of the structure of the chromatin fiber and chromosomal arrangements; we know little of how structural transformations occur. These transitions are tightly controlled by a host of proteins, which can directly bind to the chromatin fiber or induce chemical modifications of DNA and histones. These changes profoundly influence the global organization of the chromatin fiber and in turn affect DNA accessibility by the genome processing machinery. More specifically, transitions involving the nucleosome, fiber, and chromosome levels alter chromatin states from/to open, transcriptionally active to/from closed, transcriptionally silent forms and thereby affect a wide range of genome functions from cell differentiation to replication and transcription. Because these structures and transitions also impact human disease, notably many cancers; a better understanding of these processes also has strong translational ramifications on human health via epigenome-based therapeutics.

Exciting recent advances in instrumentation are providing important information into these puzzles from X-ray crystallography, Cryo-electron microscopy, in-vitro biochemistry,

2 Major outcomes

Our workshop brought together broad-thinking multidisciplinary scientists who discussed these multiscale challenges, from the level of DNA interacting with histones via the local organization of the chromatin fiber to the folding of chromosomes in the cell, from both experimental and modeling perspectives. Through a special open atmosphere, ideas from different fields were presented, assimilated, and advanced to discuss new ways to address the hierarchical structure of chromatin and the functional implication of these levels and rearrangements on human disease.

Specifically, we discussed:

1- The dynamic structure of the nucleosome: how to combine approaches from molecular and coarse-grained modeling, atomic-resolution structural analysis and in-solution biophysical techniques.

2- The organization of the chromatin fiber as a function of internal and external parameters (linker DNA length and variations, linker histone concentration, salt environment, etc.): how to merge experiment and theory and move current view from a more static to a dynamic vision of chromatin flexible in its natural cellular environment.

3- The folding of the chromatin chain into chromosomes, connecting modeling with experimental biophysics and biochemistry (e.g., proximity ligation, microscopy) by merging genome-wide association data measurements with polymer and fiber modeling.

4- Novel experimental and computational approaches to multiscale modeling of chromatin architecture: single cell views, novel models to merge fibers with gene resolution, linking supercoiling and knotting models to chromatin problems.

These concrete discussions already led to several new collaborations between experimentalists and modelers (e.g., publication in Cell by the Erez Lieberman Aiden and Tamar Schlick groups: Rao et al., Cell 171: 305 (2017)), as well as a commitment to assemble again in two years.

In addition, given the unfortunate death of organizer Jorg Langowski just one month after the meeting, a special memorial volume in Biophysical Journal has been planned (edited by A. Stasiak and T. Schlick) and will be published in spring 2018. Contributions from many attendees will be included in this special volume.

3 Community needs

Though much progress has been made and continues in our understanding of chromatin organization on the disparate length scales, a bridging between modeling and experimentation on the nucleosome and fiber levels with genome studies on the kilo-base level is lacking. New tailored multiscale computational approaches are needed to help interpret the rising volume of experimental data, especially those coming from genome-wide contact data.

As mentioned above, the current community needs are:

- Collaborations between modelers and experimentalists;
- Consideration of and merging of chromatin multiple scales;
- Moving from a static to dynamic view of chromatin, with parameter-dependent fluctuations and environment-specific context;
- New modeling and experimental approaches to probe chromatin's dynamic transitions and especially the process of chromatin loop extrusion postulated to be involved in formation of TADs;
- Better understanding of transcription-induced supercoiling and its role in shaping interphase chromosomes.

4 Funding

The CECAM workshop led to proposal of a thematic meeting approved by the biophysical society to be held in Les Houches in 2019 titled Multiscale Modeling of Chromatin: Bridging Experiment with Theory.

Other possible sources of funding for meetings on similar subjects are:

European Molecular Biology Organization (EMBO) and Gordon Research Conferences (GRC).

There were no discussions of general joint research proposals but our meeting started several collaboration projects involving participating researchers.

5 Will these developments bring societal benefits?

Because the chromatin fiber stores the genomic material for eukaryotic organisms, understanding chromatin structure and dynamics translates directly to interpreting biological function that controls all basic life's function. When the DNA is obscured from the cellular machinery in condensed chromatin, the cell is transcriptionally silent, and when the chromatin is open, the DNA is accessible to the transcription machinery and is transcriptionally active. Understanding what controls these open and closed states and how to transform one state to another affects a wide range of genome functions from cell differentiation to replication and transcription. Because these structures and transitions also impact human disease, notably many cancers; a better understanding of these processes also has strong translational ramifications on human health via epigenome-based therapeutics. Such epigenome-based strategies hold great promise for a new paradigm for future medicine since they have the potential to address many deficiencies in current drug treatments.

6 Participant list

Organizers

Everaers, Ralf
École Normale Supérieure de Lyon, France

Langowski, Jörg
Division Biophysics of Macromolecules, German Cancer Research Center (DKFZ), Heidelberg, Germany

Schlick, Tamar
New York University, USA

Stasiak, Andrzej
Center for Integrative Genomics, University of Lausanne, Switzerland

Arneodo, Alain - Laboratoire Joliot-Curie, ENS Lyon, France

Barth, Roman - CNRS, France

Benedetti, Fabrizio - UNIL, Switzerland

Bentivoglio, Alessandro - School of Physics and Astronomy - University of Edinburgh, United Kingdom

Bishop, Thomas C - Louisiana Tech University, USA

Blossey, Ralf - Institut de Recherche Interdisciplinaire, Lille University, France

Brandani, Giovanni - Kyoto University, Japan

Buitrago, Diana - IRB Barcelona, Spain

Bystricky, Kerstin - Université Paul Sabatier - CNRS, France

Clarkson, Chris - Department of Biological Sciences, University of Essex, United Kingdom

Cojocaru, Vlad - MPI for Molecular Biomedicine, Münster, Germany

De Bruin, Lennart - Lorentz Institute, Leiden University, The Netherlands

Drsata, Tomas - University of Chemistry and Technology, Czech Republic

Fudenberg, Geoff - UCSF, USA

Gkountaroulis, Dimoklis - University of Lausanne, Switzerland

Grange, Pascal - Xi'an Jiaotong-Liverpool University, China

Grigoryev, Sergei - Penn State University, College of Medicine, USA

Jost, Daniel - University Grenoble-Alpes, France

Joyeux, Marc - Université Grenoble Alpes, France

Kos, Pavel - Lomonosov MSU, Russian Federation

Lankas, Filip - University of Chemistry and Technology Prague, Czech Republic

Levene, Stephen - University of Texas at Dallas, USA

Lieberman-Aiden, Erez - Rice University, USA

Maddocks, John H. - Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland

Manley, Suliana - EPFL, Switzerland

Minhas, Vishal - NTU, Singapore

Mukherjee, Arnab - University of Tours, France, France

Nordenskiöld, Lars - Nanyang Technological University, Singapore

Olson, Wilma - Dept. of Chemistry, Rutgers University, USA

Panchenko, Anna - NIH, USA

Papale, Andrea - Sissa, Italy

Papoian, Garegin - Univ. Maryland, USA

Patelli, Alessandro - EPFL, Switzerland

Petkeviciute, Daiva - Kaunas University of Technology, Lithuania, Lithuania

Pettitt, B. Montgomery - U. Texas Med. Galveston, USA

Polovnikov, Kirill - Physics Department, Moscow State University, Russian Federation

Praprotnik, Matej - National Institute of Chemistry, Ljubljana, Slovenia

Rabin, Yitzhak - Bar-Ilan University, Israel

Racko, Dusan - Universite de Lausanne, Switzerland

Rafii Tabrizi, Arash - Weill Cornell Medicine, Qatar

Rosa, Angelo - SISSA Trieste, Italy

Saurabh, Suman - University of Tours, France, France

Schram, Raoul - ENS Lyon, France

Scolari, Vittore - Institut Pasteur, France

Silahtaroglu, Asli - Wilhelm Johannsen Centre for Functional Genome Research, Department of Cellular and Molecular Medicine, University of Copenhagen, Denmark

Spakowitz, Andrew J. - Stanford University, USA

Stevens, Tim - Cambridge University, United Kingdom

Teif, Vladimir - University of Essex, United Kingdom

Toth, Katalin - DKFZ, Germany

Vaillant, Cedric - Laboratoire de Physique, ENS Lyon, France

Walther, Jürgen - IRB Barcelona, Spain

Winogradoff, David - University of Illinois at Urbana-Champaign, USA

Zazhytska, Marianna - Center for Integrative Genomics, Switzerland

Zwahlen, Thomas - EPFL, Switzerland

Ion Transport from Physics to Physiology: The Missing Rungs in the Ladder

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1481.html
Dates: April 3, 2017 to April 5, 2017

1 State of the art

Regulated ion transport across bio membranes is crucial to a wide range of processes including neurotransmission, photosynthesis, and microbial motility. Integrating a unique combination of biological, chemical, and physical principles, ion transport has been a key area of research for biophysicists for decades. Among other things, the ability to directly measure ion channel activity via transmembrane electrical properties enabled some of the first measurements of protein function at the single-molecule level.

Despite these advances, our understanding of biological ion transport remains limited at the atomic level, due in large part to its dependence on multipass membrane proteins (e.g. channels, transporters) that pose challenges to classical methods of protein biochemistry and structure determination. Moreover, ion transport proteins undergo dramatic conformational changes such that, even at high resolution, a single structure reveals only one chapter in a complex mechanistic story. Due in part to these difficulties, computational methods have played a key role in the modeling of both electrophysiological and structural data in this field.

Ion transport research has benefitted substantially in recent years from advances in both experimental methods (e.g. resolution and accessibility of electrophysiological recordings and three-dimensional structures) and computational tools (e.g. processing power and speed, force field accuracy, and statistical models). Accordingly, the field has offered increasing opportunities for interdisciplinary collaboration—accompanied by dramatic differences in technical terminology, conceptual paradigms, and data access.

This workshop assembled ion transport experts from both experimental and computational backgrounds, with the goal of identifying specific barriers—and possible solutions—to our own research and to interdisciplinary collaboration.

2 Major outcomes

Symposium presentations in this workshop spanned experimental and computational studies on ion channels and transporters. The first session focused on ion conduction, introducing both atomistic and kinetic ion channel simulations. A second session concerned ligand gating and modulation, including biochemical, electrophysiological, and computational investigations of the molecular basis for allostery. The third and final session surveyed diverse mechanisms of ion transport, including perplexing stimuli such as light, temperature, and voltage.

Whereas several stories involved the classic use of computational methods to “explain” experimental data, some of the most notable—as recalled by multiple participants in our post-assessment survey—invoked the analysis of long-timescale simulations (particularly of voltage gating in potassium channels, and ligand binding in glutamate receptors) to generate novel hypotheses. Other high-impact stories involved the use of molecular dynamics to assess structural data (particularly for ion coordination in the channel pore, and apparent “open” versus “closed” channel states). Modern analytical methods, such as Markov state models, also received particular attention for their potential to bridge simulations and experiments.

In addition to symposium talks, the second day of this workshop included hands-on training opportunities in either molecular dynamics simulations and free energy calculations, or in statistical mechanics based on Ising and hidden Markov models. Enthusiasm for these practical experiences exceeded our expectations, with nearly all speakers and participants engaging throughout the three-hour tutorial. Some technical challenges faced during these exercises even proved useful, helping participants to appreciate the complexities of others’ work. Subsequent feedback encouraged the further development and propagation of such exercises, with possible refinement of user interface and molecular visualization tools. As atomistic simulations become increasingly accessible to both specialist and nonspecialist audiences, it may be particularly useful to develop training opportunities in trajectory analysis.

An overarching theme of workshop feedback was the common gaps in understanding and trust between experimental and computational methods. There remains a general need to set explicit expectations and risk assessments, particularly when entering interdisciplinary collaborations; specific terms “open,” “conducting,” “streaming potential,” “Q matrix,” “hysteresis,” “allostery,” etc. may require precise definition when communicating across disciplines. On the computational side, a common concern was the reliability of molecular dynamics force fields—perhaps overestimated by some computational researchers, underestimated by experimentalists. On the laboratory side, parallel concerns involved sources of error in different types of functional data, such as measurements of binding

affinities and kinetics, and the assignment of functional states to crystal structures. Clarity on both sides could aid in the oft-cited goal of incorporating experimental constraints to enhance simulations.

Several other open questions surfaced in our final roundtable, including concerns over the reliability of molecular dynamics force fields; still, participants generally called for access to more, longer simulations, with the goal of approximating timescales of electrophysiological data, and reducing bias from initial structures or conditions. Many attendees cited difficulties in the functional classification of structural models as a key challenge, which might be informed by computational methods. In light of these and other questions, one positive outcome appeared to be the collegial environment of the workshop: some described as “refreshing” the opportunity to acknowledge and (attempt to) address technical limitations with a sense of enthusiasm, common purpose, and community.

3 Community needs

Several participants voiced a need for laboratory trainees to develop solid foundations in thermodynamics, and exposure to—if not expertise in—production and analysis of atomistic simulations. Demand for training, even for experienced scientists, was reflected by attendees’ enthusiastic engagement in hands-on tutorials; some called for the further development of live and/or online education opportunities. For computational trainees, it may be equally important to gain a basic understanding of relevant biochemical and biophysical laboratory methods, enabling scientists in both fields to visualize transport processes at micro- and macroscopic scales.

Building on the open questions above, a key community need discussed in our final roundtable was for a public data repository of long-timescale molecular dynamics simulations. Calls for such repositories are not new in this field, nor limited in potential impact to ion transport; still, we believe the need to be particularly urgent, and potentially fruitful, in this context. We briefly discussed the types of data most important and feasible to share, how and where they might be accessed, and the long-term need for systematic validation tools. Parallels were drawn not only to well established databases for macromolecular structures, but also to repositories for biological reagents such as plasmids or mice: in at least some cases, atomistic simulations could be considered substrates for novel data collection and analysis, similar to a gene or rodent model.

4 Funding

Given the diverse applications and implications of ion transport, funding sources in this area have included both public and private, medical and basic science agencies. A particular topic for discussion at this workshop was possible support for a public molecular dynamics data repository, in parallel to the NSF-, NIH-, and DOE-sponsored Protein Data Bank (PDB). Such a resource would be consistent with the goals of the Open Research Data Pilot associated with Horizon 2020 projects in the EU; in the US, a PDB-affiliated group has already applied for NIH funding to develop simulation repository initiatives, though not to fund data archiving infrastructure directly. Torsten Schwede (University of Basel) has expressed recent interest in organizing a workshop around these goals.

5 Will these developments bring societal benefits?

Understanding ion transport at the atomistic level offers crucial insights into the design of novel therapeutic agents for pain, anesthesia, and neurodegenerative diseases, as well as industrial applications such as agricultural pest control. It will become increasingly important to apply state-of-the-art computational methods to understand and motivate experimental studies in ion transport, as these dynamic processes push the boundaries of what can be learned from crystal structures. Enhancing interaction between computational and experimental approaches in this field will thus crucially facilitate pharmacological applications (e.g. revealing molecular mechanisms of drug action on ion channel targets) relative to either approach in isolation.

More broadly, ion transport proteins offer valuable model systems for fundamental biological processes, such as allosteric regulation and membrane trafficking. In addition, demands in this field for long-timescale simulation repositories and widely accessible training resources likely anticipate similar needs in other fields, and could motivate the development of widely applicable data sharing and educational infrastructure.

6 Participant list

Organizers

Carnevale, Vincenzo
Temple University - Philadelphia, USA

Delemotte, Lucie
KTH Science for Life Laboratory, Sweden

Hellmich, Ute
Johannes Gutenberg-Universität Mainz, Germany

Howard, Rebecca
Stockholm University, Sweden

Rothberg, Brad
Temple University School of Medicine, USA

Aldrich, Rick - University of Texas, Austin, USA, USA

Ardevol, Albert - Max-Planck Institute for Biophysics Frankfurt, Germany

Benkerrou, Dehbia - Department of Physics, University of Cagliari, Italy

Berneche, Simon - U Basel, Switzerland

Chanda, Baron - University of Wisconsin, Madison, USA, USA

Corringer, Pierre-Jean - Pasteur Institute, Paris, France, France

de Groot, Bert - Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Domene, Carmen - University of Bath, United Kingdom

Gaudet, Rachelle - Harvard University, Cambridge, USA, USA

Giraldez, Teresa - University of La Laguna, Tenerife, Spain, Spain

Harpole, Tyler - Scilifelab, Sweden

Heusser, Stephanie - Stockholm University, SciLifeLab, Sweden

Islas, León - UNAM, Mexico City, Mexico, Mexico

Jogini, Vishwanath - DE Shaw Research, New York, USA, USA

Johner, Niklaus - SIB, Switzerland

Kasimova, Marina - SciLife Lab, Sweden

Lindahl, Erik - KTH/Stockholm University, Stockholm, Sweden, Sweden

Middendorf, Thomas - University of Texas at Austin, USA

Nimigean, Crina - Weill medical college, USA

Plested, Andrew - Leibniz-Institut für Molekulare Pharmakologie, Germany

Sigg, Daniel - dPET, Spokane, USA, USA

Stock, Leticia - Universidade de Brasilia, Brazil

Tarek, Mounir - University of Nancy, France

Voelz, Vincent - Temple University, Philadelphia, USA, USA

Westerlund, Annie - KTH royal institute of technology, Sweden

Recent advances in numerical methods for micro and macro models in fluid dynamics

Location: CECAM-IT-SIMUL
Webpage: https://www.cecam.org/workshop-0-1485.html
Dates: April 5, 2017 to April 7, 2017

1 State of the art

Linked to the incredible increase of computer speed calculation, scientific computation may be decisive enough to define the border between complex problems that can be treated and those which, on the contrary, cannot. The aim of scientific computation is the development of versatile and reliable models, detailed in closed form, and tested on a wide range of test cases, either analogical or experimental, which there are helpful reference solutions for.

A mathematical model must simulate universal concepts, such as, for instance, the conservation of mass or the momentum of a fluid, or the moment of inertia of a structure; moreover, in order to obtain a successful numerical simulation, it is necessary to define which level of detail must be introduced in the different parts of a model, and which simplifications must be carried out to facilitate its integration into different models.

Models able to simulate very complex problems should take into account uncertainty due to the lack (or uncertainty) of data (or data affected by noise) which feed the model itself. The risk analysis, which arises from uncertainty and exposition to “defeat” (i.e. profit reduction, environmental damage, health damage, and so on) is another feature that a good model should have.

These kinds of models are used to foresee natural, biological and environmental processes, in order to better understand how complex phenomena work, and also to contribute to the design of innovative products and technologies.

An important aspect of scientific computation is represented by computational fluid dynamics (CFD), a discipline which aims to solve by computers problems governed by fluids.

In aerospace, for example, CFD can be applied in many ways. Numerical models based on potential flow equations or on the more sophisticated Euler or Navier-Stokes equations can be used, for example, in the aerodynamic analysis of wing tips or for the whole fuselage for performance optimization.

Simulation implies validation

2 Major outcomes

The program of the mini symposium has included the following talks:

1. A fully semi-Lagrangian discretization for the 2D Navier-Stokes equations in the vorticity-streamfunction formulation

L. Bonaventura (1) and R. Ferretti (2)

(1) MOX - Dipartimento di Matematica Politecnico di Milano Piazza Leonardo da Vinci 32, 20133, Milano

email: luca.bonaventura@polimi.it

(2) Dipartimento di Matematica e Fisica Università degli Studi Roma Tre L. go S. Leonardo Murialdo 1, 00146, Roma, Italy ferretti@mat.uniroma3.it

2. High order ADER schemes for a unified first order hyperbolic formulation of Newtonian continuum mechanics coupled with electro-dynamics

M Dumbser, I Peshkov and E Romenski

Laboratory of Applied Mathematics University of Trento

Via Mesiano 77, I-38123 Trento (TN), Italy

E-mail : michael.dumbser@unitn.it

3. Deconvolution-based nonlinear filtering for incompressible flows at moderately large Reynolds numbers: analysis and medical applications

Alessandro Veneziani (1) and (2)

(1) Department of Mathematics & Computer Science, Emory University Atlanta, GA, USA e-mail: avenez2@emory.edu

(2) School of Advanced Studies IUSS Pavia, IT

E-mail: alessandroveneziani@iusspavia.it

4. Stokesian Dynamics of colloidal suspension in extensional flow

E. Fried, G. Giusteri, A. Martiniello and R. Seto

Okinawa Institute of Science and Technology Graduate University (OIST) 1919-1 Tancha, Onna-son, Kunigami-gun Okinawa, Japan 904-0495

E-mail : contact@oist.jp, web page: https://www.oist.jp/

5. Ab initio hydrodynamics

S. Meloni

Department of Mechanical and Aerospace Engineering, University of Rome Sapienza,

Via Eudossiana 18, 00184 Rome (Italy)

Email: simone.meloni@uniroma1.it

6. Lattice Boltzmann simulations across scales of fluid motion: classical, quantum and relativistic

S. Succi

IAC-CNR, Via dei Taurini 19, 00185, Roma, Italy, and IACS-SEAS, Harvard University,

Oxford Street 29, 02138, Cambridge, USA

For more information on the organization and the abstracts see the web page of the conference:

http://congress.cimne.com/FEF2017/frontal/Invited.asp

It is important to note that the FEF 2017 conference focuses on several topics related with advanced numerical methods for flows problems, not limited to finite element, but including spectral methods, finite volume, as well as techniques for granular flows, porous media. All the minisymposia and special sessions organised at FEF were related with fluids problems mainly solved with a macroscopic approach and several applications of computational fluid dynamics and related problems such as fluid-structure interactions, naval or aeronautical applications, as well as turbo machinery, just to cite few topics presented in the special sessions at FEF 2017. Micro approaches are less spread in FEF community with respect to the macro ones since they are more related with classical computational mechanics. In this respect the minisymposium has been a notable exception in the program of this conference. The final round-table has allowed to discuss several points of strength and weakness related to the micro and macro approaches, see the section below (Benefits) for more details.

3 Community needs

The Finite Elements in Flow (FEF) Problems Conference has a rich history that closely parallels the development and maturation of the finite element method and its application to computational fluid dynamics problems. The FEF meetings began in Swansea (U.K.) in 1972 and are the principal forum for the exchange of research results in all aspects of flow simulation using the finite element method. The scope of the conference is intentionally broad with coverage of theory, implementation, assessment and application in all of the major and emerging areas of fluid dynamics and flow-related phenomena. The methods covered at the conference are not restricted to finite elements. It has been many years since many researchers using different methods have also been attending this conference series. Our intention has been to compare the typical techniques of this conference with the micro techniques to start an active scientific interaction between the two communities.

4 Funding

The costs of this event have been very small. We have spent 1050 euros (the planned budget was 2000 euros) for the local expenses for three invited speakers. All the facilities have been provided by the Math Department inside the conference FEF 2017.

5 Will these developments bring societal benefits?

The minisymposium has attracted about 40 participants, which is a rather good result taking into account that Friday was the last day of the conference and that there were 6 parallel sessions.

The high quality of the presentations has allowed to have a general overview of advantages and difficulties in the two approaches (the pdf is available just writing to falcone@mat.uniroma1.it).

At the end of the presentations, we have run a round-table open to the participants with several interventions from the public. The main topics discussed during the round-table, which has continued for about 1 hour, have been the following:

- How can we guarantee accurate solutions and stable solution in micro models?
- How can we handle complicated geometries and boundary conditions in fluid problems when using micro models?
- How can we handle multiphysics problems in this framework?
- Which kind of theoretical results are necessary to pass to the limit in micro models to get the macro models, what can we say about the long-time behavior of the solutions?
- How can we couple atomistic and macro models?

Several contacts have been established between the participants so we hope that this mini symposium will be the starting point for some scientific collaborations.

6 Participant list

Organizers

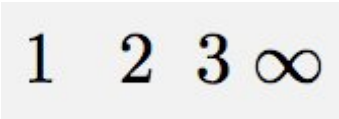
Ciccotti, Giovanni
University of Rome La Sapienza, Italy

Falcone, Maurizio
Università di Roma "La Sapienza", Italy

Perotto, Simona
Politecnico di Milano, Italy

Rozza, Gianluigi
SISSA, Trieste, Italy

Exploiting finite-size effects in simulations.



Location : CECAM-FR-MOSER. Université Pierre et Marie Curie (UPMC), Paris
Web page : https://www.cecam.org/workshop-0-1416.html
Dates : April 18, 2017 to April 21, 2017

1 State of the art

Finite size effects are ubiquitous in simulations. Sources of such effects are of different nature: finite number of particles, finite simulation box when using periodic boundary conditions, finite basis set in quantum chemistry, finite time step or grid spacing in algorithms, not even mentioning incomplete sampling of phase space due to the finite computational time. Practical consequences of such finiteness are numerous, with dramatic implications on the computed properties and the (lack of) possibility to compare simulation results with experiments, which correspond to an "infinite limit": thermodynamic, hydrodynamic, continuous, etc.

These effects are usually considered a nuisance and strategies are developed to correct for these artefacts. However, they also reflect the physical properties of the system of interest. In fact, it is also well known that in some cases one can exploit the size-dependence, e.g. in thermodynamics (detection of first-order transitions, computation of free energies), in hydrodynamics (diffusion coefficient vs system size allows extrapolating to infinite size and measuring the viscosity), in crystals (compatibility of the number of particles with boundary conditions) or in a recent quantum Monte Carlo approach (involving creation/annihilation of discrete walkers in the space of Slater determinants).

This suggests that a new perspective on some finite-size effects (some are more "promising" than others) may provide a wealth of information on the physical properties. This includes revisiting some classics (e.g. choice of boundary effects "at infinity" for the computation of electrostatic interactions or the dependence of computed properties and their fluctuations in the number of particles) as well as exporting these ideas into new fields (e.g. rare events, glasses, genetics and biochemical networks). The aim of the proposed workshop is to review the "positive power" of finite-size effects and to discuss techniques to measure them.

2 Major outcomes

This was an unusual workshop that brought together experts in very diverse areas of simulation, including hard and soft condensed matter, hydrodynamics, biophysics and data-analytics, and also a number of speakers who discussed experiments (e.g. evolution of bacterial colonies or the kinetics of heterogeneous crystal nucleation). Thanks to the wide range of expertise of the participants, the workshop was extremely stimulating, the more so as all participants were very keen to interact. As a result, several seeds for cross-fertilization have been sown, although the net effect will be judged on the basis of subsequent publications and collaborations. As the topic of the workshop covered any distinct field, one should expect diverse outcomes. The sub-title of the workshop was "1,2,3... infinity" and it is useful to look where the finite-size effects (FSE) could be mitigated so that small systems allow us to learn about the infinite system limit, and others where even the study of very large systems did not resolve FSE.

a) In some cases, the slogan "1,2,3... infinity" did indeed seem appropriate, in particular for small systems of simple liquids (Kjelstrup/Cortes-Huerto). This work had strong links with Hill's work on the thermodynamics of small systems.

b) A crucial area where FSE have to be taken into account from the start focuses on problems involving "under-sampling" of noisy (possibly correlated) datasets, be they experimental or numerical (Lee/Colwell). The tools developed in this area promise to be very useful for a wide range of (computational) problems, ranging from yielding in solids (Sengupta) to FSE in Quantum Monte Carlo (Ceperley).

c) For some systems, FSE provide crucial information that is very hard to obtain by other methods, e.g. glassy systems (Kob).

d) An area where 1,2,3 is very far from infinity is FSE of systems with hydrodynamic coupling (Hummer, diffusion in membranes). Although the importance of FSE in the calculation of diffusion constants is well known (to some), the magnitude and system-shape dependence of the effects in membrane diffusion still came as a surprise.

e) For some problems, the convergence was even worse. In the calculation of friction coefficients, even infinitely large system, computed for infinitely long times may yield the wrong results if the limits are taken in the wrong order.

f) In some cases (e.g. nucleation - Ceriotti), going to the thermodynamic limit naively makes things worse, rather than better. A careful analysis of the FSE will, however, resolve these problems.

g) Cells and mono-cellular organisms are necessarily finite and controlling FSE is essential to their mode of operation. This was clear from examples in the area of biochemical signalling (ten Wolde), persistent copying (as opposed to "passive" self-assembly – Ouldridge) and the

behaviour of bacterial of (active matter) colonies (Allen, Cates). One key lesson was that biological organisms do not get a free lunch: information storage necessarily costs energy (e.g. ATP).

h) In quantum simulations, FSE are inevitable because it is prohibitively expensive to study systems of the size that can be handled in classical simulations. The FSE effects show up in a number of ways: in FCIQMC (Alavi) the number of walkers has drastic effects on the convergence of the simulations. In other QMC calculations, controlling the boundary conditions (e.g. "twisted" boundaries) may help to mitigate FSE. However, FSE may show up in many other ways (k-space sampling, basis-set truncation). All these effects require different treatments, hence a good understanding of the causes of FSE is crucial - in particular for Fermionic systems. In this field, there may be interesting application of Bayes' theorem and, more generally, relations with signal processing and data-analytics.

On the whole, the workshop was very stimulating and it seems likely that some of the areas of overlap discussed above may result in separate future workshops.

3 Community needs

Our ability to mitigate finite-size effects obviously has the potential to reduce computing costs. Hence, we do not envisage that the outcome of the workshop will increase the use of HPC resources. Anyway, from the wide range of topics where finite-size effect arises, it is difficult to identify specific hardware needs.

However, networking activities such as CECAM workshops have an important role to play. The present workshop already attracted theoreticians with very diverse backgrounds as well as a few experimentalists, but obviously not all fields could be covered in only three days.

Based on the discussions during the workshop, it seems clear that many finite-size effects remain to be explored. There is therefore a good case to encourage the participants (or others) to organise one or more workshops to explore new directions. CECAM provides the perfect framework to do so. We feel that future workshops could benefit from interactions with applied mathematicians and data scientists.

4 Funding

While it is clear from the attendance and lively discussions that the issue of finite size effects is ubiquitous, very relevant and that they can be turned into powerful means of investigations, several participants mentioned that the work presented during the meeting was the result of side projects that emerged in the course of studies in a specific field of application.

In the current landscape of funding schemes, it is not obvious to identify one that would be fit for such transversal fundamental studies. This underlines the value of networking activities such as the present workshop.

5 Will these developments bring societal benefits?

We live in a finite world, with finite resources - and certain finite-size effects threaten us very directly. For instance, if the population of a particular animal species drops below one (or, more plausibly, below 2), the species goes extinct. In an infinite population, extinction due to finite sample size will not occur. We give this example to illustrate that finite-size effects are not just ubiquitous but also very important.

Of course, the present workshop focused on applications in "computational materials science". The topics discussed during our workshop have the potential of benefitting all the fields listed above: from hard material science (quantum chemistry & physics, crystal nucleation, yielding in solids) and soft matter (glasses, colloidal systems) to biology and health (bacterial growth in the context of biofilm formation, prediction of protein structure from sequence correlations, biochemical signaling), green chemistry and drug design (in-silico design by efficient sampling of chemical space).

However, funding opportunities will be linked to specific application areas, rather than to the study of finite-size effect in isolation. Funding should therefore be sought in the context of these applications.

6 Participant list

Organizers

Frenkel, Daan
University of Cambridge, United Kingdom

Rotenberg, Benjamin
CNRS and University Pierre and Marie Curie, Paris, France

Allen, Rosalind - University of Edinburgh, United Kingdom

Alavi, Ali - University of Cambridge and Max Planck Institute for Solid State Research, Germany

Bedeaux, Dick - University of Trondheim, Norway, Norway

Bernu, Bernard - CNRS/UPMC, France

Binder, Kurt - Johannes Gutenberg University Mainz, Germany

Bocquet, Lydéric - ENS Paris, France

Bombín Escudero, Raúl - Polytechnic University of Catalonia (UPC - Universidad Politécnica de Cataluña), Spain

Borgis, Daniel - Maison de la Simulation, France

Cates, Mike - University of Cambridge, United Kingdom

Ceperley, David - University of illinois at Urbana-Champaign, USA

Ceriotti, Michele - Swiss Federal Institutes of Technology Lausanne (EPFL), Switzerland

Ciccotti, Giovanni - University of Rome La Sapienza, Italy

Colwell, Lucy - University of Cambridge, United Kingdom

Cortes Huerto, Robin - Max Planck Institute for Polymer Research, Germany

DiCarlo, Antonio - CECAM-IT-SIMUL Node, Italy

Dobnikar, Jure - Institute of Physics, Chinese Academy of Sciences and University of Cambridge, Department of Chemistry, United Kingdom

Gruber, Thomas - Max-Planck-Institut for Solid State Research, Germany

Gruneis, Andreas - University of Cambridge, Germany

Hansen, Jean Pierre - University of Cambridge, United Kingdom

Holzmann, Markus - LPTL, Jussieu, Paris, France

Hummer, Gerhard - Max Planck Institute of Biophysics, Germany

Kjelstrup, Signe - Norwegian University of Science and Technology, Norway

Kob, Walter - University of Montpellier, France

Lee, Alpha - University of Cambridge, United Kingdom

Lelievre, Tony - INRIA and Ecole des Ponts ParisTech, France

Ouldridge, Thomas - Imperial College London, United Kingdom

Pagonabarraga, Ignacio - CECAM EPFL, Switzerland

Salazar, Marcos - ICB-UMR 6303, France

Sear, Richard - University of Surrey, United Kingdom

Sengupta, Surajit - TIFR Centre for Interdisciplinary Sciences, India

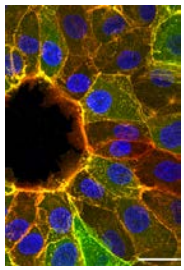
Simon, Jean-Marc - UNiversity of Bourgogne, France

ten Wolde, Pieter Rein - AMOLF, The Netherlands

Vuilleumier, Rodolphe - Ecole Normale Supérieure, Paris, France

Zeravcic, Zorana - Harvard University, France

Cell and tissue motility.



Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1390.html
Dates: May 3, 2017 to May 5, 2017

1 State of the art

In the absence of signaling, single cells on a substrate perform a gentle persistent random walk. In the presence of chemical or physical cues they move ballistically at typical speeds of μm/min. Cells move by protruding the cell front and then retracting the rear, exploiting the ability of actin to reversibly self-assemble. Moreover, there is increasing evidence that the activity of the cortex (a layer of actin under the cell membrane) also contributes to cell motility.

There is growing experimental evidence documenting the motion of confluent cellular layers. Such packed, motile cells move collectively and can initiate processes such as morphogenesis and wound healing. Increasingly physical arguments are being proposed as alternative ways to understand this motion. For example, protuberances that drive the motion of a cell front over a substrate have been attributed to the existence of `leader cells' but can also be interpreted in terms of hydrodynamic instabilities, and the motion of confluent layers has variously been described in terms of glassy dynamics and shown to resemble active turbulence. Moreover, there is now compelling evidence that the substrate has a considerable effect on cell motility: cells migrate from harder to softer surfaces. Although experiments are usually performed on ideal surfaces, in vivo cells crawl through the extra-cellular matrix which is a tangled network of fibers.

The physical modelling of cell motility is in its infancy. This is a new direction that can be addressed by the mesoscale approaches that are familiar in soft matter physics. The science is particularly timely betimely because of the advances in imaging techniques such as particle image velocimetry and traction force microscopy that are increasingly available to provide quantitative data on the dynamics of biological systems.

2 Major outcomes

Several different models of cell motility were discussed. These included analytic models, vertex models and SAMoS, phase field models and continuum approaches. All were able to reproduce several features of cell motility, but not the wide range of behaviors seen in experiment. Problems include the necessity to input some processes in an ad hoc way, the difficulty of relating model parameters to experimental parameters, and the omission of chemical signaling which regulates cellular processes.

Particular technical questions that were discussed include:

- Is compressibility being important?
- How to input connections between cells and between cells and surface in a realistic way.
- What level of coarse graining is appropriate eg do T1,T2 processes have to be modelled explicitly?
- What is the correct way to model actin driving on a coarse-grained level?

All the models had strengths and weaknesses and so at this early stage it is sensible to continue to develop them in parallel, to cross compare with each other and to experiment.

Physical questions that were identified where modelling has a role to play include:

Are collections of cells sensibly modelled as an active nematic? Should cell sheets by modelled as contractile or extensile systems? Are nematic models sufficient or is polarization important? Topological defects have now been identified in confluent cell layers. Can they be implicited in biological processes?

Cells exhibit durotaxis, a tendency to move towards harder substrates. Why is this the case and how can it be modelled? How do cells behave on structured surfaces, and can such surfaces be used to guide their motion? How do cells spread across surfaces eg in wound healing, and how do 'colliding' sheets of cells behave?

What drives the alignment of stress fibers in adherent cells? Do microtubules play a role in directing acting polymerization?

To what extent is droplet physics relevant to cells?

Confluent cell layers are a useful model system but in vivo cells move in a much more complicated fibrous environment. Will this significantly alter their behavior? Almost all experiments and models so far are in two dimensions. To model eg tumor formation, the third dimension is likely to be relevant.

How do patterns and structures form in biological systems? Are mechanical considerations of relevance to embryogenesis, or is chemistry key?

3 Community needs

This is a field is in its infancy where there is a great deal that is not yet understood. We are still at the stage of understanding the best way to model cell motility even for 'simple' model systems such as confluent cell layers. The in-silico models will not capture the full complexity of cell processes, so it is important to establish which features of cell motility are key, and which questions are usefully asked using a modelling approach.

Therefore, what is needed is funding for fundamental research, good ideas and a continued dialogue between experiment, theory and simulation. The topic is highly interdisciplinary and networking between biologists and physicists should be encouraged.

4 Funding

ERC, EU, National funding agencies, HFSP, etc.

5 Will these developments bring societal benefits?

This is currently fundamental research, but an understanding of cell motility will lead to better understanding of malfunctioning cells and tissue and hence the rational design of medical interventions. Moreover, understanding cell motility may help in the design of more efficient nanomachines, and give insight into self-assembly.

6 Participant list

Organizers

Giomi, Luca
Lorentz Institute, Netherlands, The Netherlands

Ladoux, Benoit
CNRS and Paris Diderot University, France

Yeomans, Julia
Oxford University, United Kingdom

Alaimo, Francesco - tu dresden, Germany

Alert, Ricard - University of Barcelona, Spain

Araujo, Nuno - Universidade de Lisboa, Portugal

Aronson, Igor - Pennsylvania State University, USA

Banerjee, Shiladitya - University College London, United Kingdom

Blanch-Mercader, Carles - Institut Curie, France

Bonilla, Luis - Universidad Carlos III de Madrid, Spain

Callan-Jones, Andrew - Laboratoire Matière et Systèmes Complexes/Université Paris-Diderot, France

Cerbino, Roberto - Università degli Studi di Milano, Italy

Charras, Guillaume - University College London, United Kingdom

Coburn, Luke - University of Aberdeen, United Kingdom

Discher, Dennis - UPenn, USA, USA

Doostmohammadi, Amin - University of Oxford, United Kingdom

Dufresne, Eric - ETH, Zurich, Switzerland

Ejtehadi, Reza - Sharif Univ. of Tech., Iran

Etienne, Jocelyn - Université Grenoble Alpes – CNRS, France

Henkes, Silke - The University of Aberdeen, United Kingdom

Henrich, Doris - Leiden University, The Netherlands

Koester, Sarah - Gottingen, Germany

Lio, Pietro - University of Cambridge, United Kingdom

Lugli, Francesca - Dipartimento di Chimica "G. Ciamician", Italy

Messi, Zeno - LPMV-EPFL, Switzerland

Mueller, Romain - Department of Physics, University of Oxford, United Kingdom

Nandi, Saroj - Wiezmann Institute of Science, Israel

Pagonabarraga, Ignacio - Swiss Federal Institute of Technology, Switzerland

Prost, Jacques - ESPCI, France

Riveline, Daniel - Strasbourg, France

Rosowski, Kathryn - ETH Zürich, Switzerland

Sain, Anirban - Indian Institute of Technology (IIT) - Bombay, India

Schakenraad, Koen - Leiden University, The Netherlands

Schwarz, Ulrich - Heidelberg University, Germany

Silberzan, Pascal - Institut Curie, France

Sknepnek, Rastko - University of Dundee, United Kingdom

Staddon, Michael - UCL, United Kingdom

Thampi, Sumesh - Indian Institute of Technology Madras, India

Trepat, Xavier - Barcelona, Spain

Vågberg, Daniel - Laboratoire Charles Coulomb CNRS - Université de Montpellier, France

Voigt, Axel - Technische Universität Dresden, Germany

Wondergem, Joeri - Leiden University, The Netherlands

Yashunsky, Victor - Institut Cuire, France

Theoretical Chemistry for Extended Systems: systematically improvable electronic structure methods

Location: CECAM-FR-GSO
Webpage: https://www.cecam.org/workshop-0-1442.html
Dates: May 22, 2017 to May 24, 2017

1 State of the art

Recent years have seen much progress both in Wave-Function (WFT) based and Quantum Monte Carlo (QMC) methods to treat very large or periodic systems. A common theme of the most recent and innovative approaches is the search for fruitful combinations of the best ideas of each world. Most of the standard algorithms of WFT have been revisited in the last five years to optimally exploit new supercomputer architectures and to scale up to an arbitrary number of cores. Important examples include the stochastic MP2 method, the FCI-QMC approach, the stochastic coupled-cluster theory, and the stochastic CASSCF method. Quite remarkably the stochastic version has been found on some examples to be capable of surpassing the current limits of the deterministic version. Even in the case of the most standard QMC methods, important effort is currently made to take full advantage of CI expansions of WFT to construct accurate nodes for the trial wavefunction.

For periodic systems the generalization of WFT and QMC is a crucial step to go beyond the standard DFT, HF, or MP2 levels of theory. This generalization is far from trivial, but some remarkable progress has been recently made, e.g., the transcorrelated method, the extension of FCIQMC to periodic solids, and the combination of many-body-perturbation-theory (MBPT) widely used for solids with quantum-chemistry methods, such as coupled cluster theory, in order to describe photoemission spectra of solids.

The main objective of the workshop is to compare the emerging approaches of WFT and QMC with the current state-of-the-art tools for calculations of the solid state such as MBPT, e.g., Bethe-Salpeter equation and cumulant expansion.

2 Major outcomes

As expected the workshop has been a unique opportunity to have many detailed and fruitful exchanges between various experts, and also young scientists, on the various aspects of WFT, QMC and MBPT approaches for the electronic structure of extended systems (either finite or infinite). As announced in the workshop description, a large amount of time was allowed after each presentation to promote ample discussion, a possibility which has been systematically used.

From a general point of view, it was clear that the three communities put together have each their own existence and that some people were not used to attend to presentations of the two other fields. However, the scientific connections appeared sufficiently clear that we feel that it promoted a real interest (not by simple courtesy) and that some possible interactions may follow.

Let us now highlight a number of interesting aspects that have emerged from the workshop. Regarding wavefunction theory for periodic systems, it is clear that we assist at the rapid development of theories beyond Hartree-Fock. MP2 theories are actively developed with the aim of making it practical for complex solids. We can cite a very recent work allowing to reduce the computational burden form N5 to N4 (N, number of basis functions) and also some new improved implementations using localized orbitals. Even more boldly, the development of the very expensive Coupled Cluster approach is now considered with interesting applications; during the workshop half a dozen of presentations have been devoted to this hot topic. For finite systems we can also cite the presentation of two very recent works about the implementation of MRPT2 theories where the expansive second-order (PT2) contribution is computed stochastically. Applications not feasible with the standard deterministic approach have been presented. As illustrated in the workshop, the use of stochastic techniques is now becoming a general trend, not only for the traditional QMC methods, which are of course intrinsically stochastic, but also for deterministic approaches such as, for example, the FCI approach (FCI-QMC in its stochastic version). As a remarkable consequence, we can now envision the calculation of absorption or photoemission spectra for solids using WF approaches provided that the most difficult part is treated stochastically. Two illustrative examples presented in the workshop are the use of the transcorrelated approach or of the FCIQMC approach in its real time version which is currently developed. We emphasize that these approaches create a new bridge between MBPT (the method of choice for such quantities) and WFT theories. Regarding the MBPT theories themselves some novel aspects have been presented. Let us cite for example the possibility of connecting the photoemission

spectra with some well-defined hierarchy of density matrices, such quantities that turn out to be computable with QMC, thus creating an additional new bridge between communities.

3 Community needs

Because of the type of investigations, the community needs are mainly of computational infrastructures. The researchers in this field use different types of codes, mainly written by the different groups, and in some cases more general-purpose codes with a larger diffusion. The computational needs depend in a very tight way from the type of approaches that are used. For this reason, the computational infrastructure needs span a very large range of machines. Massively Parallel Computers having distributed memories, for Quantum Monte Carlo calculations. At the other extremity, there are machines having a small number of nodes that access a very large shared memory, as it is the case for exact diagonalization of Davidson type (Configuration Interaction, Coupled Cluster). The needs of Density-Functional calculations are located in some way between these two extreme cases, since massively parallel computers can be used, although the parallelization of the codes is not a straightforward task in this case. For these reasons, it is extremely important that different types of architectures are available in the computer centers. Unfortunately, extremely massively parallel computers are becoming by far the most diffuse ones in the large computer centers, and this poses some problems to at least a part of the Quantum Chemistry community.

The other type of need of the community is for workshop where the different experiences in the field are shared. The present workshop was the second of this type, and we could witness a stronger interaction between the different groups belonging to the community.

For this reason, we believe that such a type of workshop could be organized on a recurrent basis, every second or third year, in order to continue this type of interaction.

4 Funding

The workshop brought together many established experts as well as young promising talented researchers in the field of quantum chemistry, quantum Monte Carlo and condensed-matter physics. Therefore

there are several EU programs that might fund these researchers such as

- ERC starting grant
- ERC consolidator grant
- ERC advanced grant
- ERC synergy grant

We also note that it is of utmost importance that funding agencies continue or even increase their funding of fundamental research as this will both increase knowledge and advance technology.

5 Will these developments bring societal benefits?

Progress in theory and methodology to describe extended systems is of great importance to European Industry. Theoretical chemistry brings a wealth of information and this information can be used to develop novel

materials for various innovating technological applications.

For example, several methods are being developed for the accurate theoretical description of photoemission spectroscopy, which contains information about the ionization energies and electron affinities, this is very important information in the development of photovoltaic devices.

Another example is given by the various methods that are being developed for the accurate theoretical description of absorption spectra, from which crucial information can be obtained for the development of new photovoltaic and photocatalytic devices, for which its success largely depends on the ability of the material to split the electron and the hole after their formation.

However, these considerations apply to the field globally. Concerning the more restricted focus of the workshop in particular, it is about fundamental research preparing the long-term future on a scale of, say, 10 years which is not of direct interest for companies now.

6 Participant list

Organizers

Andrae, Dirk
Physikalische und Theoretische Chemie - Institut für Chemie und Biochemie - Freie Universität Berlin, Germany

Berger, Arjan
University Paul Sabatier, France

Caffarel, Michel
University Paul Sabatier, Toulouse, France

Evangelisti, Stefano
Universite Paul Sabatier, France

Leininger, Thierry
Laboratoire de Chimie et Physique Quantiques UMR5626 CNRS Université Toulouse 3, France

Alavi, Ali - University of Cambridge and Max Planck Insitute for Solid State Research, Germany

Battaglia, Stefano - Université Paul Sabatier, France

Ben Amor, Nadia - LCPQ IRSAMC Universté de Toulouse III, France

BENMAKHLOUF, ABDENNOUR - physique des matériaux, Algeria

Berkelbach, Timothy - University of Chicago, USA

Bondo Pedersen, Thomas - Centre for Theoretical and Computational Chemistry, University of Oslo, Norway

Deur, Killian - Université de Strasbourg, France

Ehsan, Sohaib - Vienna University of Technology, Austria

Gruber, Thomas - Max-Planck-Institut for Solid State Research, Germany

Grüneis, Andreas - Max-Planck-Institute for Solid State Research, Germany

Harb, Moussab - KAUST University, Saudi Arabia

Hongo, Kenta - JAIST, Japan

Hu, Yuchen - University of Cambridge, United Kingdom

Ichibha, Tom - School of Information Science, JAIST, Japan

Liao, Ke - Max Planck Institute for Solid State Research, Germany

Loos, Pierre-Francois - Laboratoire de Chimie et Physique Théoriques, UMR5626, UPS CNRS., France

Maezono, Ryo - School of Information Science, JAIST, Japan

Maschio, Lorenzo - University of Torino, Italy

Mazouin, Laurent - Université de Strasbourg, France

Mitas, Lubos - North Carolina State University, USA

Neufeld, Verena - University of Cambridge, United Kingdom

Panholzer, Martin - Laboratoire des Solides Irradi´es, Ecole Polytechnique, CNRS-CEA, Universit´e Paris-Saclay, France

Paulus, Beate - Physikalische und Theoretische Chemie - Institut für Chemie und Biochemie - Freie Universität Berlin, Germany

Ramberger, Benjamin - University of Vienna, Faculty of Physics and Center for Computational Materials Science, Austria

Rebolini, Elisa - University of Oslo, Norway

Reinhardt, Peter - Sorbonne Universités, UPMC, France

Reining, Lucia - Ecole Polytechnique, Palaiseau, France

Romaniello, Pina - University Paul Sabatier, France

Scemama, Anthony - University Paul Sabatier, Toulouse, France

Schäfer, Tobias - University of Vienna, Faculty of Physics and Center for Computational Materials Science, Austria

SENJEAN, Bruno - Institut de Chimie, UMR7177, Laboratoire de Chimie Quantique, France

Sharma, Sandeep - University of Colorado Boulder, USA

Sottile, Francesco - Ecole Polytechnique, Palaiseau, France

Stemmle, Christian - Freie Universität Berlin, Germany

Ten-no, Seiichiro - Kobe University, Japan

Thom, Alex - University of Cambridge, United Kingdom

Tsuneyuki, Shinji - Department of Physics, the University of Tokyo, Japan

Xu, Lei - Leibniz Institute for Solid State and Materials Research, Germany

State of the art in mesoscale and multiscale modeling.

Location: CECAM-IRL, University College Dublin
Webpage: https://www.cecam.org/workshop-0-1487.html
Dates: May 29, 2017 to June 1, 2017

1 State of the art

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

The use of mesoscale models faces challenges such as

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

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

Significant areas that require special attention in order to be able to advance faster and deeply on the development of meso- and multi-scale methods include: the foundations of mesoscale and multiscale models, the use of particle-based and statistics-based static and kinetic mesoscopic approaches, the understanding of fundamental processes in non-equilibrium and heterogeneous systems, and the use of hybrid and mesoscale approaches to analyze the dynamics of complex materials. These requirements include fundamental topics related to the foundations of these type of models with the objective to understand the potential of existing approaches and their weaknesses. This is a central aspect in order to identify the major needs in the improvement of the theoretical basis for mesoscale methods.

2 Major outcomes

Given the spirit of the workshop, focused on a survey of the state of the art, the main outcomes of the discussions aim at setting the stage for promoting further development and creating the best research environment. The event recognized the needs to advance in the establishment of mesoscopic models and their proper calibration to convert them into quantitative predictive tools. The event also serves to agree that the next four years we can expect a consolidation of different mesoscopic methods developed over the last ten years and a more systematic analysis to be able to combine them with molecular methods. Specifically, the main topics explored in the SAW have been,

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

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

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

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

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

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

e) Many particles based coarse grained models need to be used to simulate non-equilibrium behavior of complex and heterogeneous materials. These systems lead to an inhomogeneous distribution of the particles that represent the different components of the materials. These asymmetry poses computational challenges, especially when exploiting mesoscopic models on HPC facilities. The discussions identified load

unbalancing as a serious limitation in the scaling of mesoscopic algorithms at the peta-scale and beyond.

The outcomes of the meeting include:

1. Overviews of recent advances in systematic coarse-graining and multiscale modelling, inclusion of electrostatic, quantum, and hydrodynamics effects in simulation

2. Identification of remaining challenges in bridging the time and length-scale gaps in soft matter modelling

3. Discussions of the foundations of mesoscale models, hybrid models, and coarse-grained liquid state models

4. Discussions linking ab initio methods with atomistic modelling

5. Identification of bottlenecks in HPC implementation of the multiscale software (AdResS, and computational packages such as ESPRESSO, DLMESO, LAMPPS, PI-GC-AdResS, MP2C, Ludwig, Votca.)

6. Discussions regarding the gaps in dialogue and interaction between academia and industry

7. Discussions regarding the need for further development of meso- and multi-scale methods and soft-ware codes

8. A proposition for a Lorentz workshop in 2018 – still under preparation.

3 Community needs

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

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

It was recognized the need to procure sufficient human resources is all the more important due to the potential recognized in meso- and multi-scale modelling to cope with complex

materials. The meeting also recognized the need of a balance deployment of resources in the foundation of these new methods and in their adaptation to a variety of industrial needs.

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

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

4 Funding

In terms of funding, the discussions carried out during the workshop have indicated that the development of mesoscale and multiscale methods will increase their potential for direct application to industrially related challenges. In this respect, Horizon 2020 is clearly a potential funding channel, and recent developments, which pave the way to material and energy-related applications, might lead to successful ERC projects. EPSRC, in the UK, is a clear source of funding for the development of new formulation initiatives.

To make progress in the development of new methods and tools for the development of multi-scale methods that build on the solid knowledge of molecular models, the expected advance in our control of mesoscopic methods and finite element approaches, a concerted community effort is needed. To fund such a community-wide effort in a sustainable way, a combined strategy is necessary. While individual PIs can apply for single investigator grants from their national funding agencies, the EU H2020 framework could provide opportunities to set up an international network geared towards method development. More specifically, within the Marie Skłodowska-Curie actions, Innovative Training Networks offer attractive possibilities to train the required human expertise with strong ties to industry. Other opportunities for funding might be available in the Future and Emerging Technologies (FET) Program of H2020.

5 Will these developments bring societal benefits?

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

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

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

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

6 Participant list

Organizers

Lobaskin, Vladimir
University College Dublin, Ireland

Mac Kernan, Donal
University College Dublin, Ireland

Pagonabarraga, Ignacio
CECAM EPFL, Switzerland

Andrienko, Denis - Max Planck Institute for Polymer Research, Germany

Asinari, Pietro - Politecnico di Torino, Italy

Buchete, Nicolae-Viorel - University College Dublin, Ireland

Casciola, Carlo Massimo - University of Rome I "La Sapienza", Italy

Cazade, Pierre - University of Limerick, Ireland

Cheung, David - NUI Galway, Ireland

Chiacchiera, Silvia - STFC, United Kingdom

Donev, Aleksandar - Courant Institute, New York University, USA

Duenweg, Burkhard - Max Planck Institute for Polymer Research, Mainz, Germany

English, Niall - University College Dublin, Ireland

Español, Pep - National University of Distance Education, Spain

Harb, Moussab - KAUST University, Saudi Arabia

Holm, Christian - Institute for Computational Physics, University of Stuttgart, Germany

Jung, Gerhard - Institute of Physics - Johannes Gutenberg-Universität Mainz, Germany

Kabedev, Aleksei - University College Dublin, Ireland

Kalliadasis, Serafim - Imperial College, United Kingdom

Kobayashi, Hideki - Max Planck Institute for Polymer Research, Germany

Kremer, Kurt - Max Planck Institut for Polymer Research, Mainz, Germany

Lemmin, Thomas - UCSF, USA

Lio, Pietro - University of Cambridge, United Kingdom

Lopez, Hender - University College Dublin, Ireland

Lyubartsev, Alexander - Stockholm University, Sweden

Maheshwari, Nikunj - University College Dublin, Ireland

Markina, Anastasia - Faculty of Physics, Lomonosov Moscow State University, Russian Federation

McCartan, Sarah - University College Dublin, Ireland

Müller, Marcus - Georg-August University, Göttingen, Germany

Nolan, David - Trinity College Dublin, Ireland

O'Reilly, Eoin - Tyndall National Institute at University College Cork, Ireland

Perez, Danny - Los Alamos National Laboratory, USA

Poggio, Stefano - University College Dublin, Ireland

Power, David - University College Dublin, Ireland

Praprotnik, Matej - National Institute of Chemistry, Ljubljana, Slovenia

Reese, Jason - University of Edinburgh, United Kingdom

Rieger, Heiko - Saarland University, Germany

Samantray, Suman - National University of Ireland, Galway, Ireland

Sanyal, Shourjya - CASL, School of Physics, UCD, Ireland

Scherer, Christoph - Max Planck Institute for Polymer Research, Germany

Seaton, Michael - Science & Technology Facilities Council, United Kingdom

Sevink, Agur - Leiden University, The Netherlands

Shields, Denis - UCD Conway Institute for Biomolecular and Biomedical Research, Dublin, Ireland

Stratford, Kevin - University of Edinburgh, United Kingdom

Tywoniuk, Bartlomiej - University College Dublin, Ireland

Xu, Liang - University of Limerick, Ireland

Zavadlav, Julija - ETH Zurich, Switzerland

Green's function methods: the next generation III.

Location: CECAM-FR-GSO
Webpage: https://www.cecam.org/workshop-0-1399.html
Dates: June 6, 2017 to June 9, 2017

1 State of the art

Green's functions have always played a prominent role in many-body

physics. In particular the one-body Green's function (GF) delivers a wealth of information about a physical system, such as ground-state energy, excitation energies, densities and other measurable quantities. Therefore, the development of approximate methods to

calculate the one-body GF has been an active research topic in many-body physics since the 60's, and many routes have been explored in order to find increasingly accurate GFs. A very popular class of methods is based on the iterative solution of an integral equation for the GF containing an effective potential, the so-called self-energy, which needs to be approximated. The well-known GW approximation belongs to this class; this approximation is the method of choice for calculating band structures, but it also shows several shortcomings, such as the wrong description of satellites in photoemission spectra, in particular in so-called strongly-correlated materials. Therefore, more refined levels of approximations are needed to keep the pace with the advances made in

experiment. Recently much progress has been made in this direction both by going beyond standard methods and also exploring completely novel routes to calculate GF. A new wave of original ideas, understanding, and solutions, has pervaded the field and therefore we think it was timely to gather these new concepts in a workshop.

2 Major outcomes

It is clear that state-of-the-art approximations are not sufficient anymore to describe new phenomena and emerging new physics that the advances in the experimental techniques allow us to explore.

The so-called strongly correlated materials, for example, exhibit remarkable electronic and magnetic properties, such as metal-insulator transitions, half-metallicity, or unconventional superconductivity, which make them among the most attractive and versatile materials. Describing these systems requires to go beyond today's state-of-the art

approaches and represents nowadays one of the greatest challenge for condensed matter theory. New strategies start to emerge which revisit fundamental equations and reformulate them in such a way to make clearer the physics they describe. New physical constraints are searched in order to obtain physical approximations. It is also clear that

collaboration with other fields is essential since similar problems are common to various domains and solutions might already exist.

According to this, the workshop has shown four big axes of development, promising to tackle the new challenges in material science:

1) Beyond GW for the description of electrons and hole in correlated materials: self-consistency, vertex, solution of the equation of motion of G, are all branches of the many-body theory heavily explored today, especially for the description of beyond-band-structure-effects, like satellites, Hubbard bands, etc. To emphasize this, one point was particularly debated: the unsatisfying (yet) level of convergence in actual GW calculations.

2) Combination of multiple approaches: the workshop really showed an ever-increasing combination of theoretical approaches for a variety of questions: one-particle spectroscopy, total energies, optical properties, fundamental behavior. The most discussed topics concentrated on combination of i) many-body perturbation theory and Dynamical Mean Field Theory, ii) diagrammatic approach and Configuration Interaction, and iii) density functional theory and quantum electro-dynamics.

3) The necessity to devise new and more efficient approaches, approximations and strategies, following alternate routes, like the solution of the equation of motion of G (as an alternative to the self-energy) brought also the problems of multiple solutions vs uniqueness of solution. The latter is a particularly nasty problem, that only recently has got the attention it deserves.

4) Non-equilibrium theories. the workshop showed the increasing interest in developing non-equilibrium theories, for two main reasons: i) the increasing interest in thermodynamic properties, and the (dynamic) process of phase transition (like the Mott transition), often in conjunction with thermal effects; ii) the description of time-resolved spectroscopies, more and more used in the new generation synchrotron radiation facilities to investigate properties of matter, that crucially require theoretical description and analysis.

Transversal to those axes, it emerged a clear direction in better code development, more distributed, more 'professional'. This is both crucial and difficult. Most of the fundamental developing benefit form a light and versatile code management. At the same time, in the moment new developments are tested and running, the more professional procedure (distributed revision control, tickets, forums, etc.) becomes important. This frontier is a new important as much as difficult topic.

3 Community needs

Many of the concepts here reported will benefit from an increase

support of fundamental research.

This is today particularly important in a moment in which public research is funded over contracts and projects. In many countries, fundamental research suffers against applied or industrial research. Very often national calls give high priority to joint research + industry applications. To this we can add the perverse ramification of calls (European, national, regional, local) that far from multiply the offer, rather it creates a frustrating scattered and highly inefficient funding procedure.

For what concerns specifically software and hardware, we have both good and bad news. Many groups have already partnerships with local software engineers, few others decided to ask support to the PRACE facilities. This is a crucial step: it is indeed true that the computer power available today (both in national and European calls) is good news to tackle bigger and more complicate systems. However, without a proper writing (and often, re-writing) of our computer codes (and this is the bad news), to take full advantage of the modern paradigms (blue-gene low memory nodes, GPUs accelerators, mics, and all hybrid architectures), there will not be any possibility to tackle such complex materials and behaviors. The scalability required to take full advantage of this new kind of resources is in fact such (1-1000000 cores) that only a professional approach can succeed.

This professional procedure comes not only in term of parallelization

of the codes, but also in their everyday maintenance and in all aspects of collaborative development (revision control, tickets, pull requests, forums, etc.), as previously mentioned.

Finally, in order to make these new codes and capabilities widely available, training strategies have to be devised, at both hard (summer dedicated schools) and soft (eLearning

platforms, MOOCS) levels.

4 Funding

As mentioned before it is crucial for the development of the fundamental research involved in this workshop, that funding agencies continue or even increase their funding of fundamental research. The workshop brought together many established experts in the field of Green's function methods as well as young promising talented researchers. At today, several channels have been analyzed, for the funding of fundamental research:

- ERC grants at the European level (starting, consolidator and advanced, together with synergy) are the most important call in which fundamental theory can be funded.
- Marie-Curie calls (Individual fellowship, CoFUND, and ITN) are still active and available also for fundamental research (even if some calls, useful in the past, like the career integration, are now closed)
- National funding agencies are uneven (good for Germany, bad for Italy, worsening in France, etc.)
- Local/regional calls are sometimes good sources of funding, but only for punctual needs.

5 Will these developments bring societal benefits?

Progress in Green's function methods is of great importance to fundamental research. However, it already shown the crucial usefulness also for European Industry. Many-body Green's functions contain a wealth of information and this information can be used to develop novel materials for various innovating technological applications.

For example, the single-particle Green's function contains information on the electron addition and removal energies, which allows for an accurate description of band gaps, band alignments etc. This is very important information in the development of photovoltaic devices. The single-particle Green's function also contains information on the current density, which can be used to describe accurately all kinds of phenomena related to electron transport. From the two-particle Green's function we can obtain information about the interaction

between two particles such as the interaction of an excited electron with the hole it leaves behind. This is crucial information for the development of new photovoltaic and photocatalytic devices, for which its success largely depends on the ability of the material to split the electron and the hole after their formation.

However, this applies to the field globally. Concerning the more restricted focus of the workshop in particular, it is about fundamental research preparing the long-term future on a scale of, say, 10 years which unfortunately is not always of direct interest for a private company.

6 Participant list

Organizers

Berger, Arjan
University Paul Sabatier, France

Romaniello, Pina
University Paul Sabatier, France

Sottile, Francesco
Ecole Polytechnique, Palaiseau, France

Al-Badri, Mohamed Ali - King"s College London, United Kingdom

AYRAL, Thomas - Physics & Astronomy Department, Rutgers University, USA

Caffarel, Michel - University Paul Sabatier, Toulouse, France

Caruso, Fabio - Humboldt-Universität zu Berlin Institut für Physik, Germany

Di Sabatino, Stefano - LSI, Ecole Polytechnique, Palaiseau, France

Draxl, Claudia - Humboldt University Berlin, Germany

Droghetti, Andrea - University of the Basque Country, Spain

DUONG, LE QUY - University of Liege, Belgium

Dvorak, Marc - Aalto University School of Science, Helsinki, Finland, Finland

Helbig, Nicole - Forschungszentrum Juelich, Germany

Kozik, Evgeny - King’s College London, United Kingdom

Kunes, Jan - Academy of Sciences of the Czech Republic, Austria

Laflorencie, Nicolas - CNRS & Université de Toulouse, France

Loos, Pierre-Francois - Laboratoire de Chimie et Physique Théoriques, UMR5626, UPS CNRS., France

Lupo, Carla - King"s College London, United Kingdom

Marmodoro, Alberto - Ludwig Maximilians Universität, Germany

Martins, Cyril - LCPQ IRSAMC Universté de Toulouse III, France

Mazouin, Laurent - Université de Strasbourg, France

Michelini, Fabienne - Aix-Marseille UniversitÃ©, IM2NP UMR CNRS 7334, France

Moller, Gunnar - University of Kent, United Kingdom

PAVARINI, Eva - Research Center Juelich, Germany

Pavlyukh, Yaroslav - Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany, Germany

Perfetto, Enrico - National Research Council (CNR), Rome, Italy

Potthoff, Michael - University of Hamburg, Germany

Rehr, John - Dept of Physics, University of Washington, USA

Reining, Lucia - Ecole Polytechnique, Palaiseau, France

Rocca, Dario - University of Lorraine and CNRS, France

Sheridan, Evan - Kings College London, United Kingdom

Stepanov, Evgeny - Radboud University, The Netherlands

Tarantino, Walter - ETH Zurich, Switzerland

Tokatly, Ilya - U. del Pais Vasco, Spain, Spain

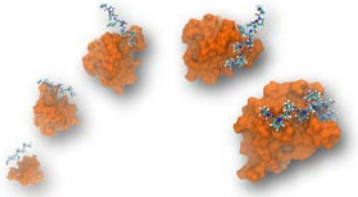
Toschi, Alessandro - Technical University of Vienna, Austria, Austria

Werner, Felix - ENS, Paris, France

Winterowd , Christopher - University of Kent, United Kingdom

zhou, jianqiang - ETSF, Ecole Polytechnique Paris, France

Beyond Kd's: New computational methods to address challenges in drug discovery



Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1460.html
Dates: June 6, 2017 to June 9, 2017

1 State of the art

With the rapid growth of computational resources, using both massively parallel and GPU-based architectures, and the development of innovative algorithms, drug discovery research teams are progressively turning from approximate to more rigorous methods. The workshop aimed at focusing on challenges in predicting the thermodynamics and kinetics of ligand binding as well as drug absorption, using state-of-the-art computational approaches. From the workshop, it is clear that all directions of computational drug discovery are moving towards more efficient and reliable free-energy calculations, incorporating enhanced-sampling methods to improve protein-ligand binding predictions. It is also increasingly recognized by both academia and industry that in order to go beyond binding affinity, new methods need to be developed to capture ligand binding/unbinding pathways in order to predict the underlying kinetics. Furthermore, rigorous physics-based calculations are applied to estimate membrane permeation. Thus, an important goal of the workshop was to establish a network of international researchers to exchange and discuss methods and algorithms for the future development of computational approaches that will impact modern drug discovery.

2 Major outcomes

During the four-day workshop, the planned time for discussion and well-prepared discussion topics were highly appreciated by the participants and proved to be a fruitful source of inspiration. A total of 33 invited oral presentations were given during the workshop. Each 20-minute talk was followed with 20-minute discussion. Each speaker was requested to prepare their discussion slides ahead of time to address key questions: What are the obstacles that keep us from going beyond Kd? What major advances are required for success? What are the key directions for development? At the end of day 1, day 3, and day 4, there were 1.5-hour general discussion sessions, led by 2-3 participants each day. On day 2, there was a poster session featuring 12 contributed posters. The following items emerged as key outcomes.

There is a consensus that with the rapid growth of computational resources and sampling methodology, force field development is critical for the future success of the computational drug discovery. Current challenges in force field development are:

a. Dataset problem. The same, very limited set of experimental data is used in parameterization of empirical force fields, leading to the danger of overfitting. In addition, the majority of the data was measured more than 50 years ago, where some experimental techniques were not as sophisticated as today. Moreover, some data were acquired from fitting instead of direct experimental measurement. To be able to develop more accurate force fields, increasingly accurate experimental data is needed. As a community, we need to carefully curate the existing data to ensure the quality of the experimental data used for developing force fields.

b. Technical issues. The combination rules used in current force fields may need to be modified. Polarizability and the number of off-site point charges were discussed. As a community, there is a need to reach a consensus regarding reasonably good validations for force field, such as NMR data, hydration free energy, osmotic pressure, or binding affinity.

c. Protonation states and tautomerization are big issues in the pharmaceutical industry and were seen as a huge problem from last SAMPL5 challenge. Possibilities to address these challenges may involve constant-pH simulations, but the best approach is yet to be determined.

One of the major challenges to go beyond Kd is modeling kinetics. Much less is known about the molecular determinants of binding kinetics than about those of equilibrium binding affinity. Capturing the correct ligand binding/unbinding pathways as well as the conformational fluctuations becomes essential to predict the underlying kinetics. Identifying the conformations involved in the (un-)binding pathways and the transition state will be key for the rational manipulation of binding kinetics to improve kinetic selectivity. The workshop identified the current challenges in kinetic modeling:

a. Benchmarking datasets. Choosing a system with more than one slow degree of freedom is very important for benchmarking. The binding kinetics study of the FKBP protein with fragments and reversible protein folding simulation from David Shaw Research could be a good benchmarking set for kinetic modeling. There will be also an industry/academia collaboration that currently generates data for 13 targets. The datasets will be released by the end of 2017.

b. Enhanced sampling for kinetics. A large number of methods have been proposed with often only subtle differences between them. Which method ought to be used for which system was discussed at length.

c. Identification of the reaction space. As a good practice it was proposed to use more collective variables first and then reduce gradually. In particular, the string method can give good starting points for further simulations. Depending on the system, when there is more than one path, a method needs to be chosen that allows an ensemble of paths to be sampled.

3 Community needs

The community needs efforts in the following directions:

a. Availability of more automatic, efficient and reliable codes is essential for reproducibility, benchmarking and usability.

b. There is a consensus that force field development is critical for the future success of the computational drug discovery. There is a need for organizing a CECAM workshop on force field development.

c. There is a need for automatic infrastructure tools for re-parameterizing small molecules.

d. New benchmarking datasets to construct kinetic models and testing various enhanced-sampling methods for kinetics.

e. More experimental data for parameterization and validation.

f. More connection with industry would also benefit the community because industry is certainly in a need to address the challenges of beyond Kd prediction.

g. Besides drug binding kinetics, bioavailability of the drug is one of the essential intrinsic properties of drugs. Prediction of the passive permeation rate and metabolism pathway is of key importance in pharmaceutical community.

4 Funding

The strong support from CECAM, academia, and industry in both Europe and the US made this workshop possible and showed the benefits that an international funding mechanism could bring. During the workshop, it was emphasized that developing and validating force field need large and long-term collaborations. However, it is currently difficult — and, in fact, nearly impossible — to get funding for force-field development, despite the importance for the field. This issue has become particularly problematic, especially for junior scientists. Funding agencies usually want to see a wide usage of a funded program or force field; however, popularity is not accuracy. Additional funding is needed to acquire newer and more reliable experimental datasets for force-field development.

5 Will these developments bring societal benefits?

The broad scope and the state-of-the-art methods presented during the workshop hold a great potential for health benefits as they can help design drugs with longer-residence time, better membrane permeability and metabolic stability. Over the course of the workshop, we had current experts from both academia and industry with different, albeit complementary mindsets to discuss the progress achieved recently as well as the current pitfalls in computational methods employed in such tasks. We had presentations about protein-ligand binding and membrane permeability, which were carried out in collaboration with industries. Companies such as Sanofi, Janssen R&D, Bayer, Roche, Actelion, Mitsubishi Tanabe Pharma, and GSK were also present during the workshop, due to their great interest in these novel methodologies. We also surveyed where the current methodological developments stand and what are the most promising methods for the next five to ten years. One of the suggested ways to fulfill this potential and expand the network of international researchers established from this workshop is to hold similar workshops regularly to sustain this kind of academia-industry connections for the future development of computational methods that will lead to a breakthrough in modern drug discovery.

6 Participant list

Organizers

Chipot, Chris
University of Illinois at Urbana-Champaign, USA, USA

Luo, Yun Lyna
Western University of Health Sciences, USA

Riniker, Sereina
ETH Zurich, Switzerland

Botello-Smith, Wesley Michael - Western University of Health Sciences, USA

Cecchini, Marco - University of Strasbourg/ISIS, France

Chang, Chia-en - Department of Chemistry, University of California, Riverside, USA

Elber, Ron - UT Austin, USA

Essex, Jonathan - University of Southampton, United Kingdom

Gallicchio, Emilio - Brooklyn College of the City University of New York, USA

Gilson, Michael - University of California, San Diego, USA

Gumbart, James - Georgia Institute of Technology, USA

Gunsteren, Wilfred van - ETH Zurich, Switzerland

Hansen, Niels - Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart, Germany

Hédin, Florent - CERMICS, École des Ponts - ParisTech, France

Hunenberger, Philippe - ETH Zurich, Switzerland

Hwang, Sunny - Institute of Georgia Technology, USA

Jorgensen, William L. - Yale University, USA, USA

Kuhn, Bernd - F. Hoffmann-La Roche, Switzerland

Lelievre, Tony - Ecole des Ponts ParisTech, France

Levy, Ronald - Temple University, USA

Liedl, Klaus - Leopold-Franzens-University Innsbruck, Austria, Austria

MacKerell, Alexander - Univ. of Maryland, School of Pharmacy, USA

Mark, Alan - University of Queensland, Australia

Martinotti, Carlo - Curtin University, Australia

Meier, Katharina - Bayer, Germany

Merz, Kenneth M. - Michigan State U., USA

Meyer, Christophe - Janssen R&D, France

Miao, Yinglong - UC San Diego, USA

Minh, David - Illinois Institute of Technology, USA

MINOUX, HERVE - sanofi, France

Mobley, David - University of California, Irvine, USA

Montalvo Acosta, Joel - University of Strasbourg, France

Noskov, Sergei - University of Calgary and Institute for Biocomplexity and Informatics, Canada

Oakes, Victoria - University of Bath, United Kingdom

Okada, Okimasa - Mitsubishi Tanabe Pharma Corporation, Medicinal Chemistry Research Laboratories, Japan

Oostenbrink, Chris - University of Natural Resources and Life Sciences, Austria

Pan, Albert - D. E. Shaw Research, USA

Pavlova, Anna - Georgia Institute of Technology, USA

Rauscher, Sarah - Max Planck Institute for Biophysical Chemistry, Germany

Rowley, Christopher - Memorial University, Canada

Schneck, Jessica - GlaxoSmithKline, USA

Shen, Jana - University of Maryland School of Pharmacy, USA

Sidler, Dominik - ETH, Switzerland

Silva Lopes, Laura - CERMICS, France

Sultan, Mohammad - Stanford University, USA

Vasilakaki, Sofia - Biomedical Research Foundation Academy of Athens, Greece

Walker, Ross - University of California, San Diego, USA

Yuan, Shuguang - Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland

The future of biomembrane simulations: hidden pitfalls and future challenges

Location: CECAM-FR-RA
Webpage: https://www.cecam.org/workshop-0-1470.html
Dates: June 6, 2017 to June 9, 2017

1 State of the art

The first molecular simulations of lipid membranes were published 35 years ago. Since then, the field has exponentially grown in ambition both with respect to size and length, as well as force field refinement and complexity. Instead of small patches of simple lipids, we can nowadays study membranes consisting of thousands of lipids, explore interesting curved geometries, study the phase behavior of mixtures, incorporate proteins, and much more. The impressive advances over the past decades owe a great deal to the often-coordinated progress made on multiple fronts, among them the massive increase in computational resources, the development of powerful simulation and analysis software, our ever-increasing abilities to compare theoretical and computational predictions with better and better experiments, and a host of refined theoretical tools and models to conceptualize the physics and chemistry of bio membranes.

The key aim of the CECAM workshop “The future of bio membrane simulations: hidden pitfalls and future challenges” was to take stock of what has been achieved, which endeavors were particularly successful, which long-lasting lessons have been learned, and how all of this informs the future of our field: Where will we go from here? What are worthwhile goals to set for our community for the next years, or the next decade? What will be the major challenges we will likely be facing? Which known pitfalls must we avoid? And how to we recognize traps we have not yet encountered, because so far, our systems were not yet complex enough to exhibit them, but which we will, therefore, encounter in the future?

To address these questions, almost 50 practitioners in the field---from senior PIs and PhD students, simulators and experimentalists---met early June in Lyon and discussed the future of our field. This report summarizes some of the key findings they arrived at.

2 Major outcomes

Atomistic force fields:

All-atom force fields (AA-FF) are becoming ever more faithful, as reported by two developers (CHARMM and AMBER) who attended the workshop. For instance, area-per-lipid (APL) or bond order parameters (BOP) are predicted much better today than a decade ago. However, the same was said last decade about what back then were state-of-the-art FF. Open-science projects (e.g http://nmrlipids.blogspot.ch) were extensively discussed as a promising avenue to compare FF progress in an unbiased way. And yet, the existence of multiple AA-FF (vs. only one nature!) reminds us that even AA simulations are approximations with inherent flaws---notably, transferability and representability issues. These are well appreciated and studied in the coarse-graining (CG) community. Due to increasingly ambitious and well-equilibrated AA simulations, and the greater availability of experimental data, they become more noticeable in the AA world, and this opens an opportunity for the AA community to learn from past decades of CG experience.

Coarse-grained force fields:

CG approaches come in two flavors: bottom-up models derive from a more finely resolved description, while top-down models explore physical principles in simplified settings. Some of the most successful models, e.g. MARTINI and SDK, incorporate aspects of both, as highlighted in updates from developers. CG models begin to look at greater complexity, e.g. complex lipid mixtures plus proteins. However, while closer to biology, it will be more difficult to validate such models: the intricate nature of ternary lipid phase diagrams has been studied for almost two decades, and much less is known at that detail about quaternary (let alone higher level) mixtures. Moreover, many CG models are specifically designed for a particular situation, and so striving for simple explanations might also tempt one to make a model do what one wants to see. More transparent falsification criteria are needed.

Linking Simulation and experiment:

Growing experimental data sets on structure (e.g. electron density profiles, BOPs, APL) and thermodynamics (e.g. partition coefficients, phase behavior, elastic moduli) provide a fantastic foundation for refining computational models. But we must eschew tuning our models too closely towards some subset of observables (say, APL), lest we hurt its ability to capture others (say, phase transitions). Representability, again! To make headway, we need more than good experimental data on these observables for well-defined standard systems; we also need model predictions for all of them. While routinely done for the “simple” ones (local structure), we often lack “difficult” (large-scale) observables (e.g. transition temperatures or elastic moduli). Focusing too strongly on the simple ones in FF-development threatens

transferability and representability. We hence discussed which "large-scale" observables might constitute a good training set.

Complexity:

The community is enthusiastic about increasing complexity: begin with mixtures of lipids, add proteins, add coupling to the cytoskeleton, etc. Many feel that the ultimate goal must be to simulate a whole cell. Even ignoring computational challenges, this will be difficult: how will representability and transferability issues fare going up the emergent hierarchy? What even is emergence in this context? Might we learn the wrong lessons? The community is eager to try anyways, and so it seems worthwhile to verbalize more clearly what one hopes to learn that cannot be gleaned from a study of the parts and their connections. In any case, much useful knowledge will be gained along the way, and so it is highly unlikely that the endeavor will not prove fruitful.

3 Community needs

Three limitations of biomembrane simulations are (i) the short simulation times, (ii) the small sizes of the simulated samples, and (3) the limited accuracy of force-fields.

Despite simulation or modeling tricks, biomembrane simulations of increasing complexity often remain too short in time or too small in size to make accurate predictions on experimental observables. Therefore, the community expresses demand of increasing HPC resources. At the time beeing, local, national, and European centers provide most resources. The molecular dynamics community benefits from the development of GPU/CPU based HPC, thanks to permanent code development, which should continue to be publicly funded. But there is still space for improvements in terms of simplicity of usage. Hardware, software, and usage have to be more and more adapted to each other, and this can become a difficulty for typical users. Contacts within hardware and software developers and users are desirable, for example within schools and tutorials.

There is also clearly a demand for accurate and transferable force-fields, both at AA and CG level. This would be promoted by a good networking with experimentalists, but also within the community, for example to share databanks, or tools to compare different force-fields. But this networking would not have the aim of FF standardization towards a unique one: Since there is no unique ideal FF, the parallel development of various FF families in different groups is paramount and should be more effectively supported by public funding. For FF development and testing, there is also a strong need to have access to precise experimental properties of relatively simple systems at mesoscopic scales (e.g., binary or ternary phase diagrams,

diffusion constants, APL, BOP, etc.), but also to have access to experimental data providing various information on the membrane structure and dynamics at the molecular level.

4 Funding

Typical funding channels for this research are standard national or international project funding grants. Two main trends emerged in the discussion. First, FF development is no high priority of grant agencies, making it extremely difficult to obtain resources for stand-alone methodological development. Rather, development must be co-packaged with compelling new applications, even though the limits of to-be-improved FFs raise questions about how reliable predictions on such complex systems are. These two aspects, development and application, often require distinct scientific competences. This long-standing issue remains a serious hurdle towards steadily improving available methodology. On the other hand, optimism was expressed that membrane simulations emerge as a high-impact topic in the larger field of cell biology, which will improve the chances of securing resources in this highly competitive field.

5 Will these developments bring societal benefits?

Economic benefits: The academic development of open code, tools, and FFs will sustain their use in industry, but the limit on predictive power may still be perceived as a bottleneck. FF development for a specific purpose often remains necessary.

Health and societal benefits: Biomembrane simulations at increasing complexity will create molecular level insight into a huge number of relevant biological phenomena. Societal benefits could emerge from the use of biomembrane simulations as a predictive screening tool in the drug development industry (e.g. membrane-permeating peptides, new membrane-disrupting antibiotics, drug-loaded liposomes, etc.). Since membrane proteins are both a major target for drugs, as well as the cause for numerous diseases, understanding lipid/protein interactions and membrane-protein extraction at the molecular level are two challenges with high societal impact. Moreover, the tremendous increase in artificial nano-objects in everyday life and in

industrial processes compels us to study the interactions between these nano-objects and biomembranes at the molecular level, e.g. to assess their toxicity.

Sustainability: Sustainability considerations provide a good motivation for resorting more regularly to natural products in formulations, due to their better properties in terms of biodegradability and toxicity. Industrial formulations are often limited to pure artificial substances because biological molecules are too expensive and/or of lower purity. Being able to predict the behavior of lipidic mixtures would permit the use of more natural lipid products.

Funding opportunities: Co-funded research between academia and pharmaceutical industry is desirable but remains difficult because of the interest differences. Fortunately, public funding opportunities exist for academics in collaboration with experimentalists in medical sciences or nano-sciences.

6 Participant list

Organizers

BARENDSON, Samantha
Centre Blaise Pascal - ENS de Lyon, France

Deserno, Markus
Carnegie Mellon University, Pittsburgh, PA, USA

Loison, Claire
Institut Lumière Matière, France

Monticelli, Luca
CNRS, University of Lyon, France

Vanni, Stefano
University of Fribourg, Switzerland

Amelie, Bacle - University of Poitiers, France

Awasthi, Neha - Georg August University, Germany

Bassereau, Patricia - Institut Curie, France

Benedetti, Florian - Institut Lumiere Matiere, Lyon University, France

Bhaskara, Ramachandra M - Max-Planck Institute of Biophysics, Germany

Böckmann, Rainer - Universität Erlangen-Nürnberg, Germany

Buslaev, Pavel - Moscow Institute of Physics and Technology, Russian Federation

Chavent, Matthieu - University of Oxford, United Kingdom

Cosquer, Robin - University of Namur, Belgium

Covino, Roberto - Max-Planck-Institute for Biophysics, Germany

Deplazes, Evelyne - Curtin University, Australia

Di Meo, Florent - UMR INSERM 850, Univ. Limoges, France

Fiorin, Glacomo - Temple University, Philadelphia, USA

Fuchs, Patrick - University Paris 7, France

Gould, Ian R - Imperial College London, United Kingdom

HOLOGNE, Maggy - Université Lyon 1, France

Hub, Jochen - Georg-August-University Göttingen, Germany

Hummer, Gerhard - Max Planck Institute of Biophysics, Germany

Klauda, Jeffery - University of Maryland, USA

Marrink, Siewert-Jan - University of Groningen, The Netherlands

Melcr, Josef - Institute of Organic Chemistry and Biochemistry, Academy of Sciences, Czech Republic

Mounir, Tarek - Université de Lorraine, Nancy, France

Müller, Marcus - Georg-August University, Göttingen, Germany

Ollila, Samuli - Institute of Organic Chemistry and Biochemistry, Academy of Sciences, Czech Republic

Paloncýová, Markéta - Regional Center of Advanced Technologies and Materials, Department of Physical Chemistry, Palacký University in Olomouc, Czech Republic

panzuela pérez, sergio - Universidad Autónoma de Madrid, Spain

Peter, Christine - University of Konstanz, Germany

Prunotto, Alessio - Laboratory for Biomolecular Modeling - EPFL, Switzerland

Reuter, Nathalie - University of Bergen, Norway

Risselada, Herre Jelger - University of Goettingen, Dept. of theoretical Physics, Germany

Rossi, Gulia - Physics Department, University of Genova, Genoa, Italy, Italy

Roth, Gunter - NVIDIA, France

Salassi, Sebastian - Physics Department, Italy

Saric, Andela - University College London, United Kingdom

Schmid, Friederike - Johannes Gutenberg Universität Mainz, Germany

Seo, Sangjae - Nagoya University, Japan

Shinoda, Wataru - National Institute of Advanced Industrial Science and Technology, Japan

Shinoda, Wataru - Nagoya University, Japan

Smirnova, Yuliya - Georg-August University of Goettingen, Institute for Theoretical Physics, Germany

Sodt, Alexander J. - NICHD, NIH, USA

Sosso, Gabriele Cesare - The University of Warwick, United Kingdom

Vacha, Robert - Masaryk University, CEITEC and Faculty of Science, Czech Republic

Voegele, Martin - Max Planck Institute for Biophysics, Germany

WALKER, Olivier - Université de Lyon, France

Zhang, Guojie - Institute for Theoretical Physics, Georg-August University, Germany

Seeking synergy between dynamics and statistics for non-equilibrium quantum processes

Location : ENS Paris
Web page : https://www.cecam.org/workshop-0-1483.html

Dates: June 6, 2017 to June 9, 2017

1 State of the art

Many different quantum dynamics techniques are being developed and refined to provide new algorithms that respond to the demand for a balance between computational efficiency and physical accuracy. Currently available techniques are typically based upon two different, but formally equivalent, formulations of many-body quantum mechanics, the wave function approach or the density matrix picture. Wave-function-based methods generate the dynamical evolution of a system by solving the time-dependent Schrödinger equation. Prominent examples of such methods are wave packet propagation techniques, such as the multi-configurational time-dependent Hartree (MCTDH) approach, and trajectory-based approaches such as Gaussian-based MCTDH, and methods based on the exact factorization approach such as the coupled-trajectory mixed quantum-classical (CT-MQC) scheme. Density-matrix-based approaches are typically developed starting with the Liouville-von Neumann equation. Numerically exact approaches such as real-time path integral methods, and approximate methods such as the family of (partially) linearized density matrix (LDM) propagation scheme, the hierarchy of techniques derivable from the quantum-classical Liouville equation (QCLE), and mapping-variable ring polymer molecular dynamics (MV-RPMD), have been applied to a variety of systems. The non-equilibrium evolution of a subset of degrees of freedom in a system can also be rigorously formulated using the quantum master equation formalism. These equations can be evaluated using information generated from either wave function-based methods or density matrix techniques. However, a disconnect between the descriptions that the two formalisms offer is created when approximations are introduced that prevent one from achieving a fully quantum mechanical treatment of the problem. It is thus of great importance to address this interstitial region between these approaches.

2 Major outcomes

Discussion on the first day of this workshop highlighted two wave-function based approaches to quantum dynamics: the exact factorization (EF), and Gaussian-based versions of the variational multi-configurational (MC) approach (vMCG, and G-MCTDH). Although the EF picture may be impractical to implement in systems with more than a few degrees of freedom, it has led to promising approximate numerical algorithms, e.g. the coupled trajectory mixed quantum classical, CT-MQC scheme. This method has recently been combined with a TDDFT based description of the electronic structure for individual small molecules such as oxirane. The initial results from this approach seem quite promising and represent a systematic improvement over the fewest switches surface hopping algorithm. Similarly, Gaussian based MC methods have also been employed in direct tandem with electronic structure codes. In this effort, the main bottleneck seems to be “good but cheap” electronic structure data (energies, gradients, couplings). Some very nice progress on the diabatization problem has been generated from this effort, and there is ongoing work in using machine learning methods and neural network algorithms to reduce the computational cost of the electronic structure part of the problem. Two different approached to nonadiabatic dynamics using the framework of the ring-polymer molecular dynamics (RPMD) ansatz were discussed during the second morning. These two methods differ fundamentally in how they are formulated, and thus have different Hamiltonians that govern the dynamics that they generate. These approaches have only been tested for a small number of simple systems, however they show very promising results. As both approaches are quite new, they have not yet been directly compared. It is still unclear if either approach will offer systematically higher accuracy or more facile simulations than the other. The use of various levels of linearization approximations within the path-integral representation was discussed on the afternoon of Day 2. The basic idea here is to calculate a correlation function of interest directly, as a more compact approach than using a method to construct the full wave-function of the system, and then subsequently obtaining the correlation function. This approach is quite versatile, and often yields surprisingly accurate results. It can also be combined with the generalized quantum master equation (GQME) formalism, to reap even further numerical benefits for condensed phase problems. These linearization techniques have also been used in the language of quantum field theory and particle physics in generating functional theory. The morning of the third day was devoted to the study of steady state transport properties such as charge and spin current in molecular junctions. It was discussed that, quite often, looking at the steady state limit can reveal larger problems with some approximate methods, as opposed to observing their behavior for the relaxation process from a non-equilibrium initial state. The use of formulas from the area of counting statistics was discussed in this respect, and connections between nonequilibrium Green’s functions and quantum master equations were considered in this setting. The afternoon of Day 3 focused on as non-equilibrium charge transfer dynamics, where quantum dynamics methods such as mean field theory, surface hopping, and Bohmian mechanics are used in conjunction with electronic structure (DFT, and TDDFT) packages. The last morning

of the workshop was devoted to generalized statistical methods for sampling the multidimensional (Wigner transform) integrals that appear in trajectory-based quantum dynamics methods, and in exposing the formal connections between many of the different theories that were discussed at the workshop. Somewhat confounding is the fact that FSSH still lacks a formal derivation or justification, whereas almost all other methods discussed can be rigorously justified in some way

3 Community needs

During this workshop, the community did not express any special need for new computational infrastructure. This is mostly due to the exponential scaling law of quantum dynamics, which requires more careful thought than brute-force computational power to be circumvented. It was a common impression amongst the participants of the workshop that the major needs in the community lie in human resources.

A major limitation in direct wave-packet based quantum dynamics, in particular, is the accuracy of the potential energy surfaces (PESs). More accurate surfaces are needed since PES accuracy influences heavily the quantum dynamics calculation accuracy. Therefore, the participants expect to benefit from developments at the interface between this field and machine learning of electronic structure in the future.

Workshops such as this one that bring together a wide spectrum of researchers active in quantum dynamics are extremely rare and the community insisted that they are key for the development of the field. We therefore strongly believe that at least one CECAM workshop on this topic should continue be conducted every year, to give the opportunity to the community to exchange on recent developments. CECAM workshops are particularly suitable for this ongoing need.

5 Will these developments bring societal benefits?

The fundamental nature of method development in molecular quantum dynamics does not prevent its use in solving industrial and/or societal problems, however it is not as mature as the electronic structure community, and hence has less visibility in the broader community. Developments of quantum dynamics are for example of great interest to industrial partners active in quantum computing, whose impact on society could be enormous. As another example, applications of these techniques to dyes and emitters have been reported and brought new insights for the design of molecules in domains such as dye-sensitized solar cells and organic light emitting diodes. Applications of quantum dynamics techniques are also central in elucidating reaction mechanisms. This has potential for a large impact in atmospheric chemistry. Atmospheric models indeed employ experimental data when available, but often complete missing information by oversimplified models. Implementing the use of quantum dynamics to circumvent the problem of missing experimental data could be transformative in that field. In the future, we expect an ever-broadening range of areas in science and society to benefit from the application of the types of quantum dynamics simulation algorithms that are being developed in this community.

6 Participant list

Organizers

Agostini, Federica
Université Paris-Sud, Laboratoire de Chimie Physique, France

Coker, David
Boston University, USA

Kelly, Aaron
Dalhousie University, Canada

Lauvergnat, David
Université Paris-Sud, Laboratoire de Chimie Physique, France

Albareda, Guillermo - Universitat de Barcelona, Spain

Ananth, Nandini - Cornell Univerity, USA

Bonella, Sara - CECAM@EPFL, Switzerland

Borgis, Daniel - Maison de la Simulation, France

Burghardt, Irene - Goethe University Frankfurt, Germany

Carof, Antoine - Ecole Normale Supérieure, United Kingdom

Curchod, Basile - Durham University, United Kingdom

Debnath, Arunangshu - Max Planck Institute for the Structure and Dynamics of Matter (MPSD) , Germany

Dijkstra, Arend G. - University of Leeds, United Kingdom

Eich, Florian - Max-Planck-Institut für Struktur und Dynamik der Materie, Germany

Faccioli, Pietro - Physics Department of Trento University, Italy

Finocchi, Fabio - Institut des NanoSciences de Paris (INSP), France

Geva, Eitan - University of Michigan, USA

Gross, Eberhard K.U. - Max Planck Institute of Microstructure Physics, Halle/Saale, Germany

Kapral, Raymond - University of Toronto, Canada

Lani, Giovanna - Université Pierre et Marie Curie, France

Mangaud, Etienne - Laboratoire Collisions Agrégats Réactivité, France

Mannouch, Jonathan - Oxford University, United Kingdom

Min, Seung Kyu - Ulsan National Institute of Science and Technology, Korea, South Korea

Nikolic, Branislav - University of Delaware, Newark, USA

Penfold, Thomas James - Newcastle University, United Kingdom

Richardson, Jeremy - ETH Zurich, Switzerland

Richings, Gareth - University of Warwick, United Kingdom

Schild, Axel - ETH Zürich, Laboratory for Physical Chemistry, Switzerland

Segal, Dvira - University of Toronto, Canada

Seitsonen, Ari Paavo - Ecole Normale Supérieure, France

Tavernelli, Ivano - IBM Research-Zurich, Switzerland

Vuilleumier, Rodolphe - Ecole Normale Supérieure, Paris, France

Worth, Graham A. - University College London, United Kingdom

Interface Morphology Prediction with Robust and Efficient Structure Search (IMPRESS)

Location: CECAM-FI, Aalto University, Helsinki, Finland
Webpage: https://www.cecam.org/workshop-0-1415.html
Dates: June 7, 2017 to June 9, 2017

1 State of the art

Determining or predicting the structure of organic ensembles on surfaces is a challenging problem that occupies basic science and engineering alike. Recently, novel machine-learning approaches have started to compete with more traditional, stochastic methods, such as basin hoping or simulated annealing. In IMPRESS we take an interdisciplinary stance and bring together assorted experts to focus on the challenges of organic/inorganic interfaces: this is the first workshop to unite different electronic structure methods, structure search approaches and machine learning. The community as a whole will discuss the challenges outlined above and propose long-term solutions.

Although the established and novel approaches have employed different strategies, no consensus has emerged to date on how to address some key challenges that all developers face, and which we plan to tackle in the workshop:

- Energy evaluation: is it better to pair accurate approaches with advanced phase space sampling algorithms, or focus on perfecting inexpensive approximations (interatomic potentials, non-self-consistent functionals)?

- Phase space exploration: coarse-graining is an effective way to remove degrees of freedom in phase space explorations, but how do we deal with the limitations?

- Pre-screening structures: offers a great advantage, but how can this be done well? Fast sampling with lower accuracy methods often miss important regions of phase space.

- Search target: can we efficiently extract not only global and local minima, but also the barriers between them? Alternatively, can we directly target desired properties?

- Parallelisation potential: how well are we taking advantages of the massive HPC resources available?

- Data storage: Structure search efforts often generate a wealth of additional, useful data. How can existing or future repositories be exploited to make most use of the computational effort?

2 Major outcomes

In the past 5 years, global structure search field has been re-energized by the influx of machine-learning techniques, which are now increasingly employed to augment or advance existing methodology and deliver unprecedented accuracy and speed up. The availability of high quality experimental data is also contributing to the growth of the field. Interface problems are a major driver of computational structure search method development on the account of structural complexity, irregularity and polymorphism.

Topics discussed included global optimization methods and the benefits of employing machine learning to enhance current techniques. A large variety of approaches were presented to address different physical problems and close collaboration with experimental groups was notable across the field. There was much discussion on how to consolidate the field, disseminate techniques with better documentation and tutorials, and promote consortium efforts to compare different simulation methods.

Most featured methods suffered from intrinsic limitations that prevent their immediate dissemination, but routes towards improvement have been identified and further years of development are expected to deliver considerable improvements. The computational cost of applying accurate computational methods to simulate realistic large-scale systems remains a limitation that will likely continue in the years to come, despite the availability of computational infrastructure.

Even after extensive discussions produced lots of interesting suggestions, many open questions remain. It remains difficult to compare different simulation methodologies and it is not clear which ones will emerge as most versatile and transferable in the years to come. In machine learning-based approaches, there is ongoing debate over the role of algorithm choices and data representations on the results obtained. It remains uncertain whether employing low-accuracy fast simulation techniques is beneficial and where, or whether on-the-fly parameterization is a better solution where accurate simulations are prohibitive. Furthermore, most techniques address a particular lenthscale (atomistic-nanoscale) and it is not clear how to extend them to multi-scale approaches for more realistic studies.

3 Community needs

The number of workshop participants from different backgrounds and the variety of approaches presented testifies to the resurgence of interest in the field of global structural optimization and increasing attention to interface problems. Presently most groups carry out this research as a side-activity but given the potential impact of novel methods and the volume of open questions, it is expected that funding applications on this topic will help to consolidate this field in future years. While funding and manpower is presently lacking in this field, existing high-performance computational infrastructure is sufficient for this community.

The workshop brought together contributors from Europe, USA and China that originate from different communities (physics and chemistry), and many of them have not met before. We have identified a clear need for more networking and discussion in this field. Given the time scales needed to advance present approaches, participants have agreed that biennial (once every two years) meetings may serve this community best. On the other hand, the close relationship between method development and experimental work has exposed a need for a scientific exchange with the experimental community. Theory-experiment meetings could be organised biennially in between method development meetings, and one is planned for 2018.

4 Funding

Small amounts of funding are readily available for networking activities. This community traditionally relies on funding from CECAM and Psi-K sources, given the good match between the subject matter and the scope of these two bodies. An emerging source of small-scale funding for this field are the novel European centres of excellence (CoEs) for computational materials design such as NOMAD and Marvel: they have an interest in the methodology produced in this field, but many contributors work outside the CoEs.

There is no present plan for joint funding proposals at this stage: it is expected that groups will apply for individual funding (national and Horizon 2020) to advance their simulation tools before the community is ready for collaborative work. However, there is one joint proposal for computational resources to compare present methodologies.

5 Will these developments bring societal benefits?

The renewed interest in structure prediction at interfaces is strongly driven by industrial applications, more concretely the need to understand and influence surface-based processes underpinning various technologies. By understanding structure and properties at the interface, the community aims to improve present industrial processes and develop new approaches for future technologies.

Renewable energy applications drive work presented on interfaces for optoelectronics and electrochemistry (batteries) in order to improve efficiencies. Much new development on oxide interfaces and nanoclusters is inspired by industrial catalysis. Organic crystal structure prediction studies contribute to the field of pharmaceutical research, inferring the crystal forms of novel compounds and helping to eliminate ineffective or harmful crystallisation mechanisms. The latter applications may attract future funding from the pharmaceuticals industry. Other research directions already fall under current strategic funding initiatives of national funding bodies and Horizon 2020.

6 Participant list

Organizers

Hofmann, Oliver T.
Institute of Solid State Physics, Graz University of Technology, Austria

Rinke, Patrick
Aalto University, Helsinki, Finland

Todorovic, Milica
Centre of Excellence in Computational Nanophysics (COMP), Aalto University, Finland

Blum, Volker - Duke University, Durham, NC, USA, USA

Ghiringhelli, Luca M. - Fritz Haber Institute of the Max Planck Society (FHI), Berlin , Germany

Goedecker, Stefan - University of Basel, Switzerland

Klapp, Sabine - Institute of Theoretical Physics, Technical University Berlin, Germany

Laasonen, Kari - Aalto University, Finland

Marom, Noa - Carnegie Mellon University, USA

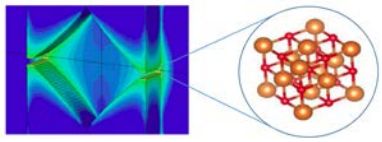
MAURER, Reinhard - Department of Chemistry, Yale University, USA

Oberhofer, Harald - Technical University Munich, Germany

Reilly, Anthony - Cambridge Crystallographic Data Centre (CCDC), United Kingdom

Sierka, Marek - Friedrich-Schiller-Universität Jena, Germany

Bridging the worlds of electromagnetic and quantum simulations.



Location: CECAM-ISR
Webpage: https://www.cecam.org/workshop-0-1432.html
Dates: June 20, 2017 to June 23, 2017

1 State of the art

Given the rapid growth in engineering applications of nanotechnology, it has become imperative for one to understand the nuances of electromagnetic field and matter interaction. The challenges in this area are fascinating from multiple perspectives; from bringing scales across domains for theoretical analysis to using this analysis for design of devices. For instance, studies on disordered optical materials have been focusing on fundamental questions, such as Anderson localization in which multiple scattering creates localized modes, or Levy flights of light, indicating diffusion with time dependence faster than linear. These fundamental concepts are becoming of increasing technological relevance, and they are important in the design of novel devices based on random lasing or on super-diffusive optical materials.

Downscaling conventional radio frequency antennas to submicron dimensions leads to the development of nanoantennas facilitating precisely controlled strong coupling of electromagnetic radiation at infra-red and optical frequencies to molecular and atomic devices. This in turn opens new venues for efficient excitation of various non-linear effects that may be useful in potentially revolutionary technologies. For example, second order non-linearities allow for second harmonic generation and rectification at optical frequencies. Nanoantennas coupled with such rectifying devices termed nano-rectennas open novel possibilities for developing energy harvesting devices with efficiencies higher than conventional photovoltaics. In a similar vein, one can envision engineered devices that use nano-magnetic arrays for a variety of applications, from MRI to THz devices. Other examples of magnetic nanotechnologies include Spin Transfer Torque Magnetic Random-Access Memories (STT MRAM), Skyrmion supporting structures, quantum Spin Hall effect, all optical switching of magnetic nanostructures.

2 Major outcomes

To help bridging the gap between the two communities of electromagnetic and quantum simulations and to develop a common language, a successful tutorial was held before the workshop with the participation of many of the workshop speakers and attendees. The main topic discussed were Hartree-Fock theory, Density Functional Theory (DFT), time dependent DFT and its applications for electron dynamics in open quantum systems. The workshop itself dealt with topics that are of interest to both communities – transport and field effects in quantum and classical systems, induced spin dynamics, mixed Maxwell and TDDFT simulations for multi-scale and multi-disciplinary modeling, and stochastic TDDFT. Strong laser interactions with molecules and solids were discussed in few experimental and theoretical talks. Multi-scale modeling was demonstrated in simulations that aim to model actual electronic devices from the atomic scale – QM/MM and tight-binding Hamiltonians were among the methods that were introduced. Methodologies and algorithms for efficient and fast time propagation in different systems were presented and discussed.

It is apparent that both communities, although coming from different disciplines and treating different time- and length-scales, have invested considerable efforts in developing advanced theory and simulation tools to solve the problem of electromagnetics in quantum nano- and meso-scale systems. It is however obvious that the two communities use different terminology to describe similar phenomena and can considerably benefit from forming a common language and strengthening scientific collaborations.

3 Community needs

The communities of electromagnetic simulations and quantum simulations are well developed and have established a considerable body of knowledge. As discussed before several issues can help synergic progress of the field of nano-scale quantum and classical methods:

- Creating a common language in the formulation of theories that combine electromagnetic and quantum methods. This is extremely important for new comers to the field but is not trivial since it is a dynamic field, where many methodologies are still in development stages.

- Fostering common culture by having more joint conferences and workshops that host people coming from both disciplines and communities.

- The creation of tutorials and courses, aimed to teach electromagnetic methods to chemistry graduate students and post-doctoral fellows as well as quantum methods to younr researchers in the field of electromagnetic simulations.

- Forming common open access repositories of efficient and scalable solvers that can serve both communities and facilitate the efficient solution of ever larger systems and complex problems.

4 Funding

Funding is needed to support this field in several aspects:

- Research grants that are specifically aimed at cross-communities collaborative efforts of multi-scale and multi-physics treatment of relevant problems.

- Funding of academia and industry collaborations is important as the electronic industry is also interested in smaller devices that should be modeled by quantum methods.

- Funding for education, promoting additional workshops, schools, conferences and also higher degrees dedicated tracks that will help to educate more professional new researchers.

5 Will these developments bring societal benefits?

The benefits that can come out of the synergic collaboration between these two communities are hard to imagine and can be well beyond the current most optimistic view of the field. Such collaborative efforts are still at their infancy but we envision great potential that can lead not only to new scientific achievement but also to novel technological breakthroughs. The growing demand of more accurate modeling of smaller electronic device is an additional practical motivation for the field. The design of new nano-scale devices requires such inter-disciplinary approaches that require understanding of both atomistic quantum and classical electromagnetic phenomena. This means that the demand for common language, multi-physics tools, and inter-disciplinary education will most definitely considerably grow in the near future.

6 Participant list

Organizers

Balasubramaniam, Shanker
Michigan State University, USA

Boag, Amir
Tel Aviv University, Israel

Hod, Oded
Tel Aviv University, Israel

Lomakin, Vitaliy
University of California, San Diego, USA

Maci, Stefano
University of Siena, Italy

Natan, Amir
Tel Aviv University, Israel

Yogev, Yael
Tel Aviv University, Israel

Chew, Weng Chow - University of Illinois at Urbana-Champaign, USA

Cohen, Guy - Tel Aviv University, Israel

Dudovich, Nirit - Weizmann Institute of Science, Israel

Engheta, Nader - University of Pennsylvania, USA

Fleischer, Avner - Tel Aviv University, Israel

Galperin, Michael - University of California, San Diego, USA

Ginzburg, Pavel - Tel Aviv University, Israel

Kosloff, Ronnie - The Hebrew University of Jerusalem., Israel

Kronik, Leeor - Weizmann Institute of Science, Rehovoth, Israel

Moiseyev, Nimrod - Technion - Israel Institute of Technology, Israel

Mukamel, Shaul - University of California, Irvine, USA

Neuhauser, Daniel - UC Los Angeles, USA

Nitzan, Abraham - University of Pennsylvania, USA

Peskin, Uri - Technion, Israel Institute of Technology, Haifa, Israel

Schapiro, Igor - Hebrew University of Jerusalem, Israel

Segev, Moti - Technion - Israel Institute of Technology, Israel

Sharma, Sangeeta - Max Planck Institute of Microstructure Physics, Germany

Silveirinha, Mário G. - University of Lisbon, Portugal

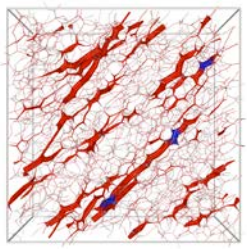
Slepyan, Gregory - Tel Aviv University, Israel

Tannor, David J. - Weizmann Institute of Science, Rehovoth, Israel

Yabana, Kazuhiro - University of Tsukuba, Japan

Yam, ChiYung - Beijing Computational Science Research Cente, China

Rheology of gel networks: combining experimental, computational and theoretical insights



Location: CECAM-FR-RA, CBP in Lyon, France
Webpage: https://www.cecam.org/workshop-0-1457.html
Dates: June 21, 2017 to June 23, 2017

1 State of the art

Gels with tunable mechanical properties and rheological behavior are at the core of new material technologies. All soft matter, in fact, from proteins to colloids or polymers, easily self-assembles into these weakly elastic solids. The nano-scale size of their building blocks makes their structure quite sensitive to thermal fluctuations, with a rich relaxation dynamic associated to spontaneous and thermally activated processes. In addition to affecting the time evolution, or aging, of the material properties at rest, those dynamical processes also interplay with an applied deformation and are crucial for their mechanical response. The result is a complex rheological behavior, with diverse, unexpected and strongly non-linear features (shear localization, stiffening, creep and fracture…).

Disentangling the impact of the structure, from dynamics and rheological response is hard, due to the complexity of the gel structures and of the microscopic dynamics at play. Theoretical and computational work in past years has been mainly focused on the self-assembly and structure formation associated to gelation of colloidal suspensions or protein solutions and on their implications for the microscopic relaxation dynamics. Nevertheless, the connections with the mechanical properties and the non-linear rheological response of the solid gel networks remain poorly understood, significantly hindering new progress for material technologies.

The idea of this conference was to bring together international experts in the field of the dynamics of gel networks, to discuss recent progress and insight from computational, theoretical and experimental approaches. In the recent years, however, the computer power and new parallel coding techniques like GPGPU or large scale MPI programming techniques

has allowed for significant progress in accessing reasonable time and length scales to address questions that were difficult to tackle before.

2 Major outcomes

The workshop was structured into six thematic half-day plus two poster sessions. At the end of each session we had detailed discussions to sort out the important open questions in the concerned field. Abstracts and some of the talks will be available on https://gel2017.sciencesconf.org/.

Aging and relaxation:

The role played by elastic and thermal stresses on aging and relaxation in colloidal and thermo-responsive gels has been amply discussed. Depending on the details of the structure and the interactions at play, gels exhibit distinct arrested states. Particular emphasis has been given to new numerical approaches able to describe an anomalous dynamic reported in different experimental works. The discussions however showed the need to find a quantitative way to compare experiments and simulations in order to discriminate between the proposed models.

Creep and precursors to failure:

Although creep and delayed failure has been observed and studied on a macroscopic scale since a long time, the specific underlying microscopic mechanisms are still poorly understood. Identifying precursors of catastrophic failure remains one of the Holy Grails in this field. In this session new experimental measurements using dynamic light scattering techniques as well as numerical efforts as first steps towards predicted failure have been presented. The discussion made clear that a combined effort of experimental and simulation techniques will be necessary to provide further answers.

Onset of rigidity and elasticity:

Whereas large part of the literature on colloidal gelation has focused on the structural arrest of the microscopic particle dynamics and its similarities with glass transition, recent works have started to address the question of how mechanical rigidity develops in soft particle gels. This session has covered theoretical approaches and connection with jamming theories, simulation studies and experiments, with a discussion mainly around the theme of rigidity percolation. The contributed talks have allowed us to expand the discussion towards biopolymer gel networks, nano composites and denser colloidal systems.

Gel rheology:

Characterizing and understanding the rheological properties of gels, both in the linear and nonlinear regimes, is crucial to applications. Recent technical developments in oscillatory rheology, such as optimal Fourier rheology or rheo-confocal imaging, as well as original experimental approaches based on splashing and simulations of the response of gels and bigels to oscillatory shear, were presented. The discussion focused the behavior of gels and glassy systems under large deformations, in particular two-step yielding in attractive vs repulsive systems and strain-stiffening in protein systems.

Mechanical instabilities:

Controlling and predicting mechanical failure of polymer and colloidal gels is a grand challenge in numerous applications. In this session new approaches for the characterization of failure modes such as crack formation, delayed yielding and gravitational collapse were discussed, where it became clear that the phenomenology of failure in respectively polymer gels and colloidal gels bares some striking similarities. Strategies such as the design of dual networks to control failure in polymer gels were presented, which also exposed that the development of strategies for the control of failure in colloidal gels are to date still missing.

Structuring and flow induced anisotropy:

The tendency to restructure under flow is fundamentally important and crucial to many technological applications. We discussed the latest experimental quantification of flow induced anisotropies in gels and the capability of newly designed numerical studies that include long range hydrodynamic coupling to correctly reproduce them. Further we learned about flow induced texture. The session finished with an investigation of nanoparticle gels and a technical discussion of recent advances in optimal Fourier rheometry.

3 Community needs

The CECAM workshop on rheology of gel networks was a success and has clearly exposed the need of meetings, where researchers working on the diverse aspects of gel networks can exchange their ideas and put their work within a broader context. All participants have expressed their satisfaction for a workshop centered on the mechanics and rheology of gel networks. A few participants had attended previous CECAM workshop on gels but found that the focus there was more on self-assembly or microscopic dynamics. All participants communicated that the choice of the focus (rheology and mechanics) was timely and excellent to create and strengthen synergies between experiments and computational approaches.

When asked specifically about upcoming events in a similar framework, none of the participants could name any future workshops or conferences. Thus, it was suggested to be highly desirable to develop a series of CECAM workshops on gel characteristics and mechanics to promote the development of unifying concepts and stimulate further collaborations between researchers exploring the behavior of gels in simulations and those exploring them in experiments.

All participants were satisfied with the set of topics covered by the workshop, that appeared sufficiently diverse without losing a coherent focus in the discussions. For future meetings, it was suggested to include related themes such as gel poroelasticity (not specifically addressed in the talks of this workshop) and gel confined in films (an important theme for food and cosmetic industrial applications). Some of the participants felt that discussions in possible future meetings would benefit from more contribution from analytical theories, and we believe that further efforts to integrate theoretical approaches, simulations and experiments in gel networks would fit perfectly CECAM workshops scope and mission.

4 Funding

Beside the CECAM main funding (12 k€), the organizers raised additional support from their local institutions and from their industrial partners as follows:

- Georgetown university: 1 k€
- Ecole Normale Supérieure de Lyon (Research Fund): 2 k€
- Université Lyon 1 (FST): 1 k€
- CNRS: 800 €
- GDR Phenix: 3 k€
- L'Oreal: 2 k€

This additional funding was used to cover travel expenses for non-invited participants, post-docs and students as well as the conference dinner, some coffee breaks and printing of the abstract booklets.

Other possible sources for funding a subsequent similar workshop include the national call for international scientific cooperation (PICS CNRS), the international laboratories program (LIA CNRS), the more local collaboration schemes such as the MIT-France seed fund (MISTI) in which some organizers are already involved.

At the end of this successful workshop, it was proposed to submit new applications for funding future conferences on the topic of gels.

5 Will these developments bring societal benefits?

The mechanics and rheology of soft gels is crucial to a wide range of technologies, for industries ranging from food to personal care products, to cosmetics and paintings. Participation and interest from industrial researchers in some of these areas demonstrated the need to develop novel fundamental understanding and complementing experiments with computational approaches to advance material design and process optimization. The research discussed in the Workshop has the potential to help develop new products or optimize and enhance existing ones; optimize industrial processes to achieve higher sustainability (in terms of solvent used, for example, or amount of resources required); enhance quality of life through better designed products and industrial processes.

In addition, creating such an environment in which academic scientists communicate across disciplines and with industrial researchers helps enhancing integration of scientific culture and communication with societal needs, with new opportunities to develop mixed academic-industrial collaborations and to access diversified funding.

6 Participant list

Organizers

BARENDSON, Samantha
Centre Blaise Pascal - ENS de Lyon, France

Del Gado, Emanuela
Georgetown University, USA

Manneville, Sebastien
ENS Lyon, France

Martens, Kirsten
LIPhy, University Grenoble Alpes & CNRS, France

Ruta, Beatrice
University Lyon 1 & CNRS, France

Trappe, Veronique
University of Fribourg, Switzerland

Angelini, Roberta - CNR-ISC Sapienza, Italy

Barrat, Jean-Louis - Université Grenoble 1 , France

Baumberger, Tristan - INSP, France

Blair, Daniel - Georgetown Washington DC, USA

Bouzid, Mehdi - Georgetown University, USA

Castaneda-Priego, Ramon - University Guanajuato, Mexico

Chaudhuri, Pinaki - Institute of Mathematical Sciences, India

Chinedum, Osuji - Yale University, USA

Cipelletti, Luca - CNRS, University of Montpellier, France, France

Creton, Costantino - ESPCI, France

Divoux, Thibaut - CRPP, Bordeaux, France

Ferrero, Ezequiel - University of Milano, Italy

Foffi, Giuseppe - University of Paris-Sud, France

Hsiao, Lilian - NC State University, USA

Keshavarz, Bavand - MIT, USA

Leheny, Robert - John Hopkins University, USA

Mao, Xiaoming - University of Michigan, USA

McKinley, Gareth - MIT, Cambridge, USA, USA

Petekidis, George - University of Crete, Greece

Puosi, Francesco - SIMAP Grenoble, France

ramos, laurence - Laboratoire Charles Coulomb, CNRS-Université Montpellier 2, France

Swan, James - MIT, USA

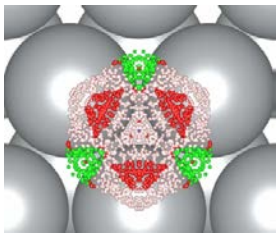
Van der Gucht, Jasper - Wageningen University & Research, The Netherlands

Vermant, Jan - Swiss Federal Institute of technology Zurich, Switzerland

Zhao, Xuanhe - MIT, USA

Zia, Roseanne - Cornell University, USA

Challenges in reaction dynamics of gas-surface interactions and methodological advances in dissipative and non-adiabatic processes



Location: CECAM-FR-GSO
Webpage: https://www.cecam.org/workshop-0-1458.html
Dates: June 26, 2017 to June 29, 2017

1 State of the art

The role of dissipation is central in surface chemistry. At short range the adsorbate motion can couple to either phonon modes or to electron-hole pairs (EHPs), which can influence the rates and mechanisms of molecule-solid energy transfer as well as the outcomes of chemical reactions. For the simplest, atomic sticking reaction, surface dissipation is a necessary condition. How excitation of a solid becomes localized on an adsorbate, and vice versa, how quenching of vibrationally or electronically excited adsorbates occurs, are central questions in surface photochemistry. The challenge is to understand the coupling of the elementary solid excitations to the elementary degrees-of-freedom (DOFs) (translation, rotation, vibration, electronic) of atoms and molecules near the surface. When translation is coupled to phonons or to EHPs, elementary processes like adsorption and diffusion can be dramatically altered. How molecular vibration, the elementary motion needed for dissociation, is coupled to the surface determines how energy flows into and out of reactive bonds. Also, excited surface modes can transfer their excitation energy to adsorbate molecules and thereby induce dissociation.

Density Functional Theory (DFT) has become a standard approach to investigate molecule-surface interactions and full-dimensional, DFT-based on-the-fly calculations (e.g. AIMD) can be performed almost routinely for the ground electronic state, but the computation of excited states and of electronic processes remains a formidable challenge. Yet, schemes such as Independent Electron Surface Hopping and AIMD with electronic friction have been

developed. Also, excited states can now be treated via Time-Dependent DFT (TD-DFT), but on-the-fly calculations are too time-consuming for simulations beyond a few typical trajectories, preventing meaningful comparison to experiment. Approximations to DFT such as Density Functional Tight Binding (DFTB) or TD-DFTB, constitute another promising route.

2 Major outcomes

The relevant task is multiple and can be decomposed in a series of steps: electronic structure determination, representation of a global potential energy surface (PES) and nuclei dynamics solving. On-the-fly dynamics such as AIMD offers an alternative, layered strategy that also avoids the second step. The workshop addressed many recent methodological advances, relevant to each of these steps or to the layering strategy.

PES representation allows not only for classical molecular dynamics but also for quantum or mixed quantum-classical schemes. The need for accurate, high-dimensional PES fits motivated the development of various descriptions such as effective medium theory, reaction-specific reactive force fields, the singular-value-decomposition multigrid POTFIT algorithm and neural networks. The main limitation is the restriction to the ground electronic state.

Most simply, dissipative and non-adiabatic processes are accounted for mostly by AIMD for phonons and by a mean-field, local density friction approximation (LDFA) either for phonons within a generalized Langevin oscillator model or for electrons within AIMDEF (AIMD with Electronic Friction). Alternatively, to LDFA, which by construction neglects directionality and hydrodynamic coupling in its description of electronic friction, a matrix of tensorial friction coefficients can be computed on the fly from Fermi's golden rule. A number of applications demonstrated the usefulness of these approaches e.g. in the scattering regime, for adsorbate relaxation and in photochemistry. The dimensionality of the system can be much increased by replacing DFT with its approximate DFTB counterpart. The main limitations are the classical dynamics approximation and the possibly poor description of excited states. The independent oscillator Hamiltonian model and the surrogate Hamiltonian method are two example strategies used to go beyond classical dynamics. Also, Ehrenfest dynamics was suggested worth to (re)investigate. Then, the main limitation is on the dimensionality of the system.

Explicit representation of the excited electronic states is achieved through turning to the time-dependent DFT versions, TD-DFT and TD-DFTB, or more accurately to wave function CAS/CI methods albeit limited to five-dimensional photochemistry studies, but with quantum wave packet dynamics. Classical dynamics is implemented with trajectory surface hopping. Quantum dynamics is accounted for by solving coupled time-dependent Schrödinger or

Liouville-von Neumann equations owing to various wave packet strategies, multi-configuration time-dependent Hartree method and its multi-layer version, Monte Carlo, reduced dynamics hierarchical equations of motion, ...

Among the high-dimensional dynamics applications those for methane scattering from and dissociating at metal surfaces demonstrated very close and detailed comparisons with experiments, accounting for lattice motion. One illustrated the importance of the accurate characterization of DFT PES, and more specifically of the barriers to reaction, which can be enhanced by the development of empirical functionals such as the specific reaction parameter scheme. Another relied on the fully quantum reaction path Hamiltonian approach in order to take explicitly into account the 15 molecule DOFs.

This dense albeit non-exhaustive summary of main methodological outcomes, furthermore deliberately omitting in good part the important knowledge gained about chemistry and physics, witnesses a highly productive field. The summary is particularly non-exhaustive regarding issues raised after each talk (30 + 15 minutes of discussion) and during the (four) dayly discussions (30-60 minutes) and final discussion (60 minutes). The confrontation of various strategies, the weighing up of their pros and cons, and the relevance in the comparison to experiment resulted in truly abundant and fruitful exchanges, which will probably and shortly give rise to new improvements and ideas.

3 Community needs

As for computing most of us use several levels of resources, including local institute clusters, regional meso-centres and national HPC infrastructures. These distinct levels of resources are complementary and provide a flexible, adequate framework for development and computational production tasks. Obviously, high-DOF scattering, AIMD and non-adiabatic dynamics require a large amount of HPC resources and will necessitate further adaptation to HPC and parallel computing.

The workshop aimed to networking theoreticians from different communities in order to bring the richest and most diverse panel of methodological expertise that can be useful to advance the community core applications. Outreach to the experimental community was explicitly sought for and implemented through inviting three renowned experimentalists gathering complementary expertise to depict a survey of the experimental state of the art and of the critical challenges in the field. In addition, they strongly contributed to the discussions and enabled for a lively interplay between experiment and theory. Thus, suggestions of both theory-theory and theory-experiment collaborative work were prolific.

Overall, the after-talk (30 + 15 minutes of discussion), the (four) dayly (30-60 minutes) and the final (60 minutes) discussions were truly intense. There were so many questions, comments and debates, that none of the discussion periods came to a sudden end and that all the round tables had to be interrupted beyond the schedule, leaving for informal sessions the opportunity to discuss further about work that was insufficiently addressed. Clearly, this first CECAM workshop was highly useful and fruitful in learning how to solve a number of problems, which in turn called for a number of new problems to be considered and solved. Hence a series of CECAM workshops would be most profitable. Some participants have proposed to organize such a follow-up workshop within one or two years, e.g. in Germany or Argentina.

4 Funding

Funding was not discussed in the official sessions. We nevertheless expect that joint research proposals will come out of the lively and fruitful discussions, of the many informal exchanges and of the overall excellent assiduousness throughout the workshop. Yet, the presentations frequently acknowledged national funding schemes as well as several existing collaborations.

5 Will these developments bring societal benefits?

The topics addressed by the workshop aim at pure fundamental research and the benefits are at the moment exclusively scientific. It is rather hard to think about a problem beyond the academic world (economical, technical, societal or cultural) that could take advantage from any development discussed in the workshop. Yet, the kind of challenging problems that were addressed is exactly the one that every once in a while, triggers developments in wider research areas, and impact on society.

While the work is fundamental in nature, in conjunction with UHV experiments it allows us to explore and understand how reactions take place on surfaces. This impacts our understanding of things like catalysis, semiconductor processing and other surface or nano technologies. What we learn about the dynamics of these fundamental processes guides those who design better catalysts, leading to industrial processes that are both more efficient and more environmentally friendly. Thus, the impact on society is significant.

More generally, the workshop addressed the theme of energy conversion that can be of relevance to scientific problems related to the production, consumption and storage of energy in all its forms.

A more specific example of potentially high impact on society is illustrated by collaborative efforts to provide specific knowledge about surface chemical systems relevant to cold plasma H- injectors that have become important to the realization of tokamak performance. The understanding developed by such collaboration could allow accurate theoretical simulation of realistic models important for the engineering development of these injectors, if not for the current ITER project, perhaps for the next DEMO generation presently at the design stage.

6 Participant list

Organizers

JACKSON, Bret
Department of Chemistry, University of Massachusetts, Amherst, USA

LEMOINE, Didier
LCAR/IRSAMC, CNRS and Université Toulouse III Paul Sabatier, France

MARTINAZZO, Rocco
Department of Chemistry, University of Milan, Italy

SPIEGELMAN, Fernand
LCPQ/IRSAMC, CNRS and Université Toulouse III Paul Sabatier, France

ALDUCIN OCHOA, Maite - Centro de Fisica de Materiales, CSIC-UPV/EHU, San Sebastian, Spain

AUERBACH, Daniel - Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

BECK, Rainer - Ecole Polytechnique fédérale de Lausanne, Switzerland

BONFANTI, Matteo - Goethe-Universität Frankfurt am Main - Institut für Physikalische und Theoretische Chemie, Germany

BURGHARDT, Irene - Goethe University Frankfurt, Germany

BUSNENGO, Fabio - Instituto de Fisica Rosario, CONICET and Universidad National de Rosario, Argentina

CRESPOS, Cédric - Institut des Sciences Moléculaires, CNRS and Université de Bordeaux, France

CUNY, Jérôme - LCPQ/IRSAMC, CNRS and Université Toulouse III Paul Sabatier, France

DONG, Wei - Ecole Normale Supérieure de Lyon, France

GALPARSORO, Oihana - Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

GERRITS, Nick - Leiden Institute of Chemistry, Leiden University, The Netherlands

IBARGÜEN BECERRA, Cesar - Institut des Sciences Moléculaires, CNRS and Université de Bordeaux, France

JUARISTI, Iñaki - Centro de Fisica de Materiales, CSIC-UPV/EHU, San Sebastian, Spain

KANDRATSENKA, Alexander - Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

KLÜNER, Thorsten - University of Oldenburg, Germany

KROES, Geert-Jan - Leiden Institute of Chemistry, Leiden University, The Netherlands

LARRÉGARAY, Pascal - Institut des Sciences Moléculaires, CNRS and Université de Bordeaux, France

LEPETIT, Bruno - LCAR/IRSAMC, CNRS and Université Toulouse III Paul Sabatier, France

MARQUARDT, Roberto - Laboratoire de Chimie Quantique, Institut de Chimie, Université de Strasbourg, France

MARTI, Carles - LCPQ/IRSAMC, CNRS and Université Toulouse III Paul Sabatier, France

MAURER, Reinhard - Department of Chemistry, Yale University, USA

MEYER, Jörg - Leiden Institute of Chemistry, Leiden University, The Netherlands

MICHOULIER, Éric - Laboratoire PhLAM, Université de Lille 1, France

Niehaus, Thomas A. - Claude Bernard University Lyon 1, France

NOUR GHASSEMI, Elham - Leiden Institute of Chemistry, Leiden University, The Netherlands

PELÁEZ-RUIZ, Daniel - Laboratoire PhLAM, Université de Lille 1, Villeneuve d'Ascq cedex, France

PEÑA TORRES, Alejandro - Institut des Sciences Moléculaires, CNRS and Université de Bordeaux, France

PETERSEN, Thorben - University of Oldenburg, Germany

SAALFRANCK, Peter - Institute of Chemistry, University of Potstdam, Germany

SERWATKA, Tobias - Institute of Chemistry and Biochemistry, Freie Universität Berlin, Germany

SHAKOURI, Khosrow - Leiden Institute of Chemistry, Leiden University, The Netherlands

SPIERING, Paul - Leiden Institute of Chemistry, Leiden University, The Netherlands

TREMBLAY, Jean Christophe - Institute of Chemistry and Biochemistry, Freie Universität Berlin, Germany

WODTKE, Alec - Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Extended Software Development Workshop (ESDW4): Meso and Multiscale Methods

Location: CECAM-ES.

Webpage: https://www.cecam.org/workshop-0-1488.html
Dates: July 3, 2017 to July 14, 2017

1 State of the art

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

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

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

future interest for the centre on the road to exascale computing. The outcome of this extreme-scale workshop has been reported in E-CAM's deliverable D7.5: Hardware Developments II (https://doi.org/10.5281/zenodo.1207613).

2 Training provided

The primary training component of this ESDW came in the form of the development of software modules for two software packages used by the E-CAM community: DL_MESO_DPD (https://www.scd.stfc.ac.uk/Pages/DL_MESO.aspx) and ESPResSo++ (http://www.espresso-pp.de/). These have been identified as important codes for mesoscale simulations within E-CAM in a recent state-of-the-art workshop in Mesoscale and Multiscale Modelling that took place in Dublin on the 29th May-1st June 2017 (workshop report available for download at https://www.e-cam2020.eu/scientific-reports/).

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

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

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

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

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

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

The second week of the workshop was dedicated to the "training by doing" component of the event, associated to module contribution within E-CAM. E-CAM programmers assisted the

participants on the development of software modules following programming best practices and with an eye on the future of the hardware where they will run such modules.

3 List of software development project

The following modules were developed at this workshop:

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

These modules have passed E-CAM's evaluation for quality standard for code, tests, and documentation and are now uploaded into the E-CAM Library at http://e-cam.readthedocs.io/en/latest/Meso-Multi-Scale-Modelling-Modules/index.html, and included in the following E-CAM Deliverables D4.2 (https://doi.org/10.5281/zenodo.1207372) and D4.3 (https://doi.org/10.5281/zenodo.1210075).

4 Future plans

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

6 Participant list

Organizers

Pagonabarraga, Ignacio
CECAM EPFL, Switzerland

Castagna, Jony - STFC Daresbury Laboratory, United Kingdom

Chiacchiera, Silvia - STFC, United Kingdom

Duenweg, Burkhard - Max Planck Institute for Polymer Research, Mainz, Germany

Khedr, Abeer - University College London, United Kingdom

Kobayashi, Hideki - Max Planck Institute for Polymer Research, Germany

O'Cais, Alan - Jülich Supercomputing Centre, Germany

Poggio, Stefano - University College Dublin, Ireland

Power, David - University College Dublin, Ireland

Seaton, Michael - Science & Technology Facilities Council, United Kingdom

Sutmann, Godehard - Research Center Jülich, Germany

Vargas Guzman, Horacio - Max Planck Institut for Polymer Research, Germany

Weik, Florian - Institute for Computational Physics, University of Stuttgart, Germany

Electronic Structure Library coding workshop: drivers

Location: CECAM-IT-SIDE
Webpage: https://www.cecam.org/workshop-0-1435.html
Dates: July 10, 2017 to July 21, 2017

1 State of the art

In the past several decades Electronic Structure methods have mostly been developed in self-contained monolithic software distributions implementing a variety of features. Currently most of these large codes contain routines with overlapping functionality and make use of non-standard data formats due to historical reasons, and as the state of the art in theory and computer hardware progresses, the complexity of these codes continues to grow separately, in a way that reduces their inter-operability with each new version.

While this independent development model has certainly been successful in the past, the current situation is far from ideal: new developers willing to contribute new ideas, who already face a steep learning curve due to the complexity of the existing software, are also required to become deeply involved with the development of a specific package.

Furthermore, extension of their new development to other codes requires repetition of the same work for each independent package over and over, with very little academic and personal reward.

The problem is widely recognized in the community as important yet it remains unsolved. Addressing it from various angles is among the goals of the E-CAM Center of Excellence, spawn by the CECAM community, and the MaX Center of Excellence, both recently funded by EU.

A few years ago the Electronic Structure Library (ESL) project was launched within CECAM, with the idea of fostering a new paradigm of library-based development for electronic structure by creating a common online repository of high-quality software libraries, programming interfaces and data standards in the field of electronic structure, which will facilitate reuse of

code, interoperability between different code bases, rapid and efficient evolution to new computer architectures, and development of new methodologies.

2 Major outcomes

The ESL initiative is a community-driven project which anyone can contribute to. It operates by holding regular hands-on workshops where code developers are encouraged to get involved and work on individual library modules, contributing new software as well as fragments extracted from codes they are developing, thus establishing collaborations and links between different code communities.

The first ESL coding workshop (July 2014) lasted six weeks and was hosted at CECAM HQ in Lausanne. Tools and infrastructure for the project were set up and the first contributions were included and made available online. In a second one-week workshop (June 2015), also in Lausanne, some of the basic standards for library contributions were discussed and implemented. Several new libraries were created and added to the ESL repository to build a "utilities toolbox" with an effort to implement existing libraries into different pre-existing codes, in order to start putting into practice the idea of cross-code interoperability and code reuse. A third two-week workshop (June 2016) took place at ZCAM in Zaragoza, Spain, and addressed the broad theme of solvers, resulting in initiation of three library bundles that target widely used routines in electronic structure codes: Kohn-Sham (KS) eigensolvers, Poisson solvers, and atomic solvers.

Adopting the successful format of previous years, the present two-week workshop gathered a small team of coders connected with a number of different electronic structure codes. The first couple of days were devoted to presentations and discussions focusing on an analysis of the available ESL "utility tools" and on the opportunities for code reuse and standardization created and realized so far and, on the actions, needed to foster them further. The rest of the workshop was dedicated to the coding effort focusing on “drivers”.

Complementary to the previous ESL workshops, which addressed solvers for a variety of specific representations of the KS problem, "drivers" targeted the problem of extracting existing KS solvers from major Electronic Structure codes and refactor them as libraries in a representation-agnostic fashion, resulting in further code-interoperability.

The two main iterative eigensolvers employed in the pw.x code of the Quantum ESPRESSO distribution have been completely disentangled from the rest of the code and converted to libraries. The solvers make efficient use on a Linear Algebra domain-specific library LAXlib developed within the MaX CoE which has been tuned to make use of the Eigenvalue SoLvers

for Petaflop-Applications (ELPA) replacement to ScalaPack when convenient. Solvers exploit MPI parallelization and in addition to basis-set component distribution, a parallelization over target states is possible, as well as a specific parallelization for the dense linear algebra operations using ScalaPack or ELPA. Generic k-point as well as Gamma specific versions of the solvers are included. The Reverse Communication Interface (RCI) paradigm, allowing for a complete abstraction from the basis type and the interface used to perform the matrix-vector operations, has also been implemented for one of the solvers.

A toy code implementing the Cohen-Bergstresser empirical-pseudopotential method has been included to exemplify the use of the solvers and allow a quick test of their functionalities. A git branch to contribute additional toy codes based on different basis set representations, tight-binding or real-space, to explicitly demonstrate the representation-agnostic nature of the solvers has been created and is under development. Contribution to the KS_Solvers library of additional solvers from other codes is also foreseen.

The software developed during the Workshop is hosted by the e-cam gitlab server as a sub-project of the ESL initiative (gitlab. e-cam2020/esl/ESLW_Drivers) and may serve as an ingredient of an Electronic Structure Library Demonstrator to be built to showcase ESL functionalities.

3 Community needs

The European Electronic Structure community has developed in the past decades a world recognized leadership in the field. Code development in several independent, scientifically competing, groups has been a fundamental element that made the community thrive. Specific funding to close the ensuing gap in expertise have lead in the US to initiatives like the ELectronic Structure Infrastructure (ELSI) whose participants can become valuable partners to further progress the field in a changing environment.

A key element in the future evolution will be sustainability of the effort, maintainability of the developed software in the evolving hardware landscape, scalability of the provided support to the growing user community.

Workshops such the ones organized by the ESL initiative, fostered by CECAM, that promote diffusion and reuse of basic and sophisticated software modules developed coordinating and networking the contributions of the different groups active across Europe and the ocean may play a role in all these aspects, contributing to enhance awareness for the community needs and the available solutions.

4 Funding

The Workshop was approved by CECAM council but was not given specific funds, neither from CECAM HQ nor from the e-cam workshop funds due to untimely funding request by the organizers. Some contribution from the CECAM-SIDE node was secured, as well as some contribution from the Trieste e-cam node and ICTP MaX node. Most importantly a 5K Euro contribution from psi-k was obtained. Due to the very small number of participants, some of which were in addition local scientists, and the very competitive prices of ICTP venue, the workshop could be run successfully in spite of the very limited funding. Reservation of some funding for such a “cheap” type of workshop in which a small number of participants gather together to pursue specific coding tasks could be considered as the cost/benefit ratio appears very favorable.

5 Will these developments bring societal benefits?

As should be evident from the previous paragraphs the Open Innovation Electronic Structure code development model, embraced by e-cam CoE and adopted by the ESL initiative, has the potential not only to confirm the European scientific leadership in the field but also to provide potential industrial partners, whose interest ranges from the simple use of already available codes--that should therefore be as efficient and reliable as possible--to the development of novel techniques suitable to their specific needs, with a range of well tested, efficient, and documented computational modules to perform a number of basic and sophisticated electronic structure tasks needed by their application. The adoption by the established codes of the same computational modules, actually originating from them, will contribute to code reuse, enhance maintenance sustainability, help to provide user support to a growing user community by concentrating the effort on common tools and overall will benefit the entire community, of users and developers alike.

6 Participant list

Organizers

Corsetti, Fabiano
Synopsys QuantumWise, Denmark

de Gironcoli, Stefano
International School for Advanced Studies (SISSA) and CNR-DEMOCRITOS IOM, Trieste, Italy

Girotto, Ivan
International Center for theoretical Physics, Italy

Artacho, Emilio - University of Basque Country, United Kingdom

Blum, Volker - Duke University, Durham, NC, USA, USA

Carnimeo, Ivan - Scuola Normale Superiore, Italy

Delugas, Pietro - Scuola Internazionale di Studi Superiori Avanzati, Italy

Genovese, Luigi - Alternative Energies and Atomic Energy Commission (CEA), Grenoble, France

Giannozzi, Paolo - University of Udine, Italy

Huhn, William - Duke University, Durham, NC, USA, USA

Kucukbenli, Emine - SISSA, Italy

Martin-Samos Colomer, Layla - University of Nova Gorica, Slovenia

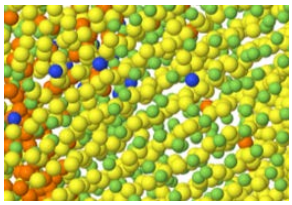
Oliveira, Micael - Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Payne, Mike - University of Cambridge, United Kingdom

Pouillon, Yann - Materials Evolution, Spain

Yu, Victor - Duke University, USA

Building links between experiments and computer simulations of crystallization



Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1379.html
Dates: July 12, 2017 to July 14, 2017

1 State of the art

Crystallization is a complex process of fundamental importance to materials science, climate science, pharmaceutical production, product stability, food science, and may other fields. Despite its widespread importance, theory and simulation fail to predict nucleation and growth rates in nearly all applications. In the past, simulation methods were simply too primitive to access the time and length scales required for studies of nucleation and growth. However, a few recent studies demonstrate that rate calculations based on importance sampling, path sampling, brute force simulations, and sometimes seeding, are mutually consistent. Moreover, these simulation methods are becoming reliable for systems of growing complexity. Likewise, although force field accuracy is a perennially persistent challenge, there are now adequate for predictions in some systems (water, NaCl, colloids, etc.).

In terms of quantitative experimental data and theoretical understanding, ice crystallisation research has surged ahead. Recent years have also seen significant progress on nucleation and crystallization of hard spheres under confinement. Other fields are typically less quantitative and are hindered by largely qualitative experiments and simulations on unvalidated force fields, but some, for example pharmaceuticals, are catching up.

Much simulation work focuses on conditions, processes, and materials that would be difficult test in the lab. A large portion of experimental work focuses on processes and materials that are too complex to simulate with any reliable accuracy. Our workshop sought to identify promising opportunities for closer synergy between experiments and theory/simulation, and so close the gap.

2 Major outcomes

The key topics discussed were:

1.Polymorphism. Many substances crystallise into two or more different crystal lattices (polymorphs). We have little understanding of why or how. Experimental techniques are advancing, allowing more quantitative data, for example via measuring nucleation times (eg Biscans, ter Horst and Veesler's talks) or advanced EM (Legg's talk) but nucleation cannot be observed in most experiments. Simulations of nucleation in simple, and ideally in more realistic, models would greatly increase our understanding and could guide future experiments (Gale). Polymorph control is fundamental to a number of industries, including the pharmaceutical industry, as discussed in Reutzel-Eden's (Eli Lilly) talk. Better understanding would make drug development cheaper and more reliable.

2.Experimental work in ice nucleation has long appreciated that a particle contacting a supercooled water droplet from the air side of the water/air interface can nucleate ice more effectively than a totally immersed particle (Kiselev and Leisner's talks). There have been no simulation studies of this, but such studies, even in a simple model (Lennard-Jones) could help suggest possible microscopic mechanisms. They would also help with understanding evaporating aerosols (Reid). Contact nucleation is important to understand due to its role in cloud formation, which in turn is a part of climate models.

3.Experimental work (Christenson, Leisner) showed nucleation occurring repeatedly on cracks or other rough features on surfaces. This recent works shows that these features are key to the nucleation of ice, and of a number of molecules - indeed this may be a very general observation. This is a real advance to our understanding of nucleation - we know have at least a qualitative idea of what sort of surface promotes crystal nucleation. But both more quantitative experiments, and computer simulations (Filion) are now needed to build on this work and develop a predictive understanding.

4.The huge dynamic range of crystal growth rates were discussed, from > 100 m/s (Harrowell) to < 1 nm/s (Rimer). We have a much better understanding of the faster rates than of the slower rates. Simulations of slow growth rates will help here but due to the range of length and timescales required, they will be highly computationally demanding. Crystallization rates in simpler systems (Fillion, Speck), as well as mixtures (Whitelam) can now be modelled.

5.Quantitative nucleation rates were presented in both simulation (Sanz, Speck, Russo) and experimental talks (ter Horst, Biscans, Veesler). But except for ice (Sanz) there has been no direct simulation/experiment comparison other than in idealized hard sphere colloid

experiments, in which there is a notorious discrepancy between prediction and experiment. Although the gap is closing, there is some way to go. Experimentalists need to study the simplest, cleanest systems possible, while simulators need to validate potentials.

6.In bulk crystallization, the crystals are often micrometers or larger which requires only one nucleation event per cubic micrometer or less. Nucleation is then a rare event, see points 2) and 3). But when nanocrystals are formed in the bulk (Owen) the density of nucleation events is orders of magnitudes higher. There was discussion that this may be a rare case where nucleation is homogeneous.

We would also like to stress that the CECAM workshop brought together leading scientists who study crystallization in a broad range of contexts. The attendees included scientists studying ice formation, pharmaceutical crystallization, biomineralization, nanoparticle synthesis, hydrothermal synthesis of zeolites, colloidal model systems and precipitation in aerosols. For many participants (organizers included) the CECAM meeting provided a first exposure to several new problems and ideas.

3 Community needs

The computational requirements of studies of the nucleation and growth vary from desktop machines for the simpler potentials, to HPC for molecules and ions in solution. Rare events methods for accessing long time scales have become quite sophisticated, but there is room for continued improvement. This is especially true for crystallization in solution where composition changes, and for transformations within solids, where elastic strain effects continue to pose major challenges. There is also a continuing need for more accurate interaction potentials. Finally, many challenges remain with models of surfaces and their interactions with molecules and ions.

From a simulation perspective, we expect that a need for two strands will emerge. Generic models, which capture the behaviour of a whole class of system. These models allow the probing of large time- and lengthscales. They might, eg, enable one to narrow down the pool of possible nucleation pathways for a given class of material. To address the limitations of such a generic approach, on the other hand specific models are required that would address a particular material, for example to identify the polymorphs of a particular drug molecule.

Crystallisation spans fields from atmospheric science, geology to drug manufacture and areas of nanotechnology such as organic photovoltaics. Perhaps more than computing limitations, progress in theory and simulation is limited by a tendency for scientists to segregate according to their chosen applications. For example, experimentalists studying ice nucleation are

familiar with 'contact nucleation' (Kiselev's talk) and expressed the view that simulations would help, but contact nucleation was a completely new phenomenon to most simulators at the meeting. This self-segregation impedes the spread of new ideas, limiting the pace of progress in crystallization as a whole. Thus, there is a real need for a workshop like ours that bring different communities together.

4 Funding

Interest in crystallisation stretches from atmospheric science to structural biology, and includes physics, materials science and chemistry. Therefore, virtually all funders fund some research involving crystallisation. Crystallisation is key to processes in industries from pharmaceuticals to electronics. Therefore, many of the more applied calls are relevant, for example the EU's Horizon 2020 MSCA ITNs and ETNs, the UK's Manufacturing the Future calls, etc.

A diverse range of national funding bodies fund crystallisation research. For example, in the USA, the US National Science Foundation provides grants for fundamental work. Other agencies support crystallization research as part of larger initiatives. Industry, particularly the pharmaceuticals industry, supports projects on the nucleation and growth of molecular crystals. In the UK, connections are being developed with pharmaceutical companies (Pfizer, GSK).

5 Will these developments bring societal benefits?

Crystallization is important in many industries: pharmaceuticals, electronics, food, construction materials, etc. For example, the need for better understanding of crystal polymorphs is well understood by the pharmaceutical industry (talk of Eli Lilly's Reutzel-Edens). A better understanding would give faster cheaper drug development and avoid highly expensive problems like that of the anti-HIV drug Ritonavir being withdrawn from sale due to appearance of a previously unsuspected polymorph. Industry itself is funding work in this area, and funding calls associated with advanced manufacturing also apply here.

Our climate is currently warming due to anthropogenic CO2 and other factors, with huge consequences for societies all over the world. The latest Intergovernmental Panel on Climate Change (IPCC) report (2104) identified uncertainties due to cloud modelling as one of the largest uncertainties in our climate predictions. Clouds are in part hard to model due to our poor understanding of ice nucleation. Our workshop addressed this and, for example, identified contact nucleation (see Major Outcomes) as a key area where new computer simulation and experimental collaborations will advance the field. This work may fall in a gap between geo-science and physical-science funding bodies but the gap between scientists is these areas is closing (something the workshop helped with) and this should help bridge the gap with funding bodies too.

In an everyday context, improving understanding of, and potentially gaining control over, crystallization means that even common problems like scaling might be tackled, perhaps in collaboration with industry.

6 Participant list

Organizers

Peters, Baron
University of California, Santa Barbara, USA

Royall, Paddy
University of Bristol, United Kingdom

Sear, Richard
University of Surrey, United Kingdom

Ahlawat, Paramvir - EPFL, Switzerland

Benjamin, Legg - Pacific Northwest National Laboratory, USA

Biscans, Beatrice - Universite de Toulouse, France

Cheng, Bingqing - EPFL, Switzerland

Christenson, Hugo - University of Leeds, United Kingdom

DeFever, Ryan - Clemson University, USA

Filion, Laura - Utrecht University, The Netherlands

Gagliardi, Luca - Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, France

Gale, Julian - Curtin University, Australia

GROSSIER, Romain - CINaM - CNRS - UMR7325, France

Harrowell, Peter - University of Syndey, Australia

Karmakar, Tarak - Postdoctoral fellow in Faculty of Informatics, USI Università della Svizzera italiana, Lugano, & ETH Zürich, India

King, Michael - University of Konstanz, Germany

Kiselev, Alexei - Karlsruhe Institute of Technology, Institute for Meteorology and Climate Research, Germany

Kurganskaya, Inna - University of Bern, Switzerland

Lee, Judy - University of Surrey, United Kingdom

Leisner, Thomas - Karlsruhe Institute of Technology, Germany

Maggioni, Giovanni Maria - ETH Zurich, Switzerland

Nalesso, Silvia - University of Surrey, Great Britain

Owen, Jonathan - Columbia University, USA

Piaggi, Pablo - EPFL, Switzerland

Quigley, David - University of Warwick, Coventry, United Kingdom

Reid, Jonathan - University of Bristol, United Kingdom

Rene Espinosa, Jorge - University Complutense of Madrid, Spain

Reutzel-Edens, Susan - Lilly, USA

Rimer, Jeff - University of Houston, USA

Rios de Anda, B. Ioatzin - University of Bristol, United Kingdom

Russo, John - Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan, Japan

Sanz, Eduardo - Universidad Complutense, Madrid, Spain

Speck, Thomas - Institute of Physics, JGU Mainz, Germany

ter Horst, Joop - University of Strathclyde, United Kingdom

Veesler, Stephane - CINaM-CNRS (Centre Interdisciplinaire de Nanoscience de Marseille), France

Whale, Thomas - University of Leeds, United Kingdom

Whitelam, Steve - Lawrence Berkeley National Laboratory, USA

Designing forcefields in an age of cheap computing

Location: Halifax Hall, University of Sheffield (CECAM-UK-HARTREE)
Webpage: https://www.cecam.org/workshop-0-1374.html
Dates: July 26, 2017 to July 28, 2017

1 State of the art

Robust, reliable forcefields are central to successful atomistic simulations. They often use functional forms that are computationally efficient to evaluate but should also model faithfully the underlying physics of atomic interactions. With the ever-increasing power of computer systems available, now is a good time to revisit that compromise. As forcefields have become more complex, debate has focused on the best ways to fit them, including moving from the traditional physics-based forcefields to purely mathematical ones. Genetic algorithms have proved useful for searching the parameter space. Multi-objective optimization (although still controversial) allows users to determine the quality of the fitting procedure with respect to structure and energy, and other user defined objectives. Machine-learning models, based on neural networks and Gaussian process regression, find non-linear relationships that can express the energy landscape in terms of atomic properties for a given configuration of atoms. They emulate directly the quantum mechanical simulations used to generate the training data. They do not, however, retain knowledge about the underlying physics except in the form of an energy partition. Physics-based models retain such knowledge; indeed, they require it. This can be a drawback in complex systems (e.g. metal-ceramic interfaces) where it is difficult to specify functional forms that include all the physics. A problem in organic forcefields is the proliferation of arbitrary atom types which identify which parts of the forcefield govern specific interactions between groups of atoms. However, the complex connectivity causes problems in unambiguously defining and using them. The increasing power of computers should shift the balance towards mathematical models since they are more flexible and rely less on intuition but we need to understand if their advantages outweigh the significant expense of fitting them and the potential lack of transferability.

2 Major outcomes

Two key areas were identified: physical forcefields, derived using the physics of the system and mathematical forcefields that parametrize functions based on structure descriptors.

Discussion of physical forcefields raised concerns about reliance on expert intuition to choose the parameter scheme. People play safe and adapt existing forcefields often designed decades earlier. Forcefields are patched up by adding extra terms ad hoc. A classic example is the number of closely-related atom types in organic forcefields needed to ensure that the nuances in bond type are correctly represented in molecules with complex connectivity. A new scheme that parses the interaction directly was proposed (Mobley). Rigid adherence to obsolete conventions in forcefield design often make matters worse. People still use Lennard-Jones 12-6 functions rather than softer short-range terms that better represent the interaction.

Machine learning methods generate a training data set of configurations and fit mathematical functions which replicate the outputs, and in essence emulate the non-linear relationship between structure and properties that is modelled by quantum mechanical calculations. This removes many of the complications of physical forcefields such as ensuring that the physics is correctly described in metal-ceramic interfaces. When combined with mathematically based models, machine learning can generate rapid, faithful representations of the energy surface. Different machine learning methods that can be used to develop the models. Goedecker uses electron density as a guide to the energetics of a system with terms to consider charge changes and electronegativity. Behler explained the neural network process involved in machine learning whereby network connections are defined with weighting functions fitted to the training set. These, together with the descriptors of the atomic configurations, constitute the forcefield. However, machine learning can over-fit, preventing transferability to other problems if the weights are too tightly linked to the training set. This is tackled by testing (not fitting) the weights with another data set that is unseen during training to ensure that convergence was achieved with both. Exponential increases in the size of the neural network inputs with the number of different atoms (due to permutation scaling) limits the size of systems that neural networks can deal with. Harke showed how a machine learning process – genetic algorithms - can be used for excited-state ReaxFF forcefields if we carefully consider the fitting system. Here, rather than discover the underlying functional form of the forcefield, genetic algorithms search for the best parameters for a user defined set of functions for the forcefield. Over-fitting and environment-specific results can cause problems. Cartsensen demonstrated automated fitting procedures to generate parameters. Electronic effects can be added to extend the power of forcefields (e.g. polarization, charge transfer, mobile charge carriers). Popelier and Gresh showed the importance of including multipolar electrostatics and how to do this.

All speakers highlighted the fitting process. In machine learning, this is limited by the accuracy of the data set. Inaccuracies in the training set will appear in a machine-learned forcefield. Similar problems occur with physical forcefields. Using the forcefield outside the domain where it has been fitted is risky, particularly for machine learned forcefields since the terms have no physical basis. Neural networks can make wildly divergent predictions outside the training domain. Gaussian process regression models default to the average expected output and so are more robust - simulations can recover and return to configurations within the training domain. A possible way forward suggested was machine learning methods where the functional form maintains some physical information, such as the masses and charges of the atoms.

3 Community needs

Challenges in understanding and implementing forcefields were highlighted. Forcefields must be published in full, with example input files for at least one commonly-used code and an indication of their domain of applicability. For mathematical forcefields fitted using neural nets, information about the hardware configuration is also necessary. This is often not provided, making it difficult to reproduce published results or to use the forcefield on other problems. Some databases exist (e.g. those provided by NIST and DFRL). Also, there are forcefields associated with particular codes (AMBER, CHARMM, Gromacs) or proprietary software (e.g. COMPASS II). Brommer drew attention to the open knowledge base of interatomic models (www.openkim.org). However, none of these fully meet the need. The new open access requirements may help force more detailed publication with example inputs. The community needs to police this and (when acting as referees) should insist on full publication of the details required to use a forcefield. The increasing integration between hardware and software in fitting forcefields will make reproducing results both more difficult and more necessary. Since the major justification for forcefields is the combination of high efficiency and accuracy within a domain of applicability, the community needs to keep aware of the hardware and software developments that can be used to produce better forcefields and simulations. An expected growth area is coarse graining for large complex systems. Finally, the challenge of developing and validating robust forcefields needs to be better understood by the simulation community as a whole. They are a necessary complement to full ab initio simulations, taking over where the weaknesses of ab initio methods (inadequate length and time scales; failure to cover enough of the phase space) become evident.

4 Funding

Funding for developing forcefields is a major problem. They are seen as unexciting and require considerable investment in time and effort. They are therefore unlikely to be the subject of a funding application, but they often appear in as part of a larger bid. The development of adequate databases is a considerable effort that is rarely funded (except organics). Government laboratories sometimes take on the responsibility of maintaining databases of forcefields. Two companies representatives (OCF and Dassault) showed that there is potential for industrial funding.

Better communication between forcefield developers and between them and users is essential. Training is needed both in the use and validation of forcefields and in methods to develop new ones. The former is best done as part of a general simulation school. The list of attendees could be used to start a network of the communities to discuss forcefields and continue to share good practice and news between groups.

5 Will these developments bring societal benefits?

Physical forcefields for organic molecules have long been supported by the pharmaceutical industry to aid the rapid development of lead compounds with desirable medical properties including low toxicological effects. More recently the same strategy has been applied to the discovery of new materials (Materials Genome project). Reliable, robust forcefields are needed in this area to permit rapid and large-scale sampling over a large domain of possible candidate formulations. However, forcefields come into their own when it is necessary to understand large, complex systems particularly at long timescales. Such problems as protein folding, docking mechanisms, diffusion in highly defective systems or at interfaces, solution chemistry at medium to low concentrations require the use of forcefields. A particular area where work is needed is in problems involving hetero-interfaces. An understanding of solid/liquid interfaces (particularly if the liquid is water) is essential for corrosion, crystallization, most drug mechanisms and chimie douce processing routes. Metal/ceramic and metal/semiconductor interfaces are central to all electronics. All these cases combine great complexity, large numbers of configurations and longtime scales. They present a challenge to forcefields (particularly physical ones) because the physics underlying the

forcefield changes at the boundary. If simulations are to tackle real industrial and social problems, better forcefields are essential.

6 Participant list

Organizers

Freeman, Colin
University of Sheffield, United Kingdom

Handley, Christopher
University of Sheffield, United Kingdom

Harding, John
Sheffield University, United Kingdom

Behler, Jörg - Ruhr University Bochum, Germany, Germany

Brommer, Peter - Department of Physics, University of Warwick, United Kingdom

Goedecker, Stefan - University of Basel, Switzerland

Gresh, Nohad - CNRS, France

Hartke, Bernd - University of Kiel, Germany

Popelier, Paul - University of Manchester, United Kingdom

Richmond, Paul - University of Sheffield, United Kingdom

Vega, Carlos - Complutense University of Madrid, Spain

Extended Software Development Workshop (ESDW6): Classical MD

Location: CECAM-NL
Webpage: https://www.cecam.org/workshop-0-1406.html
Dates: August 14, 2017 to August 25, 2017

1 State of the art

During the past decades, classical molecular dynamics (MD) simulation has become a central tool in many branches of science and engineering. In particular, in molecular biology, chemistry, and materials science, MD simulations routinely provide insights into molecular mechanisms with a spatial and temporal resolution not accessible to experimental probes. Many software packages for MD simulations have been developed, opening the possibility to carry out such simulations to a broad community of researchers. However, the relatively short time scales accessible to MD still limit its applicability. This is particularly true for processes dominated by rare but important barrier crossing events, such as protein folding and binding, chemical reactions in solution, and nucleation.

In the last few years modeling of rare events has made tremendous progress and several computational methods have been put forward to bridge the time scale gap. In particular, the trajectory sampling methods, such as transition path sampling, transition interface sampling, and forward flux sampling, promise an accurate yet efficient solution to the rare event problem in complex systems. However, these new approaches have not yet been included, with adequate efficiency and scalability, in common simulation packages. This is mostly because their implementation and application require specialized expert knowledge.

The goal of this workshop was to discuss the implementation of such methods and to create software modules that can be used in conjunction with existing programs to address the computational challenges caused by rare events. The workshop focused on the development of user-friendly modules to sample rare barrier crossing trajectories and to analyze their molecular mechanisms.

This workshop was organized in the classical molecular dynamics scientific pillar of E-CAM and focused on making state-of-the-art methods accessible to a broader audience by providing robust software modules.

2 Major outcomes

This workshop included 22 total participants, with 11 who participated in the development of modules, plus 10 senior participants, who gave instructional talks and provided advice on module development, and 1 participant from an E-CAM industrial partner.

The primary training came in the form of the development of software modules based on OpenPathSampling, which was how the majority of the time at the workshop was spent, beginning on the third day. The first few days were primarily talks to introduce essential background material, with a few other such talks interspersed over the rest of the two weeks. These talks can be categorized by their primary focus: on science, on molecular dynamics software, or on general software development. They are described below.

Talks focused on scientific topics:

- Christoph Dellago gave an in-depth lecture on state of the art rare event sampling. This included an introduction to the basics of path sampling, as well as discussion of advanced path-based sampling methods.

- Jan-Hendrik Prinz gave a talk about a novel approach, called observable operator models, which makes connections between Markov state models and transition path sampling methods. This approach is still very much in development and exposes limits in our current understanding of the connections between various methods in the field of classical molecular dynamics.

- Titus van Erp spoke about state-of-the-art methods and results for transition interface sampling, including novel path sampling moves that could be implemented as E-CAM modules. He also introduced the PyRETIS software package and demonstrated it, and demonstrated some applications of the methodology.

- Jocelyne Vreede presented about applications of path sampling methods, focusing on studies of biomolecular systems. Her presentation included work on signalling proteins, DNA, and oncogenic protein mutations.

- Peter Bolhuis discussed some cutting edge path sampling methods, as well as several possible future directions to handle remaining challenges. He highlighted a few remaining challenges for path sampling, including parallelization approaches and the need to develop better tools to extract reaction coordinates from the results of path sampling simulations.

Talks focused on molecular dynamics software tools:

- David Swenson showed how these states of the art path sampling methods could be used in OpenPathSampling (OPS) and gave an overview of how to add new tools for OPS.

- John Chodera introduced OpenMM, demonstrating how to use it to perform GPU-accelerated simulations of biomolecular dynamics, and also discussed some of the subtleties around choosing a molecular dynamics integrator.

- Gareth Tribello gave a talk about PLUMED, demonstrating the ways that it can be use to calculate order parameters.

Talks focused on general software development training:

- Jony Castagna introduced the ideas of object-oriented programming as used in Python.

- Alan O'Cais gave a talk about software development best practices, introducing software development tools like GitLab and git. In addition, that talk discussed the E-CAM concept of "modules," which were the desired output of the workshop.

- Alan O'Cais gave a second talk, focused on effective use of HPC resources.

- David Swenson presented a tutorial on software testing for scientific programming, using the Python package nose.

3 Community needs

The following modules were developed at this workshop:

- S-Shooting: An approach for calculating the rate of a reaction. It is similar to the reactive flux method, but instead of launching trajectories from constrained to a surface in phase space, it allows shots from a volume in phase space, which is easier to sample.

- Spring shooting: A Monte Carlo move for transition path sampling. It aims to push the shooting point to be close to the transition state, which provides better sampling efficiency.

- Web throwing: A Monte Carlo move for transition interface sampling. It aims to improve the decorrelation of trajectories, enhancing the exploration of trajectory space and therefore the efficiency of the algorithm.

- PPTIS: Partial path transition interface sampling, a variant of transition interface sampling that is particularly useful for diffusive rare events.

- PLUMED support: PLUMED is a powerful and widely-used package that can be used to calculate collective variables. This module creates an interface so that PLUMED can be used for collective variables in OpenPathSampling.

- Shooting Range: A variant of the shooting move that selects shooting points from the region near the top of the barrier, in order to obtain better efficiency.

Of these, the Spring Shooting modules has already been accepted into the E-CAM Library, and S-Shooting was included in E-CAM Deliverable D1.3. The remaining modules will be included in future deliverables, after they are completed and included in the E-CAM Library.

4 Funding

At the end of the workshop, six modules had made significant progress, with code mostly completed. We expect to have a follow-up meeting, to be held in Amsterdam for two days. Before the follow-up meeting, the participants are expected to complete the implementation of their modules, which as mostly done during the workshop. At the follow-up meeting, we will ensure that the modules meet E-CAM's quality standard for code, tests, and documentation. The documentation to be posted in the E-CAM library will be written, and, if possible, merged. At that point, these modules will be ready for inclusion in future E-CAM deliverables.

6 Participant list

Organizers

Bolhuis, Peter
University of Amsterdam, The Netherlands

Dellago, Christoph
University of Vienna, Austria

Swenson, David
Universiteit van Amsterdam, The Netherlands

Arjun, A - University of Amsterdam, The Netherlands

Cabriolu, Raffaela - NTNU, Norway

Castagna, Jony - STFC Daresbury Laboratory, United Kingdom

Chodera, John - Memorial Sloan Kettering Cancer Center, USA

Decherchi, Sergio - Istituto Italiano di Tecnologia, Genova, Italy

Govindarajan, Nitish - University of Amsterdam, The Netherlands

Herbert, Colm - UCD school of physics, CASL, Ireland

Jung, Hendrik - Max-planck-Institut Fuer Biophysik, Germany

Lervik, Anders - NTNU: Norwegian University of Science and Technology, Trondheim, Norway

MacKernan, Donal - University College Dublin, Ireland

O'Cais, Alan - Jülich Supercomputing Centre, Germany

Perez de Alba Ortiz, Alberto - University of Amsterdam, The Netherlands

Prinz, Jan-Hendrik - Freie Universität Berlin, Germany

Riccardi, Enrico - NTNU: Norwegian University of Science and Technology, Trondheim, Norway

Roet, Sander - University of Amsterdam, The Netherlands

Singraber, Andreas - University of Vienna, Austria

Tiwari, Ambuj - University of Amsterdam, The Netherlands

Torres Knoop, Ariana - University of Amsterdam, The Netherlands

Tribello, Gareth - Queen's University Belfast, United Kingdom

van Erp, Titus - NTNU: Norwegian University of Science and Technology, Trondheim, Norway

Vreede, Jocelyne - , The Netherlands

Synergy between quantum computing and high-performance computing

Location: CECAM-ETHZ, Zurich, Switzerland
Webpage: https://www.cecam.org/workshop-0-1464.html
Dates: August 22, 2017 to August 24, 2017

1 State of the art

Time is ripe for a dialogue between the quantum computing (QC) community and the high-performance computing (HPC) community. In fact, with humongous hardware and software progress in the past 20 years, HPC has increasingly contributed to diverse scientific fields, ranging from materials science to biology and biomedicine, including genomics and neuroscience. On the other hand, the development of QC promises to boost computational performances beyond the current technology.

Quantum technology objectives that resonate with the HPC community are:

- Development and design of new complex materials;
- Versatile simulation of quantum magnetism and electricity;
- Simulation of quantum dynamics and chemical reaction mechanisms;
- Solving chemistry and materials science problems with special purpose quantum computers > 100 physical qubits;

The quantum information community and the HPC community have proceeded so far mostly on independent tracks. Recent bridging research goals address the development of quantum machine learning algorithms that may revolutionize materials design and genomics, the application of a quantum annealer for a proof-of-concept molecular dynamics simulation and for transcription factor-DNA binding specificity, the integration of quantum processing units in current and future HPC systems and the solution of quantum algorithms on classical HPC platforms, the implementation of quantum chemistry on quantum computers.

This workshop was conceived and planned to bring together the two communities to discuss their specific expertise and to outline the bridges that may eventually identify: (1) the future role of quantum technologies in scientific fields where HPC is currently dominant; (2) the use

of existing HPC platforms to demonstrate the potentialities of future quantum technologies to simulate materials and biological systems. The ideas discussed in the workshop are the basis to identify the synergy between HPC and quantum technologies.

2 Major outcomes

7 sessions in 2.5 days, each followed by a discussion (14 45-min invited talks, 5 30-min contributed, a 2-hour tutorial).

(1) Theory and simulation of quantum systems (chair P. Zanardi);

(2) Quantum chemistry (chair S. Bonella);

(3) The status of high-performance computing (chair T. Humble);

(4) Experiments on existing adiabatic quantum computing devices (chair I. Hen);

(5) Electronic structure of materials (chair E. Molinari);

(6) Tutorial on the IBM cloud (chair R. Di Felice);

(7) Models and software for quantum computing (chair A. Seitsonen).

(1) I. Hen highlighted chaos sources that are inherent in analog computation and limit quantum advantages; R. Olsen discussed the importance of investigating correlations in quantum fluids to learn properties of quantum systems that are relevant for QC; A. Scardicchio addressed the issue of whether many-body localization is detrimental to quantum adiabatic algorithms (QAA) and showed the existence of an ergodic region in the phase diagram of many-body systems that is advantageous for QAA.

(2) N. Wiebe pointed out quantum simulation as the killer application of choice for QC, then elaborated on which quantum computer is needed for the target application; R. Babbush announced a Google quantum device with ~50 qubits in few months, then focused on the relevance of plane-wave basis sets to optimize quantum algorithms for quantum chemistry; S. Corni discussed the frontiers of quantum chemistry problems, through selected examples on biologic/inorganic interfaces; J. Romero introduced quantum autoencoders, neural networks suitable to perform tasks on quantum data; I. Tavernelli described recent advances in the simulation of Fermionic systems in analog and digital quantum computing frameworks, remarking current limitations of QC.

(3) T. Schulthess presented current HPC needs and perspectives, discussing hardware and software progress.

(4) R. Harris showed the effectiveness of analog quantum annealing to simulate the phase diagram of a 3D Ising system; P. Ronagh proposed a method to map a quantum Boltzmann machine on a quantum annealer and applied the method on D-Wave 2000Q; R. Di Felice presented the performance of quantum machine learning applied to simplified data on protein-DNA binding specificity, identifying limits in the number of qubits and incomplete connectivity of DW2.

(5) F. Wilhelm-Mauch introduced the paths to quantum computing (universal fault-tolerant, adiabatic, non-error-corrected co-designed processor) and discussed potential applications on ~100 qubits without conventional error correction (High-Tc superconductors and Hubbard model, quantum chemistry); L. Ghiringhelli outlined the NOMAD HPC initiative, devoted to creating materials databases from electronic structure calculations and interrogating the databases to predict materials performance (conductivity, structure, topology, etc.); S. Pittalis related on the use of Fermionic correlations as metric distances in materials science.

(6) P. Barkoutsos gave a tutorial on the IBM Quantum Experience, launched in 2016 with 5 qubits and upgraded to 16 qubits in 2017; the platform is open to users, who can decide whether they want to run their quantum algorithm on qubits or classical simulators; applications in quantum optimization and electronic structure calculations were shown.

(7) D. Steiger related on ProjectQ, a compiling framework for quantum computing available at www.ProjectQ.ch; T. Humble discussed hybrid models for QC+HPC and asked a provocative question: “Is all the research in QC bringing us to better HPC?”; B. Heim talked about what HPC can contribute to QC, focusing on simulated quantum annealing and the importance of having good excited-state solutions; M. Troyer identified problematic claims of quantum advantage and summarized the needs for progressing QC, namely the needs for killer applications and for people with suitable cross-disciplinary expertise.

3 Community needs

A general concept supported by many speakers and highlighted in discussions is the framework of hybrid HPC+QC, in which the most complicated task is given to the QC component but all the preparation and analysis is done on HPC platforms. This seems to be the route of choice for future development.

The needs for killer applications and specialized personnel were remarked. Possible applications were identified in: cryptography, machine learning and optimization strategies, quantum simulation; there is a wide consensus that the latter is currently the most promising

at the frontier between QC and HPC; quantum simulation ranges from the simulation of the phase diagrams of many-body systems to electronic correlations and quantum chemistry.

This particular workshop did not include experimental participants and relations with experimentalists were not discussed. However, we believe that such relations between theory and experiment are crucial, because feedback from theory and applications can help physicists and engineers to develop better and better devices.

In the closing remarks, the organizers proposed to the audience the possible publication of a position paper for a scientific journal and the organization of a follow-up workshop. We did not discuss to create a CECAM series on the topic. We would like to propose a similar workshop in two years from now (Summer 2019), while we will try to organize a related event in 2018 in the USA.

Networking between the QC and HPC communities is highly desirable to assess the computational platforms of the future. Furthermore, there is a strong need for networking among scientists who represent different disciplines, including Physics, Chemistry, Computer Science, Engineering; for pushing high-end applications the relation with other fields is also important, such as biology, medicine, business, markets, and others.

4 Funding

Since its inception, research in theoretical and experimental QC was essentially funded by public bodies. Few years ago, we witnessed a revolution that will lead to commercial quantum hardware of interesting size for real-world applications: this revolution consists of a steering in funding sources, with industry (Google, Microsoft and IBM were represented with invited speakers in the workshop.

HPC is currently funded mostly by public bodies, e.g. through the creation of large facilities, such as National Laboratories of the Department of Energy in the USA and Centers of Excellence of the European Commission. However, in the past Motorola, Intel, IBM and others strongly supported basic computational research, and nowadays NVIDIA is doing so, to push the exploitation and development of graphic processing units (GPU).

Google, Microsoft, IBM and Intel are also funding the creation of the QC/HPC interface and QC+HPC hybrid frameworks.

5 Will these developments bring societal benefits?

In principle, we would aim to achieving impact of QC+HPC in fields in which HPC is currently powerful, which include materials science, computational biology, precision medicine, genetics, finance, weather forecast, to name the main ones. In this scenario, the development of quantum technologies would have an enormous impact in terms of societal benefits, e.g. creation of new jobs and work places, economic progress through the founding of new companies and business relations, efficient medical diagnosis and therapy, and much more.

In the near-term future, we remark quantum chemistry as the application of choice, with potential benefits for clean energy production/storage, agriculture, prediction of materials with outperforming properties. Furthermore, some areas of materials science, which are currently investigated by means of HPC (e.g., vacancies in diamond and other defects), can accelerate the progress towards QC and even identify new QC hardware schemes.

We envision also educational benefits, with the creation of new curricula that incorporate quantum computation concepts in computer science departments and eventually with the introduction of quantum mechanics in early school grades.

6 Participant list

Organizers

Bonella, Sara
CECAM@EPFL, Switzerland

Di Felice, Rosa
CNR Institute of Nanoscience, Modena, Italy

Lidar, Daniel
USC, USA

Lloyd, Seth
Massachusetts Institute of Technology, USA

Molinari, Elisa
University of Modena and Reggio Emilia & CNR-NANO, Modena, Italy

Tavernelli, Ivano
IBM-Zurich Research, Switzerland

Troyer, Matthias
Swiss Federal Institute of Technology Zurich (ETHZ), Switzerland

---

Babbush, Ryan - Google Inc, USA

Barkoutsos, Panagiotis - IBM Research ZRL, Switzerland

Bassini, Sanzio - CINECA, Bologna, Italy

Corni, Stefano - CNR-NANO National Research Center, Italy

Darulová, Jana - ETHZ, Switzerland

Ghiringhelli, Luca M. - Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany

Harris, Richard - D-Wave Systems Inc, Canada

Heim, Bettina - ETZ Zurich and Microsoft, Switzerland

Hen, Itay - Information Sciences Institute, USC, USA

Humble, Travis - Oak Ridge National Laboratory, USA

Kim, Jeong San - Kyung Hee University, South Korea

Kurganskaya, Inna - University of Bern, Switzerland

Lim, Youngrong - Kyunghee University, South Korea

Malis, Momir - CECAM, EPFL, Switzerland

O'Brien, Thomas - Instituut-Lorentz, Leiden University, The Netherlands

Olsen, Raina - US Army Research Laboratory, USA

Pittalis, Stefano - Istituto Nanoscienze CNR - Modena, Italy

Robinson, Marianne - CECAM, Switzerland

Romero Fontalvo, Jonathan - Harvard University, USA

Ronagh, Pooya - 1QBit - UBC, Canada

Scardicchio, Antonello - ICTP, Italy

Schulthess, Thomas - CSCS, Lugano, Switzerland

Seitsonen, Ari Paavo - Ecole Normale Supérieure, France

Steiger, Damian - ETH Zurich, Switzerland

Tomka, Michael - University of Southern California , USA

Troiani, Filippo - CNR-NANO-S3, Italy

Wiebe, Nathan - Microsoft, USA

Wilhelm-Mauch, Frank - Saarland University, Germany

Zanardi, Paolo - University of Southern California, USA

Addressing metastability in interfacial phenomena across multiple time and length scales

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1398.html
Dates: August 29, 2017 to September 1, 2017

1 State of the art

The workshop gathered experimental and theoretical scientists working on a broad range of problems related to interfaces:

a. Metastability's and their positive/negative technological relevance, e.g. i) metastabilities preventing the formation of methane clathrate for gas transportation, ii) metastabilities allowing the preparation of thermodynamically unstable emulsions of colloidal particles.
b. Reaction paths from initial metastable to final states, e.g. the crystallization of chemical presenting polymorphism: kinetics might favor the formation of an inactive form of a drug. It was concluded that it is important to investigate locally ordered transient states, which anticipate the formation of the crystal.
c. Dynamics of liquid droplet and films in air and on surfaces, e.g. i) the sliding/rolling of liquid films/droplets on smooth or textured surface, entrapping air or liquid, ii) collision of liquid droplets and their dynamics as a function of the impact parameters, iii) wetting of ordered and random textured surfaces, iv) extrusion of liquids from porous materials.

These scientific themes have been investigated with a wide set of complementary experimental, computational and theoretical techniques. For example, confocal microscopy has been used to carefully follow the dynamics of liquid infused textured surfaces, and freeze-fracture shadow-casting cryo-scanning electron microscopy allowed to measure the wetting properties of single-nanoparticles. Several simulation techniques have been presented to study reaction path of problems in which both the initial and final state are known (double-ended problems) or only the initial one is available (single-ended techniques). The multiphase systems have been described at a micro, meso and macroscopic level, considering thermal fluctuation effects when necessary. Theories have been presented to model the wetting and extrusion of random and ordered textured surface and porous materials.

2 Major outcomes

A lively scientific discussion accompanied all workshop events, including the poster session, tea and lunch breaks, the excellent social dinner, and the final discussion. Two major directions emerged, which summarize the current and future challenges for the community: the first concerns fundamental aspects of simulating nucleation and thermally activated events; the second is moving towards systems which are closer to experiments and to technological applications in terms of complexity and of simulated time and dimensions.

Concerning the fundamental aspects, one important research avenue is to develop reduced models that allow simulations across scales. For the moment, such problems have been addressed at each scale separately, as several contributions have shown during the workshop; but true concurrent multiscale methods are still lagging behind. In addition, the larger part of the community is using gradient descent algorithms such as the string method or the nudged elastic band. While such methods are very powerful in a number of cases, they rely on the small noise approximation. The question is whether this assumption is verified in the case of very small systems or nanoscale nuclei. Another problem which is common to many participants in different areas (drug discovery, crystallization, wetting, cavitation, clathrates, etc.) is the choice of the relevant descriptors to address the thermally activated transitions from one metastable state to the other. This problem is particularly compelling for finding polymorphs of a given drug but is surprisingly important also for confined vapor nucleation.

In the second direction, i.e., moving towards real-world cases, the first important point discussed was how to find a connection between experiments and simulations. In some cases (e.g. drop dynamics and fluid flows on textured surfaces) the links between theory and experiments have matured. However, there are still a number of important areas, as in nucleation, where quantitative comparison with experiments is so difficult, owing to the different time and length scales involved, to the role of impurities, etc. To be able to make progress, we need to continue developing simulations able to access larger time and length scale (again, highlighting the need for reduced models) and, at the same time, experimental techniques that deal with small times and lengths (such AFM in liquid). Another important challenge is to deal with the full complexities of real world systems, including mixtures with a complex phase diagram (the example of crude oil has been made), the role of confinement and the unavoidable effects of impurities.

Summarizing, the community working on metastabilities in interfacial systems is investigating a broad variety of problems, going from pharmaceuticals to liquid-infused surfaces. However, common fundamental challenges emerge: dealing with several length scales, with the transition dynamics, and identifying different polymorphs. The bridge with applications is also going to be of major concern in the next years, with the challenge to being able to predict the behavior of systems with several species, impurities, etc.

3 Community needs

The participant felt that Interfaces, metastabilities, and the associated temporal and spatial multiscale problems are important for many fields ranging from soft matter (e.g. metastable states of emulsions, liquids in contact with biological membranes), engineering (drag reduction by random or ordered stable or metastable textured surfaces), energy (mechanical energy storage by intrusion/extrusion in/from porous materials), chemistry (nucleation of drugs), materials (nucleation of composite nanomaterials) and many more. Similarities in problems, techniques and theories across the fields have been identified. The participants were convinced that much can be gained by members of the communities by working together, which requires the identification of specific themes of common interest. Thus, we propose the organization of a next workshop with the main objective to identify a list of common research themes on which experimentalist, computational scientists and theoreticians can work together, possibly obtaining financial support by the H2020 programme. Of course, this should be accompanied by an even more extended search for scientific problems connected to interfaces, metastabilities and multiple scales in others domains.

Another aspect that has been discussed is that of hard and "soft" infrastructures. While there is a good provision of computer resources (National or European supercomputing centres) more complex is the situation with software and expertise to run it properly. There are communities, such as the atomistic one, in which exist a number of well-established community codes. Other communities rely more on group-level codes, which hinders the development of the community and collaborations. Concerning the temporal multiscale issue, the question is more articulate: a limited number of codes exist, e.g. LAMMPS, but they are tailored for/support only MD codes

4 Funding

The participants shared their experience with industrial partners who funded their research on subjects related to the workshop. Two representative cases were reported: the case of the oil industry funding fundamental experimental research on the wettability of surfaces by oils in the presence of ions and the case of pharmaceutical industry funding simulations to address the issue of polymorphs in the crystallization of drugs. These two success stories both suggested that long-term funding is needed for advancing substantially the field of nucleation towards a quantitative comparison with experiments. A promising funding channel to support at least a part of the common needs is the Marie Skłodowska-Curie Innovative Training Networks (ITN-ETN). This initiative aims at raising doctoral student with competences in simulating nucleation phenomena. In addition, it would be highly beneficial to promote regular meetings, development of community code for rare events, and a benchmark database.

5 Will these developments bring societal benefits?

The participants all agree that progress in understanding interfacial phenomena, including the aspect of metastability, will bring a number of benefits to society. Several concrete examples, related to the work of the participants, were discussed, in the sectors of healthcare (e.g. in computer-aided drug discovery, the use of liquid infused surfaces in hospital walls), energy (e.g. superhydrophobic coatings for drag reduction, bubble cavitation in propellers, the formation of methane clathrates during gas transportation) and consumer products (e.g. development of new class of colloidal emulsions), among others.

With these applications in mind, we also spent some time discussing good practice in creating pathways to impact, particularly in relation to industrial collaborations. ECAM was highlighted as an excellent incubator for such links, and there is an appetite to organize a sequel to this workshop with dedicated sessions on industrial problems. Several participants further emphasized the importance of building sustainable and mutually beneficial relations with companies. For example, in the Netherlands they have part time professorships for industrialists, which have been very successful. Another impact pathway that is of interest to the participants is through software. However, it was pointed out that at present we mostly

rely on group-level codes, rather than robust, well-established community codes; and it is unclear whether these group-level codes are good enough to be used as a “black box”.

6 Participant list

Organizers

Giacomello, Alberto
Sapienza University of Rome, Italy

Kusumaatmaja, Halim
Durham University, United Kingdom

Meloni, Simone
Sapienza University of Rome, Italy

Amabili, Matteo - University of Rome, Italy

Casciola, Carlo Massimo - University of Rome I "La Sapienza", Italy

Dietrich, Siegfried - Max-Planck-Institute, Germany

Eshraghi, Mojtaba - Institut für Theoretische Physik II: Weiche Materie, HHU Düsseldorf, Germany

Henkelman, Graeme - Austin University, USA

Herminghaus, Stephan - Max-Planck-Institute, Germany

Isa, Lucio - ETH Zurich, Switzerland

Kurganskaya, Inna - University of Bern, Switzerland

Lisi, Emanuele - Sapienza Universita" di Roma, Italy

Lutsko, Jim - ULB, Belgium

Marchio, Sara - Sapienza University of Rome, Department of Mechanical and Aerospace Engineering, Italy

Merabia, Samy - University of Lyon I, France

Moghimikheirabadi, Ahmad - Institute of Polymers, ETH Zürich, Switzerland

Mugele, Frieder - University of Twente, The Netherlands

Müller, Marcus - Georg-August University, Göttingen, Germany

Pagonabarraga, Ignacio - Swiss Federal Institute of Technology, Switzerland

Panter, Jack - Durham University, United Kingdom

Pepona, Marianna - Durham University, United Kingdom

Ren, Weiqing - Department of Mathematics, National University of Singapore, Singapore

Rosales, Pablo - Universidad Complutense de Madrid, Spain

Santiso, Erik - North Carolina State University, USA

Sanz, Eduardo - Physical Chemistry Department, Chemistry Faculty, University Complutense of Madrid, Spain

Satarifard, Vahid - Max Planck Institute of Colloids and Interfaces, Germany

Sear, Richard - University of Surrey, United Kingdom

Somerville, Walter - University of Hull, United Kingdom

Thijssen, Kristian - Eindhoven University of Technology, The Netherlands

Tinti, Antonio - Sapienza, Università di Roma, Italy

Tribello, Gareth - Queen's University Belfast, United Kingdom

Vollmer, Doris - Max-Planck-Institute, Germany

Wells, Gary - Northumbria University, United Kingdom

Yeomans, Julia - Oxford University, United Kingdom

Big-Data driven Materials Science

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1437.html
Dates: September 11, 2017 to September 13, 2017

1 State of the art

Many, probably most, areas in the basic and applied sciences and engineering are increasingly facing the challenge of dealing with massive amounts of data, nowadays commonly addressed as „big data “. This big-data challenge is not only about storing and processing huge amounts of data, but also, and in particular, it is a chance for new methodology and understanding, as it opens qualitatively new routes for doing research.

The number of possible materials, including organic and inorganic materials, surfaces, interfaces, and nanostructures, as well as hybrids of the mentioned systems, is practically infinite. About 200,000 materials are “known” to exist, but only for very few of these “known” materials, the basic properties (elasticity constants, plasticity, piezoelectric tensors, conductivity, etc.) have been determined. When considering 60 commercial elements blended together, there is essentially an infinite number of compounds to be explored.

It is, therefore, highly likely that new materials with superior and up to now simply unknown property profiles exist that could help solving fundamental issues in the fields of energy, mobility, safety, information, and health.

For materials science it is already clear that in terms of properties and functions, big data are structured, and in terms of materials properties and functions, the space of all possible materials is sparsely populated.

We identify these two outstanding challenges in the "big-data driven materials science":

1. Developing big-data analytics to find structures and causal relationships in big data of materials that are not recognizable by "naked eye" or standard tools.

2. Assigning error bars or uncertainty tags to the data.

The aim of the workshop is to put in contact the community that develops models and methodologies for the data analytics with the continuosly growing part of the materials science community that is applying those models and methodologies to relevant problems in the field.

2 Major outcomes

The workshop was organized in 5 sessions, devoted to 3 main subjects in the emerging field of data-driven materials science: “The central role of the descriptor”, “Extracting information from data”, and “Accuracy and error bars” (the first two topics had a “theory” and “application” session each).

The session on accuracy summarized present challenges in the standardization (in view of possible comparisons and reuse) of calculation parameters, for ground-state and beyond-ground-state methods.

This session ideally continued discussions ignited at the “Towards a Common Format for Computational Materials Science Data” CECAM/Psi-k workshop, held in Lausanne in January 2017, with the new contributions aiming both at providing reference, “numerical-errors free” data and at developing machine-learning models for the estimate of the expected error for calculation with not-fully-converged settings.

The extended time allotted for discussions, both at the end of each talk (15 minutes for Q&A) and, in the form of moderated discussion slots (30 minutes) at the end of each session, allowed the participants to ask detailed questions about the methods and results presented in the talks, but gave also room to perspective discussions.

Two discussion topics that involved most of the participants were:

- Possible convergence of the “configurational” vs “chemical space routes” in machine-learned models in materials science. The “configurational route” addresses the learning of, typically, energy and forces by using as input configurations represented in various way (Csanyi, Hirn, Tkatchenko). These methods, quite successful in predicting properties within the set of chemical species used in the training, even for configurations that are not “close” to the training one, are not constructed for extrapolate over new chemical species.

The “chemical space” way (Ramprasad, Pilania, Ghiringhelli, von Lilienfeld) uses as input the compositions of the materials and some minimal information on the structure, when necessary, in order to predict properties of interest (e.g., band gaps, or electric-breakdown field, or classifications such as “being topological or trivial insulator, or metal”). By construction, these methods attempt to predict properties also for unseen chemical species, in combination with those used in the training. However, they have difficulties in distinguishing between polymorphs of the same material.

In several talks (Csanyi, Ghiringhelli, Tkatchenko), it was pointed out the necessity that the two approaches learn from one another and possibly will converge to a unified approach.

Tkatchenko and Csanyi have presented already ideas towards this goal, but there is more work to do.

- Interpretable vs non-interpretable models. In a seminal contribution, Joachim Buhmann, a key figure in Information Science, suggested that we, humans, may "surrender" the wish to understand why modern machine-learned models (in particular, coming from "deep learning") work, as long as we can test thoroughly their validity and robustness with respect to noise. Naturally, a physicist and therefore a materials scientist would be reluctant to give up understanding and in facts several recent contributions to the field (e.g., Tkatchenko, Ramprasad, Scheffler) explicitly look for a physical "interpretability" of the model found via machine learning or other data-analytics tools. The idea is that the scientists' understanding of the physical reason why a certain model works, can lead to its improvement or allow for predictions that are completely outside the training data, i.e., discovery of novel systems (materials classes), rather than just new (better materials – with respect to a certain property or function – but similar to known ones that were "just" overlooked). Clearly the two tendencies will coexist and would benefit of each other.

3 Community needs

At the beginning of the workshop, Csanyi noted that he felt like he was participating to a "family reunion", and the family was clearly growing and thriving. Indeed, in November 2015 Scheffler and Ghiringhelli, together with Levchenko, had organized a workshop with similar scope to the present one ("Big Data of Materials Science -- Critical Next Steps") with some of the same invited speakers.

It has been indeed astonishing to witness the evolution of the field in these two years, in terms of better understanding and therefore further development of "older" approaches (one example for all, Csanyi's Gaussian Approximation Potentials, leading to structural similarity recognition tools) and the flourishing of new methods and their applications.

It seems therefore highly recommended to envision a series, perhaps with a "natural" biennial frequency, of workshops on the more and more established field of "Data-driven materials science".

Most of the classes of techniques used in this field (in particular neural networks and compressed sensing) are well-suited for on-going and future development of HCP infrastructure. The existence of ever growing repository of materials science data, allows also to decouple the intensive data production from the data analysis.

This said, the most important investment for the development of the field is the cross-breeding of data-analytics method developers (computer scientists, but also mathematicians) with "domain experts", i.e., the materials scientists that identify the physical relevance of classes of problems that may benefit from data-analytics approaches.

It is also recommendable that the future generation of materials scientist is exposed to (big-) data analytics early in their studies, in order to be prepared for an approach that it is easily foreseeable as a pillar of near and far future materials-discovery research.

4 Funding

Three Centres of Excellence, in the framework of the Horizon-2020 call for e-infrastructure, have been funded in the materials science field, with several million euros and therefore several academic positions: Materials design at the eXascale (MaX), E-CAM, and Novel Materials Discovery (NOMAD). With different focuses, all three centers share the goal of further establish high-performance computation for novel materials design and discovery.

Such initiatives will benefit of a second funding period, before being able to be fully self-funded, in particular by offering services to the industrial sector. They can further be supported by providing computational resources, e.g. by the PRACE initiative as it happens already now.

5 Will these developments bring societal benefits?

The potential benefits of data-driven materials science cannot be overemphasized. According to some actors and observers, more than a field, data-driven (materials) science is a new paradigm. In other words, clever data-analytics tools may and should become of common use for accelerating research. Simply because learning algorithms can identify pattern in multidimensional data that exceed human intuition. It has to be noted that, even though possibly requiring intensive HCP resources, data-driven research has the intrinsic benefits to reuse existing data. This in turns introduces several positive “side effects”: fully accessible “raw data” used for some published analysis fully unlocks scientific reproducibility, not easily attained in the past; furthermore, open data access propels the achievement of “standard” or “best” practice for the data production. In a, possibly near, future scenario, several concurrent data-analytics programs will run on servers over the growing materials databases in search of not yet seen trends, and outliers in the data. It is easy to foresee that such approach cannot but lead to new discoveries. Since the target of such discoveries would be materials optimizing certain properties or optimal for certain process, the positive fallout on industry and the society is evident.

6 Participant list

Organizers

Ghiringhelli, Luca M.
Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany

Scheffler, Matthias
Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany

Bereau, Tristan - Max Planck Institute for Polymer Research, Mainz, Germany

Bhattacharya, Sandip - Ruhr University Bochum, Germany

Botu, Venkatesh - Corning Incorporated, USA

Bromley, Stefan T. - University of Barcelona, Spain

Buhmann, Joachim - ETH Zurich, Institute for Machine Learning, Switzerland

Chen, Linjiang - Department of Chemistry, University of Liverpool, United Kingdom

cozzini, Stefano - CNR - Istituto Officina dei Materiali, Italy

Csanyi, Gabor - University of Cambridge, United Kingdom

Cuko, Andi - Université Pierre et Marie Curie, France

Curtarolo, Stefano - Duke University, Durham, , USA

de Gironcoli, Stefano - International School for Advanced Studies (SISSA) and CNR-DEMOCRITOS IOM, Trieste, Italy

Fazzio, Adalberto - Instituto de Fisica - Universidade de Sao Paulo, Brazil

Geurts, Amber - Aalto University, Finland

Goedecker, Stefan - University of Basel, Switzerland

Gulans, Andris - Humboldt-Universität zu Berlin, Germany

Hammerschmidt, Thomas - ICAMS, Ruhr-Universität Bochum, Germany

Heidar Zadeh, Farnaz - McMaster University, Hamilton, Canada

Hirn, Matthew - Michigan State University, Department of Computational Mathematics, Science & Engineering, USA

Kurganskaya, Inna - University of Bern, Switzerland

Legrain, Fleur - CEA-Grenoble, LITEN, France

Mace, Amber - Swiss Federal Institute of Technology Lausanne (EPFL), Sweden

Margraf, Johannes - TU Munich, Germany

Marzari, Nicola - Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Pankajakshan, Praveen - Shell India Markets Private Limited, Bangalore, India

Pilania, Ghanshyam - Los Alamos National Laboratory, USA

QUERLEUX, Bernard - L"OREAL Research & Innovation, France

Race, Chris - Manchester University, United Kingdom

Ramprasad, Rampi - University of Connecticut, USA

Sauceda, Huziel E. - Fritz Haber Institute of the Max Planck Society, Germany

Schleder, Gabriel - Federal University of ABC, Brazil

Sutton, Christopher - Fritz Haber Institute, Germany

Thygesen, Kristian S. - Technical University of Denmark, Lyngby, Denmark

Tkatchenko, Alexandre - University of Luxembourg, Luxembourg

von Lilienfeld, Anatole - University of Basel, Switzerland

Vreeken, Jilles - Exploratory Data Analysis, Cluster of Excellence MMCI, Saarland University, Germany

Winston, Donald - Lawrence Berkeley National Laboratory, USA

Ziletti, Angelo - Fritz Haber Institute of the Max Planck Society (FHI), Berlin , Germany

Multiscale modelling of organic semiconductors: from elementary processes to devices

Location: IMAG building, University Grenoble Alpes (see https://batiment.imag.fr/en/contact-addresses-access)
Webpage: https://www.cecam.org/workshop-0-1383.html
Dates: September 12, 2017 to September 15, 2017

1 State of the art

Organic semiconductors are small molecules or polymers. Modelling charge and energy transport in these materials and in devices such as transistors, organic light-emitting-devices and photovoltaic cells, will identify a new generation of materials by combining ideas from different sectors and disciplines. The aim of the modelling is to develop models that can screen organic host and dopant materials, avoiding the need for the costly and lengthy process of synthesizing and testing new materials. Films contain pristine and doped materials and are heterogeneous, e.g. include a donor/acceptor interface and have disordered and crystalline regions. Since charge and energy transport in these materials is highly sensitive to molecular and polymeric packing, modelling of structural, electronic, optical and transport must be at the mesoscopic level with embedded microscopic electronic structure and morphology calculations. Interfaces between the layers in a device must be considered. It is therefore important to provide parameter sets for drift diffusion models including densities of states, injection barriers at interfaces and rates of bimolecular processes. A predictive model should reduce the number of parameters fitted to experiment, noting that large scale defects rule out a solely microscopic approach.

Many fundamental questions remain from understanding of transport and doping mechanisms in organic semiconductors, to the problem of exciton dissociation or singlet fission in photovoltaic processes. Charge and ionic (nuclear) degrees of freedom are coupled, causing localization of charge carriers and excitons, with a strong impact on transport. This interplay between localization and delocalization, between a band-like or a localized picture, and the distinction between coherent or thermally activated scenarios places strong constraints on the theoretical methods that must be accurate but general enough to allow for the correct behavior to emerge.

2 Major outcomes

Applications: (see section on societal benefits), motivating the research, e.g. high-performance light-emitting diodes based on carbene-metal-amides.

Computational materials design: microscopic questions such as how localisation from quantum interference is destroyed by molecular motion, coherence of wavepackets in charge transport, breakdown of polaron hopping picture in crystalline pentacene, doping mechanisms, new intragap features due to charge transport complexes, GW theory accounting for electron-hole interactions, infrared active phonon modes modulating bond length alternation, microscopic origin of thermally activated delayed fluorescence

Mesoscopic approaches to understanding charge mobility variations with applied bias from kinetic Monte Carlo, influence of molecular packing via coarse grained molecular dynamics e.g. determining inter-chain and intra chain hops in polymer films, kinetically trapped morphologies, influence of side chains, network theory applications to understanding charge transport, percolative transport including filamentary transport, polarization disorder arising from electrostatic interactions, timescales in glassy solids, exciton diffusion and annihilation in light emitting devices.

Experimental input: reliable measures of charge mobility e.g. via impedance spectroscopy, transient measurements such as charge carrier extraction by linearly increasing voltage, growth conditions, neutron scattering measurements to determine phonon spectra, measurements of charge transfer in dopants, dopant efficiency and diffusion, modification of charge injection at anodes via interlayers, device fabrication by screen printing and blade coating.

3 Community needs

Networking and training: the workshop was expanded to take 70 participants following a very strong demand for places. Participants from outside the EU came from the US (including 5 invited speakers), China and Japan. The workshop was recognized as the major event this year focusing on organics modelling. Commonality of coding difficulties was addressed but there was no focus on particular codes, since in this area much coding is required and there is less reliance on running software packages such as VASP. Experimentalists were given invited talks to stimulate discussion of their modelling needs with the groups that develop the models. The workshop was attended by a mix of senior staff, early career researchers and graduate students. Most talks were 25 minutes, allowing for plenty of discussion of their work. Many early career researchers were given talks. The informal nature of the workshop allowed the younger participants to join in the discussions and they asked many questions. Computational infrastructure questions became apparent in the 2-hour hands-on tutorial by Nanomatch which attracted an enthusiastic group of around 20-30 participants. This workshop followed on from the CECAM/Psi-K Workshop on “Charge transport in organic materials”, Bremen, March 31 - April 4, 2014 but is not part of a series. Its topics are addressed in symposia at the European and US Materials Research Society meetings.

5 Will these developments bring societal benefits?

Organic semiconductors are a success story amongst the technologies that first appeared in the last decade of the 20th century/ first decade of the 21st century. Many firms and consequently jobs have been created in the EU. These firms vary from display suppliers and, large materials suppliers such as Merck, BASF and Osram to more specialist suppliers such as Novaled, Cynora, FlexEnable and software vendors addressing organics such as Nanomatch, Simbeyond, Silvaco UK, Fluxim, Tibercad.

Applications include:

- Displays: €10 billion market, e.g. Apple and Google are using OLED displays for their new smart phones,
- Automotive and aerospace applications due to their flexibility and light weight

- Lighting: €2.5 billion market for large area diffuse lighting,
- Medical: sensors on skin that can provide early warning of diabetes, increase signal to noise ratio in magnetic resonance image scans,
- Photovoltaics.

Organic semiconductors are made from sustainable easily sourced materials and in the case of polymers and some small molecule materials can be printed so have a low energy budget.

Many funding calls on organic materials and devices have been made by international science funding agencies such as the EU Horizon2020 program which funded the two consortia Extmos and Mostophos that collaborated to organize this workshop, the EoCoE project that includes work in organic photovoltaics and European Research Council grants. National funding agencies such as in Germany, France, US and UK have also funded extensive research and development activity on this topic.

6 Participant list

Organizers

Andrienko, Denis
Max Planck Institute for Polymer Research, Germany

BARENDSON, Samantha
Centre Blaise Pascal - ENS de Lyon, France

Blase, Xavier
Institut Néel, CNRS, Grenoble, France

Bobbert, Peter
TU Eindhoven, The Netherlands, The Netherlands

Deutsch, Thierry
French Alternative Energies and Atomic Energy Commission (CEA), Grenoble, France

Mercuri, Francesco
CNR-ISMN, Italy

Walker, Alison B.
University of Bath, United Kingdom

Wenzel, Wolfgang
Karlsruhe Institute of Technology (Germany), Germany

Alessandri, Riccardo - University of Groningen, The Netherlands

Altazin, Stephane - Fluxim AG, Switzerland

Ana Claudia, Arias - Berkeley, USA, USA

Antoine, Kahn - Princeton, USA, USA

Antonio, Facchetti - Northwestern University, USA, USA

Auf der Maur, Matthias - University of Rome “Tor Vergata”, Italy

Baldoni, Matteo - Consiglio Nazionale delle Ricerche (CNR), Istituto per lo Studio dei Materiali Nanostrutturati (ISMN), via Gobetti 101, 40129 Bologna, Italy, Italy

Beljonne, David - University of Mons, Belgium

Cazzaniga, Marco - Istituto di Scienze e Tecnologie Molecolari - CNR-ISTM, Italy

Ciuchi, Sergio - Dept. of Physical and Chemical Sciences University of L"Aquila, Italy

Coehoorn, Reinder - Eindhoven University of Technology, The Netherlands

Cornil, Jerome - University of Mons, Belgium, Belgium

D'Avino, Gabriele - Institut Néel, CNRS, France

Da Como, Enrico - University of Bath, United Kingdom

de Vries, Xander - TU/e, The Netherlands

Duchemin, Ivan - CEA, France

Escudero Masa, Daniel - Université de Nantes, France

Faller, Roland - UC Davis, USA

Fediai, Artem - Karlsruhe Institute of Technology, Germany

Fratini, Simone - CNRS, France

Friederich, Pascal - Karlsruhe Institute of Technology, Germany

Furno, Mauro - Navaled GmbH, Germany

Gertsen, Anders - Technical University of Denmark, Denmark

Golrokh Bahoosh, Safa - University of Konstanz, Germany

Guilbert, Anne - Imperial College London, United Kingdom

Hattori, Shinnosuke - Sony corporation, Japan

Heimel, Paul - TU Braunschweig, IHF, Germany

Hellweg, Arnim - COSMOlogic, Germany

Jenatsch, Sandra - Fluxim, Switzerland

Jing, Li - CNRS, France

Konrad, Manuel - Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

Kotadiya, Naresh - Max Planck Institute for Polymer Research, Germany

Lebedeva, Irina - Universidad del Pais Vasco, Spain

Leitherer, Susanne - DTU Nanotech, Denmark

Leo, Karl - Dresden University of Technology, Germany

Liero, Matthias - Weierstrass Institute Berlin, Germany

Ligthart, Arnout - Eindhoven university of technology, The Netherlands

Lin, Xin - Princeton University, USA

Liu, Feilong - Eindhoven University of Technology, The Netherlands

Liu, Lei - Max Planck Institute for Polymer Research, Germany

Lorenzoni, Andrea - CNR, Italy

Mangalore, Deepthi Kamath - Max Planck Institute for Polymer Research, Germany

Melnyk, Anton - MPIP, Germany

Mondal, Anirban - Max Planck Institute for Polymer Research, Germany

Muccioli, Luca - University of Bologna, Italy

Muhieddine, Khalid - imec, Belgium

Nejim, Ahmed - Silvaco Europe Ltd, United Kingdom

Nelson, Jenny - Imperial College London, United Kingdom

Neumann, Tobias - Nanomatch GmbH, Germany

Oleg, Prezhdo - ochester University, USA, USA

Olivier, Yoann - University of Mons, Belgium

Pecchia, Alessandro - The National Research Council (CNR), Italy

Querciagrossa, Lara - Bologna University, Italy

Reineke, Sebastian - Technische Universität Dresden, Germany

Ricci, Matteo - Universita di Bologna, Italy

Rodin, Vadim - Materials Science Laboratory, Sony Europe Limited, Zweigniederlassung Deutschland, Germany

Roscioni, Otello M - Universita" di Bologna, Dipartimento di Chimica Fisica ed Inorganica, Italy

Rossi, Daniele - University of Rome "Tor Vergata", Italy

Ruhstaller, Beat - Zurich University of Applied Sciences, Wintertur, Switzerland

Sami, Selim - University of Groningen, The Netherlands

Smith, Alexander - University of Bath, United Kingdom

Strunk, Timo - Nanomatch GmbH, Germany

Symalla, Franz - Karlsruhe Institute of Technology, Germany

Thompson, Ian - University of Bath, United Kingdom

TONNELE, Claire - University of Bordeaux, France

Troisi, Alessandro - University of Warwick, United Kingdom

Wang, Linjun - Zhejiang University, Hangzhou, China

Wetzelaer, Gert-Jan - Max Planck Institute for Polymer Research, Germany

Will, Paul-Anton - Technische Universität Dresden, Germany

Yang, Hui - University College London, United Kingdom

Yves, Geerts - Bruxelles, Belgium

Zannoni, Claudio - Universita' di Bologna, Dipartimento di Chimica Industriale "Toso Montanari", Italy

Extended Software Development Workshop in meso and multiscale methods (ESDW8) :

Location: CECAM-DE-MMS
Web page: https://www.cecam.org/workshop-0-1408.html
Dates: September 18, 2017 to September 29, 2017

1 State of the art

As the overview from the CECAM web page stated the state of the art is: Both Markov state models and balanced model order reduction are well established coarse graining techniques that can handle large- and multiscale dynamical systems, given certain equilibrium or stochastic stability assumptions like reversibility or the fluctuation-dissipation relation. If these assumptions are met, MD trajectory data can be used to derive coarse-grained representations of a molecular system and to quantify its uncertainly. The systematic use and the incorporation of general MD data, driven or open boundary MD is a relatively new aspect.

Model/Dimension Reduction, broken down to its basics, is basically describing any complex system with its relevant set of suitable observables or collective variables. Balanced model order reduction (MOR) is a rational approximation technique that seeks an approximation of given observables as functions of external input variables (e.g. external forces or noise), by identifying a subspace of variables that are both sensitive to the inputs and strongly coupled to the observables. For linear and bilinear systems, finding a reduced-order system boils down to solving a set of coupled Lyapunov matrix equations for the corresponding controllability and observability Gramians, for nonlinear systems in equilibrium, the problem can be rephrased in terms of a Monte-Carlo sampling procedure.

Markov State Model (MSM) is linking molecular dynamics with a time series analysis tool that allows for extracting the essential conformation dynamics from a trajectory that has been generated by any reversible and ergodic dynamical system. The generalization of the MSM approach to reversible open systems, that is currently undertaken in the Berlin node of the E-

CAM project, is a natural next step. As explained in more detail on the webpage the MSM discretisation of GC-AdResS is theoretically well described and the ESDW concentrated on MSM as a time analysis tool.

2 Major outcomes

The major goal of this workshop was to show how to systematically use several different methods and to further the idea that a new combination and/or the incorporation of several methods can lead to uncover new aspects. The take-a-way message was: (i) the participants should leave with a basic understanding of the different methods, (ii) the development of software packages/modules to optimize/simplify simulations and (iii) to identify the problems/advantages of connecting the different methods.

We provided 4 topics to start/develop. We have two very basic programming projects (1 & 4). The main aspect of projects 2 & 3 was to simplify the corresponding simulations. GC-AdResS, MSM, MOR are very effective models, which, however, require still a lot of manual adjustment of input parameters, i.e. mostly only the method developers are using those tools.

Project 1: Alternative Partitioning of space in adaptive resolution simulations

Project 2: Interface to simplify the usage of adaptive resolution simulations

Project 3: Interface to couple Markov State Model to adaptive resolution simulations

Project 4: Gentle stochastic thermostats for molecular simulation

The details regarding these projects were uploaded onto the CECAM web page as pdf file. (original file name: project-school.pdf)

These projects required the understanding of those methods involved. Thus, we divided the workshop basically into 2 parts. The first part was dedicated to the teaching of the different methods. We had an introduction into GC-AdResS, the Markov State Model from a very basic mathematical/conceptual point of view, then an explanation of the MIST library and how to patch MD codes with it, as well as what stochastic thermostats are and finally the model reduction from a mathematical standpoint. The second part was solely for the participant to work and discuss the different projects. We had 13 participants in total (PhD students and postdocs), out of which only 5 were actively involved in the development of software modules.

Limitations:

There were a very limited number of participants from groups belonging to the E-CAM project who are interested in similar or complementary subjects. As a consequence, the productive engine of the school was concentrated on those who already hold expertise in the field and could help non-expert by sharing the work to enter in the field. A higher number of students from other E-CAM projects would have enhanced the concreteness of the outcoming and enforced the network within and outside the E-CAM framework. The concept of 2 weeks of un-interrupted workshop has proved not to be ideal. Even though the combination of lectures, tutorials and project work seams reasonable given the aim of software development, the participants get overwhelmed with too much new material that they have to digest before they can use it. Therefore, it might be more useful to have two separate workshops, each of which lasts one week, and let the students work on their projects in the meantime (including the possibility for having regular web chats or the like).

3 Community needs

list of modules developed (or at least started) during the meeting, interest from industry? Will they be documented through the deliverable?

We proposed 4 software projects.

Project 1: On going work. We had 2 participants interested (at least partially). They did not reply if they

Project 2: One participant finished the interface and extended the project to incorporate the thermodynamic force calculation. This might lead to one or two modules, depending on how he uploads the code. He has submitted his interface onto gitlab and is currently focusing on project 1.

Project 3: For an interface to couple Markov State Model to GC-AdResS or simulations in general we had initially 4 people interested and, in the end, only 2 survived without having made much progress. From 1 participant I got positive feedback that he is continuuing working on it.

Project 4: No one was interested.

To sum it up, the further integration of a new mapping scheme into Espresso++ and the interfaces to simplify the usage of Markov State Models got the most interest. One participant worked on an interface to control and simplify the usage and setup of GC-AdResS, he even expanded on it. And he shifted his focus onto project 1 and is in contact with us about this.

4 Funding

We plan to invite the participants, which are either working on the projects or related topic again for face to face discussions. We would like to further those started projects, but we are also looking or future possible cooperation and new aspects developed from those projects.

While this ESDW8 was to teach PhD students and PostDocs what methods are available and how they can be connected. A face-to-face meeting must entail more concrete cooperation. How that looks like has to be evaluated for each person separately.

6 Participant list

Organizers

Delle Site, Luigi
Institute for Mathematics, FU Berlin, Germany

Hartmann, Carsten
BTU Cottbus-Senftenberg, Germany

Krekeler, Christian
Freie Universität Berlin, Germany

Banisch, Ralf - Freie Universität Berlin, Germany

Bethune, Iain - Edinburgh Parallel Computing Centre, United Kingdom

Beyerle, Eric - University of Oregon, USA

Castagna, Jony - STFC Daresbury Laboratory, United Kingdom

Donati, Luca - Freie Universitat, Germany

Erlekam, Franziska - Zuse Institute Berlin (ZIB), Germany

Kobayashi, Hideki - Max Planck Institute for Polymer Research, Germany

Krajniak, Jakub - KU Leuven, Belgium

Kuclar, Matija - national institute of chemistry, Slovenia

O'Cais, Alan - Jülich Supercomputing Centre, Germany

Popadić, Aleksandar - National Institute of Chemistry, Slovenia

Quer, Jannes - Zuse-Institut Berlin, Germany

Richter, Lorenz - BTU Cottbus-Senftenberg, Germany

Strehlau, Markus - B-Tu Cottbus-senftenberg, Germany

Wang, Weiqi - Fritz-Haber institute, Germany

Weber, Marcus - Zuse Institute Berlin, Germany

Wrzalek, Sandro - Freie Universitaet Berlin, Germany

Zhou, Yuanyuan - Fritz-Haber institute of Max Planck Society, Germany

From the atom to the material

Location: CECAM-UK-JCMAXWELL
Webpage: https://www.cecam.org/workshop-0-1489.html
Dates: September 18, 2017 to September 20, 2017

1 State of the art

One of the buzz phrases currently in fashion is ‘From the atom to the material’. It is one of the major drivers of the Materials Genome Initiative which has, amongst its objectives, the aim of reducing the time to market for materials from the current value of 20 years or more through increased use of modelling, simulation and data. It is also one of the objectives of the European Materials Modelling Council, and there are many calls from industry for such capability. The Workshop aimed to bring a sense of reality and achievability to the field by discussing and reviewing:

(i) Examples of use case requirements from industry for modelling and simulation under the general objectives of ‘From the atom to the material’ and the timescales for these requirements;
(ii) Which of these requirements can already be fulfilled by current simulation and modelling capabilities;
(iii) Which of these requirements will be fulfilled by methods and technologies currently under development;
(iv) Gaps in capability.

The primary aim of the Workshop was to open up dialogue between modelers and industrial users of modelling with the intention that:

(i) Current modelling and simulation capability is used to its maximum effect;
(ii) Future development of modelling and simulation capability is aligned closely with fulfilling the objectives of ‘From the atom to the material’;
(iii) We jointly educate and lobby Funding Councils to ensure that research is funded to address the gaps in the capability ecosystem which will thus allow us to achieve the ultimate goal of designing, testing and verifying real world materials using modelling and simulation and thus realize the ambition of ‘From the atom to the material’.

2 Major outcomes

The meeting was divided into themes with clear steers given to the speakers:

Industry requirements – review some of your industry's materials challenges, existing applications of modelling which have been helpful and provide a 'wish list' for future modelling capability.

Virtual materials design – be positive about your achievements - but at the same time be realistic about the limits of an entirely 'in-silico' approach to creating materials. This session also stressed the importance of the ‘translator’ – the individual who can connect (in both directions) a complex product challenge to a set of feasible materials modelling tasks.

Emerging methods – please talk about the materials modelling methods you are developing and how they can address challenges in virtual materials design.

'Poacher turned gamekeeper' - please talk about both your experience of materials design/discovery in an industrial context and in an academic context and how the two sides could most effectively work

International initiatives – in addition to outlining the activity you are presenting please could you explain how this activity can respond to the various materials design challenges described in the meeting.

The talks and comments from industry-based participants showed that there is a very broad range of requirements from industry for materials modelling, in terms of types of material, properties of interest and, interestingly, the level of accuracy needed. This ranged from one extreme of a requirement for quantitatively accurate predictive simulations to, in the middle, not being worried about the absolute value of a predicted quantity but only about trends under change of composition to only using modelling and simulation to provide insight into complex physical problems without requiring quantitative accuracy. It became apparent that even in large companies in most cases materials modelling is a very small-scale activity at present and in many companies it does not exist at all. It is also not unusual to have no company-wide view of modelling activities, so that there is no information exchange between different divisions of the same organisation.

The first talk in the Virtual Materials Design section showed how a novel material had been not only designed using ab initio calculations but how the same calculations helped to guide the fabrication process for this new material and were also used to demonstrate a wider range of improved properties possessed by the new material. The second talk showed how a data led approach based on the application of advanced neural networks and taking companies existing data sets had successfully predicted materials with improved properties. A particularly interesting feature of this talk was the ability of this advanced neural network approach to fill in missing data in datasets – a feature that is particularly relevant for materials data, which are rarely complete.

The emerging technologies talks covered a number of methods that should become important tools for materials modelling with a strong emphasis on machine learning approaches. The talks emphasised that many materials properties require large numbers of modest size calculations that collectively require peta to exascale resources; owners of such resources should be made aware of such needs.

The 'Poacher turned Gamekeeper' session reiterated many of the points raised in the Industry talks but also clearly demonstrated how the value of materials modelling was, in these cases, only realised when these tools were integrated into the entire design process. This is something that academics cannot do alone and, hence, there is a significant challenge to making a real economic impact from academic research unless it leaves the academic sphere. There was some related discussion about Open Source software; there was a view that very few companies would use Open Source software though they would be willing to use a supported version of the same software.

3 Community needs

The Materials Modelling Initiative session showed just how large an investment is being made in research in this field. Most of the initiatives are under pressure to show industry engagement and take up. In some cases, this is with a view to creating long term sustainable efforts – a goal that, historically, has rarely been fulfilled.

There was a general feeling that there are many initiatives in this area on the academic side. There is also a profusion of computational resources becoming available though there are issues about the suitability of proposed exascale machines for running most materials codes. At the meeting, the industrial participants were asked whether they felt that exascale machines (as opposed to exascale resources) were of interest to them and the answer was universally 'no'. The issues in this area focussed around two major subjects;

1. In every example of significant impact of materials modelling presented at the meeting, the role of the Translator was seen as absolutely crucial. There was significant concern that even at companies where very successful materials modelling project had run, subsequent re-organisations had often led to the loss of such translators and/or the loss of critical mass in materials modelling

2. Despite (or because of) the large number of well-funded research projects in this area, there is a problem of lack of connectivity and continuous re-invention of the wheel many times over. This is wasteful of resources but, particularly on the data/informatics side it is positively dangerous as it significantly reduces the possible impact of big data – particularly in a field where the amount of data available is very modest bearing in mind the complexity of materials space.

4 Funding

As mentioned previously, this field of research is very well supported in academia with numerous initiatives. It was encouraging to hear that the European Materials Modelling Council had recognised the role of the translator and that there will probably be an EC call for funding in this area in due course. However, it is important that any such call is inclusive and does not just fund a tiny fraction of the community of translators. It was agreed that it is important to provide more easily accessible case studies of successful materials modelling projects which could be used to encourage further adoption of such methods in industry. Along similar lines, it was pointed out that providing Cloud access to materials modelling tools could have a significant impact in allowing companies to experiment with these tools without incurring a significant start-up cost.

5 Will these developments bring societal benefits?

Just the small number of examples presented at this meeting give some indication of the potential impact of materials modelling though the fact that significant gains require a broad raft of tools and methods means that it is difficult to quantify the benefits that result from any one method alone. However, it is stated that Ford's 'Virtual Aluminum Castings' project has provided $millions of benefits to the Company and it was also stated that materials modelling has played a significant role in the continuation of Moore's Law for at least the last decade.

If we were truly to realise the promise of 'From the atom to the material' the economic benefit would be many $billions per year with numerous further benefits, such as reduction of toxicity. However, this goal is still many years away. There was a general consensus at the meeting that even with its current limitations, materials modelling has significant economic impact (as evidenced in the various reports from Goldbeck Consulting) and that this impact would be much higher if more companies used this modelling where appropriate – common problems being that too often companies do not know when modelling is appropriate and that academics are prone to overselling their methods and do not give sufficient advice about which methods are appropriate.

6 Participant list

Organizers

Milman, Victor
BIOVIA, United Kingdom

Payne, Mike
University of Cambridge, United Kingdom

Bonella, Sara - EPFL, Switzerland

Collins, Ian - BP, United Kingdom

Conduit, Gareth - Cambridge University, United Kingdom

Csanyi, Gabor - University of Cambridge, United Kingdom

Curtin, William - Swiss Federal Institute of Technology of Lausanne (EPFL), Switzerland

de Gironcoli, Stefano - International School for Advanced Studies (SISSA) and CNR-DEMOCRITOS IOM, Trieste, Italy

Dellago, Christoph - University of Vienna, Austria

DENNIS-SMITHER, Benjamin - BP, United Kingdom

Ghiringhelli, Luca M. - Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany

Goldbeck, Gerhard - EMMC/Consultant Goldbeck Consulting, United Kingdom

Hytha, Marek - Atomera, USA

Kyoung, Woomin - Hyundai Motor Company, South Korea

Marzari, Nicola - Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Petit, Leon - Daresbury Laboratory, United Kingdom

Probert, Matt - University of York, United Kingdom

Quigley, David - University of Warwick, Coventry, United Kingdom

Rugg, David - Rolls-Royce plc, United Kingdom

Sadasivan, Shankar - Harvard University, USA

Shenai, Pratamesh - Shell, India

Stan, Marius - Argonne National Laboratory, USA

Tildesley, Dominic - E-CAM, United Kingdom

Todd, Stephen - Biovia, United Kingdom

Vitale, Valerio - University of Cambridge, United Kingdom

Wolverton, Chris - Northwestern University, USA

Ab initio Spin-orbitronics

Location: The conference will take place at Hotel Promenade in Montesilvano, Pescara (Italy)
Webpage: https://www.cecam.org/workshop-0-1492.html
Dates: September 25, 2017 to September 29, 2017

1 State of the art

The main purpose of this Psi-k/CECAM research conference (with about 120 participants) has been to highlight the very recent theoretical and computational developments related to the interplay of spin-orbit interaction with electronic structure, magnetism, transport as well as its link to strongly correlated materials and ultrafast currents in diverse materials. We have focused on discussing spin-orbit coupling (SOC) as a means of engendering fundamentally novel physical phenomena in exotic systems. The Conference therefore spanned several research dimensions, ranging from Materials (in the form of bulk compounds, surfaces and interfaces, thin films and heterostructures) to Functionalities (associated with topology, spin-momentum locking, valley degrees of freedom, skyrmions, coupling to electric currents by Berry phases, etc.) to method developments (in terms of dynamical processes in out-of-equilibrium quantum matter, Berry phase physics, etc). A brainstorm about concepts and ideas in a little understood phenomenon, such as orbital magnetization, was carried out under the guidance of Prof. Ivo Souza. While the main focus was on ab initio simulations, a few leading scientists in experiments were invited (Prof. Stuart Parkin, Prof. Claudia Felser, etc) and a strong interface to many-body physics treated on the basis of realistic model Hamiltonians was included.

2 Major outcomes

The 10 major scientific points discussed at the meeting were addressed in the corresponding sessions (for all of them, a comprehensive view of the state-of-the-art as well as of the most promising perspectives were given): 1) Topological solids, with talks given by S. Murakami, B. Yan and O. Yazyev, tackling mostly topological semimetals, in terms of symmetry,

topology, and related emergent phenomena; the session also focused on Berry phase related physics and the spin current in antiferromagnetic Weyl semimetals, as well as High-throughput search for novel materials realizing topological electronic phases. 2) Complex magnets, where C.Felser discussed non-collinear spin structures and skyrmions in topologically non-trivial Heusler compounds and T. Jungwirth focused on antiferromagnetic spintronics; 3) Ultra-fast magnetism with talks given by P.Elliott (replacing S. Sharma), focused on ab-initio approaches to all-optical ultrafast switching of magnetic order and by P. Oppeneer, presenting a Theory of ultrafast laser-induced magnetic processes; 4) Two-dimensional spin-orbit solids, where E.Chulkov discussed mainly Quantum spin and anomalous Hall effects in topological insulators (for example prototypical Bi2Te3 doped with magnetic impurities) and V. Pardo focused on rutile-based superlattices, with emphasys on spin-orbit effects and non-trivial topological properties; 5) Chiral magnets in which L. Szunyough addressed chiral spin-textures in nanomagnets, B.Dupé addressed the physics of Skyrmions in 3d-5d metallic multilayers and R. Arita put forward a new order parameter, cluster multipole, to characterize anomalous Hall effects in antiferromagnets; 6) Correlation, cooperative phenomena and SOC, where J. van den Brink addressed the “effective J-half” physics in iridates and potential Kitaev spin-liquids, as recently discussed in RuCl3 , K. Yamauchi focused on the coupling between ferroelectricity, spin texture, and topological properties in transition-metal oxides, with emphasys on novel multiferroics and N. Kioussis addressed topological effects in chalcogenides-based alloys and heterostructures. 7) Theory of spin-orbit torque, where M. Stiles addressed spin-orbit torques from different modeling points of view (ranging from classical to semiclassical to first-principles approaches), F. Freimuth described the formalism developed to treat Dzyaloshinskii-Moriya interaction and spin-orbit torques in noncollinear magnets from first-principles density-functional theory and B. Nikolic discussed spectral functions and spin textures in magnetic heterostructures to get hints on the physics related to spin-orbit torque; 8) Dynamical spin excitations were addressed by M. dos Santos Dias focusing on time-dependent density functional theory simulations to treat Dynamical spin excitations in magnetic nanostructures and by A. Bergman to discuss the theoretical formalism (within atomistic spin dynamics) and results for magnetic excitations in low-dimensional and complex systems; 9) round table on (little understood) Orbital magnetism, magnetoelectric response and related “Berry-ology” (with large and active participation by the audience) and 10) Theory of spin transport, where J. Zelezny (replacing S. Sanvito) discussed calculation of spin-Hall conductivity in topological materials, P. Kelly focused on spin transport from fully relativistic scattering theory at finite temperatures and A. Mook presented his activity on the development of the formalism, related implementation and simulations in the field of Spin and heat transport by magnons.

3 Community needs

In terms of computational infrastructures, we remark that the community has recently invested sizeable efforts - and plans to invest in the future - on the development of first-principles codes to implement recently proposed spin-orbit-related features (i.e. to evaluate Dzyaloshinskii-

Moriya interaction, various Hall conductivities, topological invariants, magnetic excitations, etc). In terms of HPC resources, some of the simulations (presented at or stimulated by the conference, such as for example the evaluation of symmetric and anti-symmetric exchange coupling constants within perturbation theory) certainly require the availability of massive grants at HPC supercomputing centers. The “ab-initio Spin-orbitronics” community is overall well connected to other closely-related communities, such as experimentalists and various theoreticians, ranging from those working on many-body to phenomenological Hamiltonian-modelling to micromagnetic simulations. However, the field is so fastly growing that concerted interdisciplinary efforts need to be carried out at all levels; to this end, a better integration with close communities has definitely to be encouraged, including the interface to industrial partners possibly interested in spin-orbitronics.

4 Funding

Typical funding channels in “Ab-initio spin-orbitronics” are available at the European level in the H2020 program (in closer detail, within open-FET – Future and Emerging Technology - calls and within the European Research Council, ERC). We note that several FET and ERC grants were recently awarded in the “spin-orbitronics” field. At the national scale the situation is quite heterogeneous. We however note that especially in Germany, several initiatives adequately took into account topics of interest for the community, such as topological matter, spintronics, spin-orbitronics. Many possible collaborations and perspectives for joint applications in the upcoming H2020 calls were discussed among Conference attendees.

5 Will these developments bring societal benefits?

Information and communication technology in charge-based electronics is rapidly approaching the limits in terms of capacity, speed, as well as energy consumption. Novel paradigms based on spin, topology and electronic correlations (all topics largely discussed at the conference) are appearing as future ingredients to efficiently store and process information. Further promising directions are represented by possible energy efficiency achieved by exploiting multifunctional materials (such as multiferroics) and by the integration of memristive functions based on metal oxides and chalcogenides (i.e. “spin-orbit-active” materials) in view of applications as memory and logic devices and neuromorphic computing. In this framework, the spin-orbitronics field is relatively young and efforts need to be put in the

coming years on the understanding of basic physics and related microscopic mechanisms underlying exotic phenomena occurring in spin-orbit materials. To this end, first-principles simulations, in parallel with developments of theoretical formalisms (especially in subfields such as spin-dynamics, spin-transport, magnetoelectric responses, etc) and their related implementation in existing DFT codes, appear of paramount importance.

6 Participant list

Organizers

Blügel, Stefan
Forschungszentrum Jülich, Germany

Mertig, Ingrid
Martin Luther University Halle, Germany

Picozzi, Silvia
Consiglio Nazionale delle Ricerche CNR-SPIN, Chieti, Italy

Khmelevskyi, Sergii - Center for Computational Materials Science, Austria

Achilli, Simona - Università degli Studi di Milano, Italy

Alippi, Paola - CNR-ISM, Italy

Arita, Ryotaro - RIKEN, Japan

Artyukhin, Sergey - Italian Institute of Technology, Italy

Autieri, Carmine - CNR-SPIN, Italy

BAADJI, Nadjib - DÃ©partement de Physique, UniversitÃ© de M''sila , Algeria

Barati, Ehsan - University of Twente, The Netherlands

Barone, Paolo - CNR-SPIN, Italy

Bergman, Anders - Department of Physics and Astronomy, Uppsala University, Sweden

Bihlmayer, Gustav - Forschungszentrum Jülich, Germany

Blonski, Piotr - Regional Centre of Advanced Technologies and Materials and Palacky University in Olomouc, Czech Republic

Borge de Prada, Juan - Universidad del Pais Vasco, Spain

Bragato, Marco - Università degli Studi di Milano, Italy

BRUYER, Emilie - Institute of Physics of the Czech Academy of Sciences, Czech Republic

Buhl, Patrick M. - Forschungszentrum Jülich, Germany

Cardias, Ramon - Uppsala University/Federal University of Pará, Sweden

Cargnoni, Fausto - CNR - Istituto di Scienze e Tecnologie Molecolari, Italy

Ceresoli, Davide - CNR-ISTM, Italy

Chakraborty, Jayita - IISER Bhopal, India

Chang, Po-Hao - Univ. of Nebraska-Lincoln , USA

Chulkov, Eugene - University of the Basque Country, San Sebastián, Spain

Cuoco, Mario - CNR-SPIN, Italy

DAHANI, Ameur - Laboratory of computational material physics (LPCM), Algeria

Di Marco, Igor - Uppsala University, Sweden

Di Sante, Domenico - Institute für Theoretische Physik und Astrophysik, University of Würzburg, Germany

Dine, Khaled - Technology faculty - University of Saida , Algeria

Djani, Hania - centre de developement des technologies avancées, Algeria

DJERMOUNI, Mostefa - Computational Material Physics Laboratory, Algeria

Dolui, Kapildeb - University of Delaware, USA

dos Santos Dias, Manuel - Forschungszentrum Juelich, Germany

Dupé, Melanie - Johannes Gutenberg Universität, Institute of Physics, Germany

Dupé, Bertrand - Johannes Gutenberg University, Germany

Elliott, Peter - Max Planck Institute of Microstructure Physics, Germany

Fechner, Michael - Max Planck Institute for the structure and dynamics of matter, Germany

Felser, Claudia - Max Planck Institute Chemical Physics of Solids, Dresden, Germany, Germany

Fiorentini, Vincenzo - Cagliari University, Italy

Freimuth, Frank - Research Center Juelich, Germany

Frost, Jarvist Moore - Imperial College London, United Kingdom

Fu, Huixia - Institute of Physics, Chinese Academy of Sciences , China

Ganguli, Nirmal - IISER Bhopal, India

Gao, Heng - Shanghai University, China

Garcia Castro, Andres Camilo - Université de Liège, Belgium

Gayles, Jacob - Max-Planck Institute Dresden, Germany

Ghimire, Madhav Prasad - IFW-Dresden, Germany

GOVINDAN, SARAVANAN - DEPARTMENT OF NUCLEAR PHYSICS, UNIVERSITY OF MADRAS, India

Guerra, Delia - Università degli studi di Salerno, Dipartimento di Fisica "E:Caianiello", Italy

Gupta, Kriti - University of Twente, The Netherlands

Haldar, Soumyajyoti - Christian-Albrechts-Universität zu Kiel, Germany

Hanke, Jan-Philipp - Forschungszentrum Jülich, Institute for Advanced Simulation, Germany

Heiliger, Christian - University of Giessen, Germany

Hu, Shunbo - shanghai university, China

Jia, Fanhao - Shanghai University, China

Johansson, Annika - Max Planck Institute of Microstructure Physics, Germany

Jungwirth, Tomas - Institute of Physics ASCR, Prague and University of Nottingham, Czech Republic

Kanga, N'goye Bre-Junior - Laboratoire physique des hautes énergie Modélisation et simulation, Morocco

Katsumoto, Hiroshi - Osaka University, Japan

Kelly, Paul - Computational Materials Science, Faculty of Science and Technology, University of Twente , The Netherlands

Kioussis, Nicholas - Department of Physics/California State University Northridge, USA

Lafargue-Dit-Hauret, William - ISCR UMR CNRS 6226 Université de Rennes 1, France

Lamari, Saadi - Universite Ferhat Abbas -Setif 1, Algeria

LAREF, Slimane - King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Saudi Arabia

Lazar, Petr - Department of Physical Chemistry, Palacký University Olomouc, Czech Republic

Lima Fernandes, Imara - Forschungszentrum Jülich GmbH, Germany

Lounis, Samir - Jülich Research Centre, Germany

Lux, Fabian Rudolf - FZ Jülich / PGI-1, Germany

Marmolejo-Tejada, Juan - Universidad del Valle, Colombia

Meyer, Sebastian - Christian-Albrechts-Universität zu Kiel, Germany

Ming, Xing - College of Mathematics and Physics, Huanggang Normal University, China

Mokrousov, Yuriy - Forschungszentrum Jülich, Germany

Momida, Hiroyoshi - Osaka University, Japan

Mook, Alexander - Max Planck Institute of Microstructure Physics, Germany

Müller, Tristan - Max-Planck-Institute for Microstructure Physics, Germany

Murakami, Shuichi - Department of Physics and TIES, Tokyo Institute of Technology, Tokyo 152-8551, Japan, Japan

Nawa, Kenji - Mie University, Japan

Nikolic, Branislav - University of Delaware, Newark, USA

Niu, Chengwang - Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

Nordström, Lars - Uppsala University, Sweden

Oppeneer, Peter - Uppsala University, Sweden

Palotas, Krisztian - Institute of Physics, Slovak Academy of Sciences, Slovakia

Pardo, Victor - Universidade de Santiago de Compostela, Spain

Parkin, Stuart - Max Planck Institute of Microstructure Physics and Martin Luther University Halle-Wittenberg, Germany

Pentcheva, Rossitza - University of Duisburg-Essen, Germany

Petrovic, Marko - University of Delaware, USA

Ponet, Louis - Istituto Italiano di Tecnologia, Scuola Normale Superiore di Pisa, Italy

Pradipto, Abdul Muizz - Kyoto University, Japan

Rauch, Tomas - MLU Halle-Wittenberg, Germany

Ren, Wei - Shanghai University , China

Risius, Philipp - Institute for Theoretical Physics, University of Giessen, Germany

Rocquefelte, Xavier - ISCR UMR CNRS 6226, France

Sacksteder, Vincent - Royal Holloway University London, United Kingdom

Sanvito, Stefano - Trinity College Dublin, Ireland

Sasidharan Nair, Rohit - University of Twente, The Netherlands

Sasioglu, Ersoy - Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Germany

Schleife, Andre - University of Illinois at Urbana-Champaign, USA

Sharma, Sangeeta - Max Planck Institute of Microstructure Physics, Germany

Singh, Sobhit - Physics and Astronomy Department, West Virginia University, USA

Slawinska, Jagoda - Consiglio Nazionale delle Ricerche, Italy

Smejkal, Libor - Uni Mainz, Germany

Soave, Raffaella - ISTM-CNR, Italy

Soriano, David - International Iberian Nanotechnology Laboratories (INL), Portugal

Souza, Ivo - University of the Basque Country, San Sebastián, Spain

Souza Mendes Guimaraes, Filipe - Forschungszentrum Jülich, Germany

Staunton, Julie - University of Warwick, United Kingdom

Stiles, Mark - National Institute of Standards and Technology, USA

Stroppa, alessandro - CNR-SPIN, Italy

Szilva, Attila - Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden

Szunyogh, Laszlo - Budapest University of Technology and Economics, Hungary

Trioni, Mario Italo - CNR-ISTM, Italy

Turek, Ilja - Institute of Physics of Materials, Academy of Sciences, Czech Republic

van den Brink, Jeroen - IFW Dresden, Germany

Wehling, Tim O. - University of Bremen, Germany

Woźniak , Tomasz - Department of Theoretical Physics, Wrocław University of Science and Technology , Poland

Yamauchi, Kunihiko - ISIR-Sanken, Osaka University, Japan

Yan, Binghai - Weizmann Institute of Science, Israel

Yazyev, Oleg - Swiss Federal Institute of Technology Lausanne , Switzerland

Zanolli, Zeila - RWTH Aachen University, Germany

Zelezny, Jakub - Institute of Physics AVCR, v.v.i., Czech Republic

International Workshop on ‘New challenges in Reduced Density Matrix Functional Theory: Symmetries, time-evolution and entanglement'

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1448.html

Dates: September 26, 2017 to September 29, 2017

1 State of the art

Since electrons interact only pairwise by Coulomb repulsion, the energies and other electronic properties of atoms and molecules can be computed directly from the two-electron reduced density matrix (2-RDM), only. "Banishing" this way the N-electron wave function with its exponentially many degrees of freedom, the entire quantum problem can be recast in the form of a very simple linear functional on the 2-RDM. However, the description of the 2-electron picture involves highly nontrivial representability conditions, and new approaches of the reduced electron pictures need to be explored. The most successful one so far is Density Functional Theory (DFT), an approach based on the Hohenberg-Kohn and Kohn-Sham theorems. Although DFT has seen a tremendous success in many-body physics, the search for accurate functionals has suffered from an intrinsic difficulty: not only the exact functional for the exchange-correlation is unknown but also the one for the kinetic energy. In 1975, Gilbert established in the form of "Reduced Density Matrix Functional Theory" (RDMFT) a natural extension of DFT. RDMFT exploits the 1-electron picture by seeking a functional on the whole 1-electron reduced density matrix (1-RDM). The big advantage compared to DFT is that the kinetic energy can be described in an exact way and any scientific effort can be solely spent on improving the exchange-correlation functional. In contrast to the 2-electron picture, the representability conditions for the 1- RDM are known. While DFT resorts to a large zoo of hundreds of engineered density-functionals only about a dozen of 1-RDM-functionals have been proposed so far. Remarkably, those few and less developed functionals already allowed one to describe closed-shell systems with accuracies higher by one order of magnitude than DFT. Moreover, RDMFT has succeeded in predicting more accurate gaps of conventional semiconductors than DFT does and has demonstrated insulating behavior for Mott-type insulators.

2 Major outcomes

This international interactive workshop discussed and explored new aspects and open challenges in RDMFT, such as:

(1) new insights about RDMFT from recent progress on the 1- and 2-body N-representability problems,

(2) new insights from finite uniform electron gases, random phase approximation, and exact systems,

(3) implementation of 1-particle symmetries and translational invariance,

(4) extension of RDMFT to open-shell molecules, finite temperatures, and time evolution,

(5) electronic correlations, entanglement, and recent developments on fermionic orbital optimization, and

(6) separation and quantification of dynamic and static electronic correlations.

Among the major outcomes and new results, we can mention:

1. New functionals: in the last years, much effort has been put in finding new functionals and new observable functionals, such as ionization/affinity energies and spectral functions. Some outcomes are promising, but there is a clear need of a more universal functional, in particular for solids. In the traditional RDMFT, a major development at the workshop was a new functional of the PNOF family, namely, PNOF7.

2. Electronic correlations: There is also a quest for a better definition of correlation, from an intuitive point of view but also from a quantitative one. In this vein, it is quite promising the ability of RDMFT to capture static electronic correlation.

3. New developments: RDMFT served at the workshop as a springboard to ab initio development, such as turning density matrix renormalization group (DMRG) theory to a mathematically advanced version of multi-configuration self-consistent field (MCSCF) approach. There was also an important discussion on the idea of using the adiabatic connection ERPA (AC-ERPA) for DMRG between Ors Legeza and Kasia Pernal that has triggered a joint on-going collaboration.

4. Simplification of the orbital self-consistent field equation in case of symmetries: we discussed the recent work in finding the correct ground-state properties of transition metal

oxides (TMO). The good news is: RDMFT is able to capture the correct insulating state of TMO under ambient conditions. As well, away from ambient pressure, RDMFT correctly captures the physics of the insulator-metal phase transition. The bad news is that the minimization process in RDMFT must be upgraded in order to be used in infinite systems, for it is not fast enough to beat DFT or Hartree-Fock.

3 Community needs

RDMFT still needs a standard software to carry out calculations with the most recent energy functionals as well as an efficient implementation. In particular, there is a clear need for open codes to be shared by the members of the community. A good idea to start with is to establish a library of codes to test, use and improve current functionals.

Some participants pointed out the need for a major synergy in order to, working together, generate a reliable and fast code for RDMFT calculations which can later be included in usual available codes. Although it is quite promising the application of RDMFT in solids, it can only be done by improving the actual speed of the convergence.

A series of CECAM workshops on the topic of RDMFT should be considered as a meaningful vital alternative to, on the one hand, thoughtless empirical fitting of zillion of the parameters in density functional theory (DFT) and, on the other hand, to a too stiff algorithm crunching in the current ab initio theory.

4 Funding

Discussion of joint research proposals as well as to schedule more frequent workshops were, certainly, the most important outcomes of the present workshop.

There are now some groups working on RDMFT which could benefit a lot from stronger collaborations. As well, the community could benefit from a close collaboration with other communities, especially from the scientists working with 2-body reduced density approaches.

CECAM and Psi-k would probably invest money in the community. In particular, to enhance the strength of the collaborations.

5 Will these developments bring societal benefits?

Well, as all theoretical developments, societal benefits are not immediate. We all know how much important theory is for everyday life, even if its impact is not immediately tangible. However, since RDMFT explains metals and their oxides properties much better than DFT, this can lead to their higher demand in industrial research. In this latter sense, the cooperation with industry can speed up the research in solids and translational-invariant systems within RDMFT, which ultimately can alleviate, if not solve, the problem of convergence in RDMFT real calculations.

The present and similar workshops serve as a much-needed antidote to the current retreat of the academic spirit of sheer human curiosity under the outrageous pressure of the business-like approach to science.

Overall, this international conference was an interesting and stimulating meeting of scientists working in different areas of physics and chemistry connected with or inspired by reduced density matrices. It was, by and large, a great opportunity to discuss and point out new challenges for RDMFT. We hope this meeting will prompt the community to pursue new collaborations, boosting the versatility, development, and applications of RDMFT.

Some of the participants mentioned the possibility of another such meeting in two or so years, and we strongly hope that it can be repeated in the near future.

6 Participant list

Organizers

Benavides-Riveros, Carlos L.
Martin-Luther-Universität Halle-Wittenberg, Germany

Gross, Eberhard K.U.
Max Planck Institute of Microstructure Physics, Halle, Germany

Marques, Miguel
Martin-Luther-Universität Halle-Wittenberg, Germany

Schilling, Christian
University of Oxford, United Kingdom

Ayers, Paul - McMaster University, Canada

Banafsheh, Mojdeh - University of Geneva, Switzerland

Bano, Amreen - Barkatullah University, Bhopal, India

Berakdar, Jamal - Martin-Luther University Halle-Wittenberg, Germany

Buchholz, Florian - MPI for the Structure and Dynamics of Matter, Germany

Chiarotti, Tommaso - École Polytechnique Fédérale de Lausanne, Switzerland

DePrince, Eugene - Florida State University, USA

Donsa, Stefan - Technical University Wien, Austria

Gidopoulos, Nikitas - Durham University, United Kingdom

Giesbertz, Klaas - Vrije Universiteit Amsterdam, The Netherlands

Gill, Peter - Australian National University, Australia

Gonçalves Marques, Mário Rui - Martin-Luther-Universität Halle-Wittenberg, Germany

Gritsenko, Oleg - Vrije Universiteit Amsterdam, The Netherlands

Helbig, Nicole - Forschungszentrum Juelich, Germany

Hollett, Joshua - University of Winnipeg, Canada

Huran, Ahmad - Martin-Luther-Universität Halle-Wittenberg, Germany

Jafari, Homayoun - Iran University of Science and Technology, Iran

Knowles, Peter - Cardiff University, United Kingdom

Krumnow, Christian - Freie Universität Berlin, Germany

Lathiotakis, Nektarios - Theoretical and Physical Chemistry Institute Athens, Greece

Legeza, Ors - Hungarian Academy of Sciences, Hungary

Matito, Eduard - Ikerbasque, Basque Science Foundation, Spain

Mauser, Norbert - Wolfgang Pauli Institute, Austria

Mirza, Wasif Baig - J. Heyrovsky Institute of Physical Chemistry, Czech Republic

Mitxelena, Ion - Universidad del País Vasco-Euskal Herriko Univertsitatea and Donostia International Physics Center, Spain

Pastorczak, Ewa - Technical University of Lodz, Poland

Pernal, Kasia - Technical University of Lodz, Poland

Piris, Mario - University of the Basque Country, Spain

Risueño, Pablo - University of Hamburg, Germany

Rodríguez Mayorga, Mauricio Antonio - Universitat de Girona, Spain

Romaniello, Pina - University Paul Sabatier, France

Savin, Andreas - University Pierre and Marie Curie, France

Schade, Robert - TU Claustahl, Germany

Schmidt, Jonathan - Martin-Luther-Universität Halle-Wittenberg, Germany

Sharma, Sangeeta - Max Planck Institute of Microstructure Physics, Germany

Theophilou, Iris - MPI for the Structure and Dynamics of Matter, Germany

van Meer, Robert - RIKEN Advanced Institute for Computational Science, Japan

Disordered protein segments: revisiting the structure-function paradigm

Location: CECAM-FR-MOSER, Institut Henri Poincaré, Paris, France.
Webpage: https://www.cecam.org/workshop-0-1373.html
Dates: October 3, 2017 to October 6, 2017

1 State of the art

The structure-function relationship has represented a powerful paradigm for the study of macromolecules and their association for more than three decades. Yet, pioneering studies on intrinsically disordered proteins (IDP) or protein segments (IDS) have revealed that neither the organization in structured folds nor the establishment of stable interactions are always necessary for molecular association involving IDPs or IDSs to take place. These emerging phenomena are highly heterogeneous, ranging from stable interactions resulting from disorder to order transitions, to fuzzy interactions involving conformational ensembles. Furthermore, IDS-containing proteins can simultaneously present globular folds, which are central to the structure-function paradigm, and the most extreme cases of disorder.

Such situations are found for proteins containing disordered terminal or regional segments or flexible loops or linkers of various lengths. Linkers are essential agents of the ubiquitous modular reorganization of protein domains upon binding, while disordered loops enable interface remodeling in response to a variety of partners. While this generally results in these segments presenting a stable structure in the complex, terminal or regional protein segments can remain completely disordered even when the protein is embedded in large macromolecular assemblies. They can often be highly charged and play a fundamental part for aggregating associated proteins or even for the control of the superstructure assembly itself, in ways that escape the structure-function paradigm. An intermediate situation between disorder to order transition and completely disordered segments is encountered when specific binding motifs are embedded in disordered segments. The IDPs can then act as control moieties for network hubs or scaffolding.

2 Major outcomes

IDPs and IDSs are now recognized as key players in the cell machinery, notably as mediator or modulator of macromolecule interactions or as signaling hubs. This opens a new area of research where the classical structure function paradigm comes short. The purpose of this meeting was to push further our understanding of the role of disorder in biological processes, by bringing together IDP experts from various experimental and theoretical fields of

research. For this workshop, we particularly focused our attention on the interplay between order and disorder, which can be found within single proteins, playing prominent roles in mediating dynamic interactions, notably via the presence of binding motifs embedded in IDPs.

The meeting highlighted the following key issues for current and future studies

- The sequence dependency of the dynamic behavior of IDSs; this includes the identification of relevant descriptors of the physicochemical and dynamics characteristics of IDPs that can be related to their sequence and interactions
- Intramolecular interactions between folded protein regions and their disordered segments; interplay – and competition - between intramolecular and intermolecular interactions; stable versus dynamic interactions; IDSs may alternate between intra-inter-protein interactions when mediating protein assemblies: how can this phenomenon influence the protein aggregation process?
- How do protein disordered segments control aggregation processes, leading to specific superstructure architecture? What are the roles of entropy and kinetics in the aggregation process?
- The experimental characterization of the dynamics of disordered protein segments; the identification of contact patterns between folded and disordered regions within a protein or between two protein partners. Novel experimental approaches including e.g. mass spectrometry for ensembles
- The prediction of contact motifs via bioinformatics methods; how does context contribute?
- The development of theoretical methods to characterize IDSs disorder and to generate meaningful conformational ensembles for these systems. This question is being tackled by several leading groups who develop advanced algorithms and new all-atom physical models specifically adapted to addressing IDP dynamics.
- The effect of ionic environment in modulating IDS properties and interactions. Can the specific binding of ionsfavor disorder to order transitions? Do ions explicitly participate to regulation processes together with IDSs?

This interdisciplinary workshop brought together experts from both experimental and theoretical fields of research who

gave high-level lectures of excellence and the meeting favored extensive exchange between the participants during two

poster sessions, with 14 poster presentations covering novel and combinatory aspects of IDPS characterization (both

experimental and theoretical), and addressing issues such as conformational ensembles generation, interactions between

proteins presenting disordered regions, using single-molecule studies, biophysical studies, molecular and coarse grained

simulations of IDPs and IDRs, bioinformatics analyses, and biological data.

A final round table summarized the workshop and opened new perspectives for the modeling of IDSs. In addition to the 19 invited speakers talk, 6 slots in the program were reserved for contributions from younger participants (postdocs) that were selected from submitted abstracts. The effort to set up a gender balanced list for the invited speakers was also noticed and highly appreciated by the participants.

3 Community needs

Diversity of experimental approaches for IDPs/IDSS studies

The workshop highlighted the large number of experimental techniques (such as e.g. NMR, EPR and circular dichroism spectroscopies, mass spectrometry, AFM, FRET, and SAXS) that are available to retrieve information regarding what is also referred to as the Dark Proteome (1), i.e. the fraction of the proteome that cannot be characterized by the traditional methods of structural biology (such as X-ray crystallography). Experimental data can give us information about the structure and dynamics of disordered systems (2), but also on how they are likely to interact. In particular, experimental results presented during the workshop clearly showed how disorder is an essential aspect of protein function, and many disordered protein regions are involved in the regulation of biomolecular interactions, including those with proteins, DNA, RNA and lipids)

4 Funding

A key issue regarding IDPs and IDSs for theoreticians is the generation of adequate conformational ensembles, which involves both producing structural pools for a given protein and determining a statistical weight for each of these structures (3, 4). This can be achieved by integrating the physical models used for the generation of the ensemble with data obtained

by experimental approaches (such as X-ray, NMR or cryo-EM). Another essential point for the proper modeling of proteins containing disordered segments is the development of force fields that are suitable both for the ordered and disordered fragments that can coexist in a single protein, or for proteins that will oscillate between ordered

and disordered states along time (5).

5 Will these developments bring societal benefits?

Most classical force-fields were developed for modeling folded, globular proteins,

which leads to a bias toward folded states when generating conformational ensembles via Molecular Dynamics simulations. In addition, ensembles generated for disordered systems turn out to be very sensitive to the force field used during the simulation (6). Another issue regarding current force-fields is the quality of ions modeling (which is still unsatisfying, in particular regarding multivalent ions), that plays an important role since disordered regions in proteins usually contain a large number of charged residues. Once again, the integration of experimental data is likely to be a central part in the development of suitable force-fields for these complex systems. Last but not least, accessing dynamic properties of disordered systems via simulations requires long timescale calculations that are still not always accessible. Possible approaches and developments for addressing these issues in future work were discussed throughout the workshop and in the final round-table session.

6 Participant list

Organizers

Ha-Duong, Tâp
BioCIS - Faculté de Pharmacie - Université Paris Sud, France

Kragelund, Birthe
University of Copenhagen, Denmark

Papaleo, Elena
Danish Cancer Research Center, Denmark

Prevost, Chantal
Laboratoire de Biochimie Theorique LBT - CNRS UPR 9080, France

Sacquin-Mora, Sophie
Laboratoire de Biochimie Théorique, CNRS-UPR9080, France

Schuler, Ben
University of Zurich, Switzerland

Ando, Toshio - department of Physics, Kanazawa University, Japan

Barran, Perdita - University of Manchester, United Kingdom

Barrera-Vilarmau, Susana - Institute of Advanced Chemistry of Catalonia - Spanish Council for Scientific Research, Spain

Belle, Valérie - CNRS UMR7281, Aix-Marseille University, France

Best, Robert - Laboratory of Chemical Physics, NIDDK, National Institutes of Health, USA

BOIRE, Adeline - INRA-BIA Nantes, France

Bonomi, Massimiliano - University of Cambridge, Department of Chemistry, United Kingdom

Callebaut, Isabelle - IMPMC, CNRS UMR7590, Université Pierre & Marie Curie, France

Chavali, Sreenivas - MRC Laboratory of Molecular Biology, Cambridge Biomedical Campus, United Kingdom

Cortés, Juan - LAAS-CNRS, France

Crehuet, Ramon - Institute of Advanced Chemistry of Catalonia IQAC - CSIC , Spain

Emperador, Agusti - Institute of Advanced Chemistry of Catalonia, CSIC, Spain

Estana, Alejandro - Laboratoire d''analyse et d''architecture des systèmes, CNRS UPR8001, France

Fuxreiter, Monika - University of Debrecen, Hungary

Gkeka, Paraskevi - Sanofi, France

Holehouse, Alex - Washington University in St. Louis, USA

HOLOGNE, Maggy - Université Lyon 1, France

Kadeřávek, Pavel - ENS - CNRS, France

Karttunen, Mikko - Dept. of Mathematics and Computer Science, Eindhoven University of Technology, Canada

Lambrughi, Matteo - Danish Cancer Research Center, Copenhagen, Denmark

Lee, Jennifer - NHLBI, National Institutes of Health, USA, USA

Lemke, Edward - EMBL, Heidelberg, Germany

Levy, Yaakov - Weizmann Institute of Science, Rehovot, Israel

Lindorff-Larsen, Kresten - University of Copenhagen, Denmark

Longhi, Sonia - CNRS UMR7257, Aix-Marseille University, France

Martin, Erik - St Jude Children's Research Hospital, USA

Mukhi, Nitika - University of Delhi, India

Nagy, Gabor - Max Planck Institute for Biophysical Chemistry, Germany

Nygaard, Mads - Danish Cancer Society Research Center, Denmark

Perez-Riba, Albert - University of Cambridge, United Kingdom

Rhoades, Elisabeth - Deparment of Chemistry, University of Pennsylvania, USA

Robustelli, Paul - D. E. Shaw Research, USA

SAHLI, Line - INRA, France

Sinnaeve, Davy - Ghent University, Belgium

Skovgaard Sørensen, Charlotte - Aarhus University, Denmark

Teixeira, João MC - BioNMR Laboratory, Inorganic and Organic Chemistry Department, Universitat de Barcelona, Spain

Tosatto, Silvio - University of Padova, Italy

van Heijenoort, Carine - ICSN, CNRS UPR2301, France

Veenhoff, Liesbeth - University of Groningen, The Netherlands

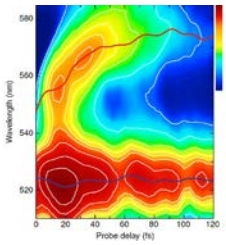
Vendruscolo, Michele - University of Cambridge, United Kingdom

Vranken, Wim - ULB-VUB - Interuniversity Institute of Bioinformatics in Brussels (IB)2, Belgium

WALKER, Olivier - Université de Lyon, France

Zosel, Franziska - Department of Biochemistry, University of Zurich, Switzerland

Charge carrier dynamics in nanostructures: optoelectronic and photo-stimulated processes



Location: University of Bremen
Webpage: https://www.cecam.org/workshop-0-1443.html
Dates: October 9, 2017 to October 13, 2017

1 State of the art

Advances of time-resolved experimental techniques, needed for a detailed understanding of charge carrier dynamics as they occur in real time, require matching progress in theoretical approaches. Applications to novel, emerging nanoscale materials, which ultimately lead to faster, more efficient and miniaturized devices, pose multiple theoretical challenges. Modeling time-resolved experimental data becomes a major goal of a theorist.

The proposed workshop became a forum to brainstorm ideas about solutions to important computational problems and identify new directions for time-dependant electronic structure method development and challenging applications. In this way, we have been able to create an exchange mechanism to unite a core of developers in an interactive environment, in order to initiate design of a new generation software tools for quantum modelling of realistic complex systems and nanostructures in electronic ground and excited states. The delivery of this technology to a broad community will facilitate breakthroughs on high-impact materials science problems.

We have been successful to achieve the following key objectives:

- Bring together researchers from experiment and theory working on time-dependent charge carrier dynamics related to optoelectronic and photo-stimulated processes, in order to highlight recent progress, and to discuss challenges and opportunities in the materials aspect of tailor-made nanostructures and hybrid interfaces for highly efficient energy applications.

- Foster the exchange of methodological expertise and new developments between scientists working on different aspects of charge dynamics at surfaces, interfaces, and in 2D-materials and hetero-structures.
- Discuss possibilities for optimizing the materials properties and device design. The interdisciplinary character of the workshop did help finding solutions for overcoming current limitations.
- The Workshop has provided opportunity to form new worldwide interdisciplinary co

2 Major outcomes

Currently, theoretical studies of light-induced processes at interfaces usually fall in one of two broad categories: i) modelling of the atomic structure and ground state electronic properties of complex interfaces and ii) simulation of light-matter interactions and electronic excited states in relatively simple systems. For example, several talks at the conference addressed the atomic surface structure of photocatalysts, such as titanium dioxide, and discussed the complex interaction of these surfaces with adsorbed atoms and molecules. Other talks addressed excited states of such photocatalysts with high-level methods, such as many-body perturbation theory. For a full understanding of photocatalysis and other light-induced processes at interfaces, it is necessary to combine these two aspects. We therefore expect and hope that in the near future more studies will attempt to bridge and connect these categories, i.e. simulate the interaction of light with matter at realistically complex systems.

For the light-matter interaction, there has been an increasing number of studies using the real-time formalism. These studies give important insights into the kinetics of light-induced processes at interfaces. However, the increased numerical effort of these simulations usually necessitates the use of approximate theories, such as time-dependent density-functional theory with its well-known limitations. Conversely, higher-level methods, such as quantum chemical wavefunction approaches or the Bethe-Salpeter equation, can only be applied with a linear-response framework. We expect that the next 2-3 years will see the transfer of high-level methods from the frequency-domain to the real-time domain. This would open up the description of exciton dynamics in heterogeneous systems, which are highly relevant to photocatalysis and photovoltaics.

Experiment

On the experimental side, the workshop has demonstrated enormous effort in the advancement of time-resolved experimental techniques probing the transient electronic structure after excitation of charge carriers with light or intense pulsed laser fields on nano- and attosecond scales.

- E.g., this includes the study of resonant energy transfer of triplet excitons from pentacene to lead selenide (PbSe) nanocrystals, where Akshay et al. [1] report on efficient resonant-energy transfer of molecular spin-triplet excitons from organic semiconductors to inorganic semiconductors. They use ultrafast optical absorption

spectroscopy to track the dynamics of triplets, generated in pentacene through singlet exciton fission, at the interface with PbSe nanocrystals.

- The direct imaging of microscopic structural changes on ultrafast time scales is another particular challenge in the natural sciences. Alongside ultrafast X-ray techniques, time-resolved electron microscopy, diffraction and spectroscopy yielded unprecedented insights into rapid physical, chemical and biological processes. Various incvited speakers in most recent years follow a variety of imaging approaches with ultrashort, highly coherent electron pulses to investigate the dynamics of ultrafast electronic and structural phenomena. Over the past few years, Feist and Schäfer et al. [2] have developed a novel implementation of Ultrafast Transmission Electron Microscopy ("UTEM"). The instrument employs a "pump-probe" scheme, in which two laser pulses are coupled into the column of a transmission electron microscope (TEM). A first laser pulse excites an electronic or structural change in the investigated sample. In a special photocathode, a second, delayed laser pulse generates an ultrafast electron pulse, which then probes the induced sample change in microscopy, diffraction or spectroscopy. By varying the relative pulse delay, the dynamics can be followed in time.
- Transition metal dichalcogenides (TMDs) are emerging as promising two-dimensional (2D) semiconductors for flexible optoelectronic, spintronic and photovoltaic devices. Their photophys

3 Community needs

A major obstacle to the accurate description of light-induced processes at interfaces is the intrinsic interdisciplinarity of the subject. The study of such processes requires knowledge of physics, chemistry, materials science and even biology. Therefore, advancing our understanding of photo-induced processes necessitates a joint effort from experts in different fields, including both experimental and computational studies. To enable such collaborations, it is of crucial importance to organize interdisciplinary workshops like ours to act as platforms for exchanging ideas and for bringing together researchers from different subject areas who work on different aspects of the same topic. In the future, we will try to continue organizing workshop to achieve this goal on a biannual basis.

The workshop became a forum to discuss about possible solutions of improving the quality of hybrid interfaces for studying real time electron dynamics and charge transfer reactions and correlating experiment and theory on a highly predictive level.

4 Funding

Progress in the field of many body physics, time-dependent electron dynamics and wave function based correlated quantum chemistry is fundamental to many European industries connected to high-tech materials design and device applications. Examples are

- Advanced hybrid photovoltaics
- Nanomaterials with vibronically-enhanced transport properties for improved photovoltaics or quantum sensing
- Photo-catalytic processes in energy storage and pollutant degradation
- Hybrid nano/bio-systems for medical applications
- Molecular scale electronic devices and quantum computing
- Single-defect-based quantum optical and spintronic sensors and devices
- Ultrafast switchable photonic devices operating at THz speed
- Bio-inspired sensor concepts for ultrasensitive detection of electric and magnetic fields.
- Such directions can be strengthened by focused research projects for the development of new materials and devices in key enabling technologies.

5 Will these developments bring societal benefits?

As discussed above, the advancement of theories of light-induced processes at interfaces requires the development of novel theories and codes which can i) capture the inherent complexity of realistic interfaces and ii) contain sufficiently accurate description of physico-chemical processes, including photon-electron interactions, electron-hole coupling, electron-phonon coupling, etc. The development of such theories and the resulting computer software will benefit the broad community of theoretical researchers, but also have important impacts on experimental studies and industry. However, to achieve this, a continued investment is required, as method and code development usually occur on a longer time scale compared to the study of applications. This also requires the training of masters and PhD students not only in physics, materials science or biology, but also in computer programming (including parallelization of software) and use of high-performance computing resources.

6 Participant list

Organizers

Frauenheim, Thomas
University of Bremen, Germany

Lienau, Christoph
University Oldenburg, Germany, Germany

Prezhdo, Oleg V.
University of Southern California, Los Angeles, USA

Yam, Chiyung
Beijing Computational Science Research Center, China

Andermatt, Samuel - Swiss Federal Institute of Technology Zurich, Switzerland

Appel, Heiko - Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Bahmani, Mohammad - University of Bremen, Germany

Bálint, Aradi - University of Bremen, Germany

Balzaretti, Filippo - University of Bremen, Germany

Bang, Junhyeok - Korea Basic Science Institute (KBSI), South Korea

Berges, Jan - University of Bremen, Germany

Blumberger, Jochen - University College London, United Kingdom

Bonafé, Franco - National University of Córdoba, Argentina

Bozzini, Benedetto - University of Salento , Italy

Bretscher, Hope L. - University of Cambridge, United Kingdom

Brixner, Tobias - University of Würzburg, Germany, Germany

Burghardt, Irene - Goethe University Frankfurt/Main, Germany, Germany

Carof, Antoine - Ecole Normale Supérieure, United Kingdom

Čerņevičs , Kristiāns - Jacobs University Bremen, Germany

Cerullo, Giulio - Polytechnic University of Milan, Italy, Italy

Chatterjee , Sangam - University of Giessen, Germany

Cheminal, Alexandre - University of Cambridge, United Kingdom

Chen, Guanhua - The University of Hong Kong, Hong Kong, Hong Kong

Cocker, Tyler L. - University of Regensburg, Germany

Cundiff, Steven T. - University of Michigan, USA

de Sio, Antonietta - University of Oldenburg, Germany

Deák, Peter - University of Bremen, Germany

Debnath, Arunangshu - Max Planck Institute for the Structure and Dynamics of Matter (MPSD) , Germany

Dumitrica, Traian - University of Minnesota, USA

Erben, Daniel - University of Bremen, Germany

Esteban Puyuelo, Raquel - Uppsala University, Sweden

Florian, Matthias - University of Bremen, Germany

Franco, Ignacio - University of Rochester, USA

Ghosh, Dibyajyoti - University of Bath, United Kingdom

Giannini, Samuele - University College London (UCL), United Kingdom

Goebel, Alexandra - Max Planck Institute for the Structure and Dynamics of Matter Hamburg, Germany

Golrokh Bahoosh, Safa - University of Konstanz, Germany

Gross, Eberhard K.U. - Max Planck Institute of Microstructure Physics, Halle/Saale, Germany

Groß, Lynn - University of Bremen, Germany

Groß, Petra - University of Oldenburg, Germany

Gupta, Verena - University of Bremen, Germany

Gütlein, Patrick - Technical University of Munich, Germany

Hartmann, Malte - University of Bremen, Germany

Hinrichsen, Ture - University of Cambridge, United Kingdom

Horsfield, Andrew P. - Imperial College London, United Kingdom

Huber, Bernhard - University of Würzburg, Germany

Huran, Ahmad - Martin-Luther-Universität Halle-Wittenberg, Germany

ismael, Ortiz Verano - National University of Colombia, Colombia

Jiang, Xiuyun - University College London, United Kingdom

Kamil, Ebad - University of Bremen, Germany

Kanai, Yosuke - University of North Carolina at Chapel Hill, USA

Karasch, Patrick - University of Bremen, Germany

Khalili, Khadijeh - Technical University of Denmark , Denmark

Khorasani, Elham - University of Bremen, Germany

Kleinekathoefer, Ulrich - Jacobs University Bremen, Germany

Koch, Tobias - University of Münster, Germany

Köhler, Christof - University of Bremen, Germany

Kuehn, Oliver - University of Rostock, Germany

Leitenstorfer, Alfred - University of Konstanz, Germany

Li, Donghai - University of Würzburg, Germany

Lischner, Johannes - Imperial College London, United Kingdom

Lorke, Michael - University of Bremen, Germany

Louie, Steven G. - University of California at Berkeley, USA

Madjet, Mohamed El-Amine - Hamad Bin Khalifa University, Doha, Qatar

Meziane, Mehdi - Univerity of Lyon 1, France

Mirbach, Philip - University of Bremen, Germany

Molina-Sánchez, Alejandro - University of Valencia, Spain

Molinari, Elisa - University of Modena and Reggio Emilia & CNR-NANO, Modena, Italy

Mukamel, Shaul - University of California, Irvine, USA

Niehaus, Thomas A. - Claude Bernard University Lyon 1, France

Pandya, Raj - University of Cambridge, United Kingdom

Perfetto, Enrico - National Research Council (CNR), Rome, Italy

Popescu, Bogdan S. - University of Delaware, USA

Popmintschev, Tenio - University of California, USA

Potthoff, Sebastian - University of Bremen, Germany

Rahman , Hasan - Jacobs University Bremen, Germany

Ramzan, Muhammad Sufyan - Jacobs University Bremen, Germany

Rao, Akshay - University of Cambrigde, United Kingdom

Rozzi, Carlo Andrea - National Research Council (CNR), Modena, Italy

Ryndyk, Dmitry A. - University of Bremen, Germany

Sánchez, Cristián G. - National University of Córdoba, Argentina

Sanyal, Biplab - Uppsala University, Sweden

Schäfer, Sascha - University of Oldenburg, Germany

Scholes, Gregory D. - Princeton University, USA

Schönhoff, Gunnar - University of Bremen, Germany

Schröter, Marco - University of Rostock, Germany

Schulze, Jan - University of Rostock, Germany

Shao, Bin - University of Bremen, Germany

Sommer, Ephraim - University of Oldenburg, Germany

Steinhoff, Alexander - University of Bremen, Germany

Steinke, Christina - University of Bremen, Germany

Stournara, Maria E. - Wiley VCH Verlag GmbHC. KGeA, Germany

Sundaraman, Ravishankar - Rensselaer Polytechnic Institute, USA

Sung, Jooyoung - University of Cambridge, United Kingdom

Syzgantseva, Olga - Swiss Federal Institute of Technology Lausanne, Switzerland

Tavernelli, Ivano - IBM Research-Zurich, Switzerland

Torun, Engin - University of Luxembourg, Luxembourg

Trabattoni, Andrea - Center for Free-Electron Laser Science-DESY, Germany

Tretiak, Sergei - Los Alamos National Laboratory, USA

Verma, Deepti - University of Minnesota, USA

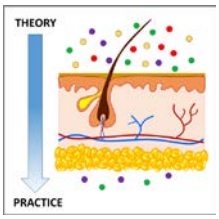
Verma, Sachin Dev - University of Cambridge, United Kingdom

Viñas Boström, Emil - Lund University, Sweden

Wehling, Tim O. - University of Bremen, Germany

Xian, Lede - Max Planck Institute for the Structure and Dynamics of Matter Hamburg, Germany

Insights into skin permeation: from theory to practice



Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1418.html
Dates: October 16, 2017 to October 18, 2017

1 State of the art

The topmost layer of the skin, the stratum corneum, comprises rigid non-viable corneocyte cells embedded in relatively rigid lipid multilayers. It is believed to provide the main barrier against passive permeation. There are three different routes for molecules to cross the stratum corneum: intercellular (via lipid phase only), transcellular (via both lipids and corneocytes) and appendageal (via sweat glands or hair follicles). Further down into the skin are the tight junction proteins (discovered recently) that are thought to play an important role in preventing large molecules entering the bloodstream and hence limiting possibility of sensitisation. Even though the sweat glands and hair follicles occupy only 0.1% of the total surface area of human skin, the appendageal route may be an important delivery pathway for slowly diffusing compounds and high molecular weight substances.

Various computational approaches have been employed for modelling transdermal permeation. Early modelling studies reported on quantitative structure property relationships (e.g. Potts and Guy model). Traditionally finite element models and compartment models have been also used to model skin permeation with varying degree of success. Over the last decade atomistic molecular dynamics simulations have been used to probe at the phase behaviour, stability, mechanical and permeation properties of the Stratum Corneum lipids – mainly when the lipids are in a hydrated bilayer structure. Atomistic simulations also give insights into understanding of the role of different lipid components, lipid mobility and the possible arrangements of the intercellular lipid matrix. Recently, the structure and interactions between intermediate filaments of keratins, the major skin proteins, has also been addressed by use of SCF coarse-grained approach and atomistic molecular dynamic simulations. A main challenge is that many models are limited to confined conditions and not fully predictive.

2 Major outcomes

- Proteins in the skin and their interactions with lipids need more attention. They probably play a significant role in transport and mechanical properties. Role of proteins in facilitating junction points in the SC lipid region.

- Corneo-desmosomes and the potential of transport routes into corneocytes: At the transition level between stratum granulosum and stratum corneum (SC), normal desmosomes turn into corneo-desmosomes. Eventually at the outer layers of SC, all corneo-desmosomes are degraded in healthy skin, possibly helping the desquamation process. How far in the SC these corneo-desmosomes survive and at what density is still an open question Because corneo-desmosomes are derived from proteins, their locations probably provide easy transport route across the corneocytes.

- Enzymes in the lipids region that break down the desmosomes, provide anti-microbial activity, or aid is desquamation. There is evidence that they change their activity in diseased states. But there is not much water in the extracellular region. How can the enzymes work in these conditions? Or are the enzymes located inside the cells (water-rich regions).

- Need to have a good and reliable coarse-grained model validated against experiments and atomistic simulations. This will give access to larger systems and move onto higher lengthscales. The coarse-graining process should retain the right level of detail for specific application in consideration.

- Interpretation of experimental data with atomistic modelling: Extensive data is available from cryo-EM, X-ray and neutron diffraction, but it needs to be matched with atomistic simulations.

- How to move from structural knowledge to barrier-function prediction?

- What is the structure and the barrier function of the Corneocyte bound Lipid Envelope (CLE)? It is commonly assumed that some ceramide fatty acids are covalently bound to the lipid matrix in corneocyte via the fatty acid tail. No information is available regarding the grafting density, conformation (extended chain or hair-pin arrangement), or the composition (are there free-fatty acids or cholesterol?). Can an atomistic model be produced that incorporates the protein network inside corneocyte separated from the extracellular lipid lamellae via the CLE?

- How do small molecules impact lipids structure and mobility? Effect of penetration enhancers and/or formulation additives and/or nano-particles. There are implications on impact of pollution, or dirt particles in the air.

- Hair follicles: Cellular structure at the bottom of the follicle and permeation through that boundary has not received enough attention. Is this a “highway” for systemic delivery? The follicle can act as a reservoir for actives on the surface of skin. What is the protective role of sebum against penetration? Note that at the bottom of the follicle there is less/no sebum. Not clear what is the status of keratinisation of the cells at the bottom of the follicle.

- COSMOmic (alternative) approach to calculating free-energies. (http://www.cosmologic.de)

- Tissue engineering for artificial skin substitutes. Many of these exist already that reproduce the cellular diversity and spatial arrangement of the different skin layers, can be created with 3-D printing, and appendages can be introduced. However, these artificial skins do not reproduce long-period periodicity of extracellular lipid arrangement and show reduced permeation barrier compared to in vivo.

- Natural variability: Lipid composition and barrier properties vary greatly across skin sites and across individuals and needs to be considered in modelling.

- Experimental challenges in reproducing the 1:1:1 lipid mixture (ceramide: cholesterol: free fatty acid). Cholesterol tends to crystallize out in vitro. Chain-length and lipid type polydispersity probably make large difference. More work is needed to determine accurate in vivo lipid profile.

- How does the structure change in a diseased state?

3 Community needs

- Access to computing resources is needed for modelling advances.
- Is there a broad skin network within Europe facilitating personnel and knowledge exchange?
- Access to skin/tissue cryo-EM facilities to validate the MD simulations.
- Structural biology network INSTRUCT offers access to facilities for simple systems. Needs to be extended to tissue?
- Increased communication between biologists and modelers – what's worth studying? What are the key questions to ask? What's the impact of the model?
- Organize exchange visits across groups (within the same country and across countries). Opportunities can arise through workshops and similar meetings.
- A CECAM workshop two years in the future will be beneficial. The ability to have focused discussions and the diversity of expertise of the participants made the current workshop unique. A number of new computational (for example mechanical annealing in bilayer simulations by Clare McCabe, fast calculation of permeation properties with COSMOmic by Karel Berka) and experimental (for example stimulated Raman to visualize percutaneous absorption) studies were presented in the workshop. It will be helpful to have a follow-on meeting at a later date to cross fertilize the new techniques to different groups.

4 Funding

- Funding opportunities for cross-country collaborations (Global Challenge Research Funds), e.g. UK – China, UK-India.
- Consortia across Academia and Industry sponsored self-funded by partners.
- CEFIC 2-3-year projects directed at industry partners to fill gaps in the knowledge. In-vitro and in-silico model development, linking with risk assessment.
- There may be opportunities arising from regulatory agencies (e.g. OECD).
- Opportunity: organize discussions/workshops with these organizations. Critical to involve funding agencies in these discussions. Need to raise the profile of the field with funding agencies program managers.
- CCP5 provides small amounts of funds to organize workshops (computational and UK focused)

- EPSRC and/or BBSRC (UK), NIH (US)
- FSA – food and safety agency.
- Welcome Trust and other charities.
- Risk: What is the impact of Brexit onto funding schemes?

5 Will these developments bring societal benefits?

Modelling is already being used in understanding and partially predicting the permeability of specific compounds for cosmetic and medical industries. There is room for improvement both in algorithm generation for faster computation and improvement in skin model for quantitative agreement.

- Work is needed to understand immature skin. Further knowledge is required for the developmental biology in young children (less than 2 years of age) and in understanding the mechanisms of skin barrier formation and early developments.

- Targeted protection for “older” skin: skin structure in ageing population is different and needs separate consideration both from experiments and modelling. The same is true for diseased skins.

- Sunscreens: Exposure to sunlight is the leading cause of skin ageing. Questions about the content of the sunscreen cream and also on the application protocols. Can modelling help in determining the ingredients and the optimal application protocol?

- Chemical protection: Can a protective cream be formulated against exposure to toxic chemicals (either from the environment or from industrial accidents), or being in extreme environments (like high altitude)

- Alternative to animal testing. Extending from cosmetic to pharma. Reduce, replace, refine. Need to engage with the relevant agencies. Look for landing points downstream. Practical demonstration.

6 Participant list

Organizers

Akinshina, Anna
University of Salford, United Kingdom

Das, Chinmay
University of Leeds, United Kingdom

Noro, Massimo
Unilever, United Kingdom

Anwar, Jamshed - University of Lancaster, United Kingdom

Belsey, Natalie - NPL, United Kingdom

Berka, Karel - Department of Physical Chemistry, Palacky Univerzity in Olomouc, Czech Republic, Czech Republic

Bouwstra, Joke - Leiden University, The Netherlands

Chen, Tao - University of Surrey, United Kingdom

Coleman, Lucy - University of Surrey, United Kingdom

Conway, Barbara - University of Huddersfield, United Kingdom

Detroyer, Ann - L"Oréal R&I, France

Devgan, Mohit - Imperial College London, United Kingdom

Fitsiou, Eleni - Lancaster University, United Kingdom

Hoshino, Takuma - Tokyo Metropolitan University, Japan

Kasting, Gerald - University of Cincinnati, USA

Lane, Majella - University College London, United Kingdom

Lian, Guoping - Unilever, United Kingdom

Lundborg, Magnus - ERCO Pharma/SciLifeLab, Sweden

McCabe, Clare - Vanderbilt University, USA

Nägel, Arne - Goethe-University, Germany

Narangifard, Ali - ERCO Pharma/Karolinska Institutet, Sweden

Norlen, Lars - Karolinska Institutet, Sweden

Notman, Rebecca - University of Warwick, United Kingdom

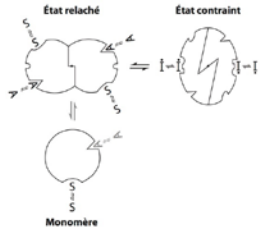
Sparr, Emma - Lund University, Sweden

Tascini, Anna Sofia - Imperial College, United Kingdom

Vattulainen, Ilpo - University of Helsinki, Finland

Wennberg, Christian - ERCO Pharma/SciLifeLab, Sweden

Computational approaches to investigating allostery



Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1414.html
Dates: October 30, 2017 to November 1, 2017

1 State of the art

Allosteric regulation plays a key role in many biological processes, such as signal transduction and transcriptional regulation and is rooted in fundamental physical properties of macromolecular systems. The detailed mechanism whereby these physical properties underpin allostery is not fully understood. Furthermore, allosteric effects are modulated by the cellular context. Computational approaches have all along played an important role in the investigation of allosteric mechanisms. They have provided insights into some of the underpinnings of allostery and have recently shown great promise in various practical applications, such as engineering regulatory modules in proteins and identifying allosteric binding sites that can be targeted by specific drugs. Notable examples include re-sensitizing resistant hepatitis C variants by a combination therapy that involves binding to the allosteric site of NS5A, allosteric inhibitors of HIV integrase, or the discovery of allosteric drugs that inhibit PARP-1 without hampering its action on cancer related DNA repair deficiencies. On a molecular level however, computational approaches have as yet not been able to yield information on the kinetic and thermodynamic drivers of allostery, an area where they could ideally have complemented experiment. This may be changing with increased access to massively parallel computers and the availability of more powerful methods for exploring the energy landscapes of complex systems. Recent bioinformatics approaches analyse sequence information (patterns of sequence conservation or correlated mutations) with the goal of uncovering signals of evolutionary pressure that may either inform or validate mechanistic aspects of allosteric processes. The increase in available protein sequences from different organisms and on human polymorphism is providing unprecedented (and still largely untapped) opportunities in investigation the role of evolution in shaping allosteric regulation.

2 Major outcomes

The CECAM workshop brought together about 30 computational biophysicists, protein modellers and bioinformaticians as well as experimentalists for an inspiring 2.5 days of stimulating talks and discussions. Among the important topics addressed were the new insights gained into the mechanistic underpinning of allostery from computational and experimental analyses of real protein systems, as well as from very simple in silico toy materials. Also presented were informative examples describing how allostery enables information processing in cellular signalling cascades. Real excitement was generated by reports on the rational design of allosteric systems that can be modulated to produce desired activity and cellular behaviour or engineered to act as sensitive molecular sensors. Encouraging results were also described on the rational discovery of allosteric drugs by combining computational and experimental approaches.

Discussions

Participants much appreciated the ample time that was allocated to questions and discussions during and after each oral presentation. Discussions also took place during breaks and at the poster session (where a total of 12 posters were presented).

All participants also actively contributed to the general discussion period that took place at the end of Day 2 of the workshop, during which the following topics were addressed:

- What are optimal method-system matches?
- Can we come up with a few allosteric systems where different computational methods can be applied, results compare, let alone, evaluated against experimental data?
- Is there a particular set of 'system-level' properties of allosteric systems that evolution tends to select? For example: FE differences/relative population levels of states? What is the relative important of local and global dynamic? What are the typical kinetic barriers between states (transition rates; is there a 'referred' range? Is there a general role for intrinsically disordered regions (IDR's)?
- Is there value in mapping the so-called allosteric 'communication' paths or 'community structures' in protein systems?
- What is the level of agreement between 'communication paths' computed by different methods for the same protein? Can identified paths be really validated? What should one map instead?
- Can concepts from protein folding theory be exploited to understand allostery?
- How can the massive protein sequence data inform us on the evolutionary pressures on protein properties important for allostery?
- What do we need to know about the allosteric mechanism of a given system to customize its allosteric regulation?

3 Community needs

Discuss the needs of the community in terms of computational infrastructure (e.g. existing codes, use of HPC resources), networking (e.g. outreach to other communities including experimentalists), event organization (e.g. should a series of CECAM workshops on this topic be considered and if so why?)

Allostery is a dynamic phenomenon. Hence, molecular dynamics simulations are critical for studies of allosteric phenomenon. Computational approaches have all along played an important role in the investigation of allosteric mechanisms. They have provided insights into some of the underpinnings of allostery and have recently shown great promise in various practical applications, such as engineering regulatory modules in proteins and identifying allosteric binding sites that can be targeted by specific drugs. Due to high importance of allosteric phenomenon, scientific community has been developing protocols to map allosteric pathways in proteins. While there are a number of approaches, no unified platform has yet been developed. Hence, CECAM workshop series on allostery would facilitate the community to select most promising approaches, to solidify the outcomes, and to develop new and more advanced requirements for future software packages. In addition, CECAM workshops are extremely important for brainstorming some of the biggest challenges in computational approaches to rapidly map allosteric communications in proteins.

4 Funding

The workshop provided the occasion to start new collaborations, including interdisciplinary ones between researchers that never considered their potential benefits. The possibility of joint research proposals was not discussed in details during during meeting sessions, but it will be certainly a central topic of a follow-up workshop. One opportunity that was discussed was that of preparing a bid for a Horizon 2020 ITN training network to establish a doctoral training centre that includes most principal investigators present as the workshop that are based in Europe.

5 Will these developments bring societal benefits?

Allosteric phenomenon is a common to many biological macromolecules. Nature has utilized allostery to control protein function via remote binding sites. Despite the fact that this phenomenon has been known for decades, we still lack full understanding of physical mechanisms resulting in specific intramolecular communication routes that result in coupling of the distal sites. Understanding allosteric coupling will pave the way to shedding light on molecular function, as well as it will enable new pharmaceutical strategies that utilize allosteric binding site to regulate protein function in living organisms. For pharmaceutical industry, allosteric drugs present an enormous potential as they do not directly interfere with the active sites of the proteins yet offering a direct regulation routes of these proteins. Furthermore, some of the most targeted proteins, G-protein coupled receptors (GPCR), representing ~50% of all drug targets, are intrinsically allosteric, yet binding sites, due to shared similarity, are promiscuous, thereby making conventional drug targeting prone to side effects due to off-target binding. Hence, targeting allosteric sites provides an enormous opportunity to regulate GPCRs. National Institutes of Health strongly supports allosteric research in the USA.

6 Participant list

Organizers

Dokholyan, Nikolay
University of North Carolina, Chapel Hill, USA

Paci, Emanuele
University of Leeds, United Kingdom

Wodak, Shoshana
VIB, Brussels and University of Toronto, Belgium

Aguilar Sanjuan, Broncio - University of Bristol, United Kingdom

Bahar, Ivet - School of Medicine, University of Pittsburgh, USA, USA

Barth, Patrick - EPFL, Lausanne, Switzerland

Berezovsky, Igor - A-STAR, Singapore

Berneche, Simon - U Basel, Switzerland

Bolhuis, Peter - University of Amsterdam, The Netherlands

Bravi, Barbara - Ecole Polytechnique Federale Lausanne, Switzerland

Brito, Carolina - Universidade Federal do Rio Grande do Sul (UFRGS), Brazil

Cecchini, Marco - University of Strasbourg/ISIS, France

Clarke, Declan - Yale University, USA

D'Achille, Matteo - CEA-Saclay ; Collège de France ; Université de Versailles, France

De Los Rios, Paolo - Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland

Dejaegere, Annick - Institute of Genetics and Molecular and Cellular Biology (IGBMC) and University of Strasbourg, France

Di Pizio, Antonella - The Hebrew University of Jerusalem, Israel

Faccioli, Pietro - Physics Department of Trento University, Italy

Gkeka, Paraskevi - Sanofi, France

Hamm, Peter - University Zurich, Switzerland

Hilser, Vincent - Johns Hopkins University, Baltimore, USA

Hodaei, Armin - KOC University, Turkey

Horovitz, amnon - Weizmann Inst. of Science, Israel

Karanicolas, John - Fox Chase Cancer Center, USA

Kozakov, Dmitry - Laufer Center, USA

Lyu, Wenping - RWTH Aachen University, Germany

Macpherson, James - The Francis Crick Institute, United Kingdom

Maggi, Luca - Forschungszentrum Jülich, Germany

McLeish, Tom - Durham University (UK), United Kingdom

Milenkovic, Stefan - University of Cagliari, Italy

Nussinov, Ruth - National Cancer Institute, Frederick, USA and Tel Aviv University, USA

Palermo, Giulia - University of California Riverside, USA

Panecka, Joanna - Centre of New Technologies, University of Warsaw, Poland

Patrick, Lisa - The University of Edinburgh, United Kingdom

Plaxco, Kevin - UC Santa Barbara, USA

Ravasio, Riccardo - EPFL, Switzerland

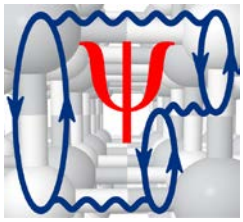
Rivalta, Ivan - Ecole Normale Superieure Lyon, CNRS, France

Stock, Gerhard - Albert Ludwig University, Freiburg, Germany

Stote, Roland - CNRS, France

Wyart, Matthieu - EPFL, Switzerland

Quantum-chemistry methods for materials science



Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1387.html
Dates: November 8, 2017 to November 10, 2017

1 State of the art

Together with the rapid growth of computational capacity, the high desire for general-purpose and accurate electronic-structure methods in materials science has drawn attention to the sophisticated quantum-chemistry methodologies rooted in wave-function theory (WFT). The implementation of popular quantum-chemistry methods to condensed matter systems, including the second-order Møller-Plesset perturbation method (MP2) and the coupled-cluster approach with singles, doubles, and perturbative triples (CCSD(T)), has been done in several mainstream computational platforms, and their applications in solids and surfaces have been presented in recent years. This workshop brought together six world's leading researchers in materials science to share their knowledge about the state of the art, challenges and the future of using quantum-chemistry methods in computational materials science.

Compared to popular density functionals, the quantum-chemistry methods face much greater challenges regarding numerical accuracy, efficiency, and reproducibility. In quantum chemistry, these challenges are well documented, stimulating a bunch of novel methodologies and algorithms with higher accuracy and efficiency. This workshop thus invited other six renowned experts with outstanding expertise in quantum chemistry to share the recent progress in their community and to deepen the coalescence of two communities and also of two theories: density-functional theory and wave-function theory.

2 Major outcomes

The workshop began with presentations on the development of sophisticated electronic-structure methods in materials science. Georg Kresse and Juerg Hutter presented the analytic gradient implementation of advanced electronic-structure methods in VASP and CP2K, respectively. Numerical convergence of quantum-chemistry methods for solids was discussed comprehensively by Denis Usvyat using Gaussian-type basis functions and by Xinguo Ren in the numeric atom-centered basis framework. Andreas Gruneis gave an overview over their recent effort to improve the computational efficiency and numerical stability of coupled-cluster theories using the plane-wave basis functions. Beate Paulus' talk then focused on the application of quantum-chemistry methods and also density-functional methods to graphene-based systems. These talks cover all the state-of-the-art developments in the field and thus sparked a heated discussion in these two sessions. By comparing the implementation of quantum-chemistry methods in different numerical frameworks and code packages, it has led to the consensus on the challenges of using quantum-chemistry methods for solids, including the slow basis-set convergence issue, the large finite-size error in the reciprocal space, and the expensive computational cost together with a huge memory consumption for large systems. These challenges have been significantly impeding the popularization of accurate quantum-chemistry methods in materials science.

In the following two sessions, the experts from quantum chemistry shared their wisdom to solve these pressing challenges in simulating finite molecules. Edward Valeev introduced his recent work on the explicitly correlated F12/R12 approach, which has been demonstrated to be very effective to reduce the basis-set error in quantum-chemistry methods for molecules. Frank Neese, Fred Manby, and Xin Xu presented their contributions to significantly enhance the computational capacity of quantum-chemistry methods towards large and complex molecular systems, including the uses of domain-based local pair natural orbital (DLPNO) methods, embedding algorithms, and the force-based extended ONIOM approach to realize linear scaling and robust performance of these quantum-chemistry methods for molecules. Ali Alavi's talk focused on the most accurate quantum-chemistry method, the full configuration interaction method in the quantum Monte Cario framework and its connection to the fixed-node DMC approach. Garnet Chan introduced their new electronic-structure package that allows for the coupled-cluster calculations of both molecules and solids on an equal footing. After lively discussions in these two sessions, these current progresses in quantum chemistry found their values in materials science, which highlights the importance of deepening the coalescence of two communities to solve the timely challenges of using quantum-chemistry methods for solids in the future.

3 Community needs

The substance of this workshop is the quantum-chemistry methods for materials science. As an emerging field with strong interdisciplinary nature, it is in the pioneering stage and full of challenges. To foster development towards routine uses of these sophisticated electronic-structure methods for solids, it needs more contributions in and outside of the community.

- At first, we should continue to strengthen the connection to quantum chemistry. As the home of quantum-chemistry methods and one of the most active communities in computational science, it is constantly giving rise to progress and new concepts in the field. This workshop demonstrated that these developments in quantum chemistry have been exhibiting a promoting role in solids or are considered to be feasible to solve the timely challenges in computational materials science.
- We should establish a stable connection to computer science. The key challenge of using quantum-chemistry methods for solids is their prohibitively expensive computational cost for large systems. Beside the development of mating lower-scaling algorithms, it is essential to grab the progress in computer science, particularly on the massively parallel supercomputer.
- Also important is an active connection to the computational scientists in materials science. Their feedback of using quantum-chemistry methods in daily research is crucial to speed up the methods development. However, it is difficult to convince the users in especial to overcome inertia and try a new method in its unstable developing stage.

4 Funding

The workshop benefited from the CECAM funding (8800 CHF) and 5000 EUR from the Psi-k society. As mentioned above, it is a fresh multidisciplinary field, which needs the contributions from different communities. However, most of the important developments described in this workshop are being undertaken in their communities and often independently. As such, funding is needed to support the exchange of scientists between 1) materials science and quantum chemistry; 2) computational science and computer science; and 3) methods development and application.

5 Will these developments bring societal benefits?

The workshop stimulated an interdisciplinary exchange of ideas and knowledge about the development of advanced electronic-structure methods transferring from chemistry, solid-state physics, and materials science. The electronic-structure theory is the foundation for many developments and investigation in these fields and the corresponding methods development drives progress. Despite its small and intimate scale, the workshop will have a lasting impact on materials science, because the description of many novel materials of experimental and/or industrial interest has been out of the capability of widely used density functional approximations, while the quantum-chemistry methods have great potential to handle the complex many-body electronic correlation correctly. The workshop reviewed the current state-of-the-art, challenge and the future of using quantum-chemistry methods in materials science and inspired new avenues for more accurate approaches and computational more efficient implementations that will facilitate future discoveries.

6 Participant list

Organizers

Scheffler, Matthias
Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany

Zhang, Igor Ying
Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany

Alavi, Ali - University of Cambridge and Max Planck Insitute for Solid State Research, Germany

Balzaretti, Filippo - University of Bremen, Germany

Bocharov, Dmitry - Institute of Solid State Physics, Department of Theoretical Physics and Computer Modeling, Latvia

Buccheri, Alex - University of Bristol, United Kingdom

Chan, Garnet - Princeton University / Caltech, USA, USA

Chen, Ji - Max Planck Institute for solid state research, Germany

Grüneis, Andreas - Max-Planck-Institute for Solid State Research, Germany

Hutter, Juerg - University of Zurich, Switzerland

Katukuri, Vamshi Mohan - EPFL, Switzerland

Kresse, Georg - University of Vienna, Austria

Manby, Fred - University of Bristol, United Kingdom

Meli, Rocco - University of Bristol, United Kingdom

Neese, Frank - MPI Bioanorganic Chemistry, Germany

Paulus, Beate - Physikalische und Theoretische Chemie - Institut für Chemie und Biochemie - Freie Universität Berlin, Germany

Ren, Xinguo - University of Science and Technology of China (Heifei/P.R. China), China

Rybkin, Vladimir V. - University of Zurich, Switzerland

Tsatsoulis, Theodoros - Max Planck Institute for Solid State Research, Germany

Usvyat, Denis - Institute for Physical and Theoretical Chemistry, Regensburg University, Germany

Valeev, Edward - Virginia Tech, USA

Xu, Xin - Fudan University, China, China

Ferroelectric Domain Walls

Location: CECAM-ISR
Webpage: https://www.cecam.org/workshop-0-1430.html
Dates: November 13, 2017 to November 15, 2017

1 State of the art

Ferroelectrics are materials with a spontaneous electric polarization that can be reoriented by an external electric field, a property that lends itself to key applications in electronics. This polarization typically points in different directions for different regions of the ferroelectric. In analogy with ferromagnetism, each region with a uniform polarization is called a domain, and the thin boundary between adjacent domains is a domain wall. Domain walls dramatically affect the properties of ferroelectrics.

Experimentally, it is difficult to characterize domain walls with atomic resolution, since in many cases this involves measuring atom positions with better than 0.05 Å accuracy. In this context, atomistic simulation calculations have emerged as a powerful complementary tool to experimental studies in unravelling the properties of these walls and how they affect the material where they are present. Moreover, ferroelectric domain walls are one of the simplest two-dimensional defects in crystals, so they represent a good test case in the quest of computational methods to tackle defects in solids, a necessary step towards the goal of modelling realistic materials.

Many of the recent works regarding ferroelectric domain walls report experimental results together with theoretical or computational analyses to help to their understanding. Typical computational methods used include those based on thermodynamic Landau-Ginzburg-Devonshire theory, effective Hamiltonians, molecular dynamics with classical potentials, and density-functional theory.

Computational methods have also provided general insights into the structure, energetics, and behaviour of domain walls, starting with pioneering work on simple perovskites and reaching recently more complicated configurations. These methods have been used to make predictions such as that domain-wall motion can give rise to negative capacitance.

2 Major outcomes

The major scientific points discussed in the meeting were the following:

(1) Recent contributions from computational groups to the understanding of the behavior of domain walls. Discussions concerned recent publications about ferroelectric reversal and domain walls in corundum derivatives; first-principles-based molecular dynamics simulations of ferroelectric domain-wall motion; and second-principles simulations of counter-rotating vortices pairs in oxide superlattices.

(2) State-of-the-art experimental techniques for imaging domain walls. These include imaging domain walls by Raman scattering, low energy electron microscopy, X-ray nanodiffraction, and transmission electron microscopy.

(3) Complex ordering in ferroelectric domains, analyzed both from the computational and the experimental point of view: properties of magnetic and electric skyrmions, unusual phenomena induced by time-dependent toroidal moments, topological vortex domains in hybrid improper ferroelectricity, and counter-rotating vortices pairs in superlattices.

(4) Electronic properties of domain walls for their possible use as electronic components and energy devices: photoelectric processes in domain walls, studies of piezoelectric behaviour, and domain walls as emulators of electronic components.

(5) Connections between domain walls and other surface/interface systems in ferroelectrics and related materials: probing ferroelastic walls in strontium titanate, and exploring superconductivity and spin-orbit interactions in superlattices of strontium titanate and lanthanum aluminate.

(6) Ferroelectric domain walls in hexagonal rare-earth manganites: insights from computational methods on their topological defects.

The workshop highlighted how collaboration between experiment, theory, and computation leads to understanding of the properties of domain walls. In this respect, density-functional theory and second-principles methods based on it provide the state-of-the-art methodology for helping characterize domain walls where experimental access to the sub-Angstrom features is not yet possible.

3 Community needs

As was shown in the workshop, the community is now addressing complex material science problems involving dynamics and defects. Computational studies of such problems are enabled by the advances in the computational methodology but still require heavy use of computational resources, making HPC resources indispensable for the continuation of research in the field. Typical simulations runs are now in the range of ns and require the use of 100-1000 processors in parallel for reasonable wall-time job length. This can only realistically be achieved at supercomputer centers. Thus, further access to HPC resources is vital.

The workshop brought experimentalists and computational scientists together for a very fruitful discussion of various problems in the field. Such discussions are very helpful for identifying new areas and problems that require modeling, which in turn stimulates new methodological development, opening up new areas of study and leading to greater relevance of computational studies and interactions with experimentalists. Additionally, perhaps biannual CECAM workshops would be very helpful for promoting this kind of virtuous circle of interactions, methodology development and applications.

The workshop also revealed the need for further development of computational methodology. While first-principles calculations are well-established in the field, the complex multiscale problems at the forefront of current research require the use of second-principles (atomistic or tight-binding models parameterized from first-principles data) simulations for which the trade-off between accuracy and computational efficiency must be addressed. Several key problems such as bond-breaking and vacancies in the materials cannot be simulated by these methods, representing a key bottleneck for further advances that must be addressed in future methodological development.

4 Funding

Typical funding channels are:

- Research grants that are specifically aimed at cross-communities collaborative efforts of multi-scale treatment of relevant problems. The Israel Science Foundation funds this kind of research.

- Funding of academia and industry collaborations, as the electronic industry is also interested in smaller devices that can be modeled using computational methods. There exist in Israel channels to achieve this through, e.g., programs between Research Authority offices of university and companies.

- Funding for education, promoting additional workshops, schools, conferences and also higher degrees dedicated tracks that will help to educate new researchers.

5 Will these developments bring societal benefits?

Ferroelectric domain walls play an important role in a variety of applications such as non-volatile memories, dielectrics and piezoelectric devices. They have also recently been investigated for possible application in photovoltaics. A better more detailed understanding of ferroelectric domain wall dynamics enabled by advances in simulation methodology and the extension of simulations to ferroelectric domain wall problems at greater length and time scales will enable improvements in device efficiency as well as development of entirely new devices that could make some previously impractical technologies suitable for widespread use.

For example, achievement of higher piezoelectric energy conversion efficiency can enable wide use of energy harvesting, contribution to more sustainable and efficient energy use and reducing the need for fossil fuel consumption. Better piezoelectric can also improve the effectiveness of medical imaging, leading to improvements in health care and enable the

replacement of toxic lead-based materials which are a key component of current piezoelectric devices with more environmentally-friendly materials.

Finally, the simulation techniques such as second-principles modeling developed in the context of studies of ferroelectric domain walls will be extended to a wide range of materials science problems where highly accurate treatment of effects on several lengths scales is necessary for understanding the energetics and dynamics that underlie the material properties, such as for example in composite materials. The use of such methods will provide advances for a wide range of material science problems related to energy use, sustainable development and replacement of toxic and expensive elements.

6 Participant list

Organizers

Dieguez, Oswaldo
Tel Aviv University, Israel

Grinberg, Ilya
Department of Chemistry, Bar Ilan University, Israel

Iniguez, Jorge
Institut de Ciència de Materiales de Barcelona (ICMAB), Spain

Yogev, Yael
Tel Aviv University, Israel

Alexe, Marin - University of Warwick, United Kingdom

Artyukhin, Sergey - Italian Institute of Technology, Italy

Bellaiche, Laurent - University of Arkansas, USA

Cano, Andrés - Institut de Chimie de la Matière Condensé de Bordeaux, France

Chen, L.Q. - Penn State University, USA

Cheong, Sang-Wook - Rutgers University, USA

Dagan, Yoram - Tel Aviv University, Israel

Damjanovic, Dragan - Ecole Polytechnique Féderale de Lausanne (EPFL), Switzerland

Gorfman, Semën - University of Siegen, Germany

Guennou, Mael - Luxembourg Institute of Technology, Luxembourg

Hlinka, Jirka - The Czech Academy of Sciences, Czech Republic

Ivry, Yachin - Technion, Israel

Junquera, Javier - University of Cantabria, Spain

Kalisky, Beena - Bar Ilan University, Israel

Liu, Shi - The Carnegie Institution for Science (USA), USA

Luk'yanchuk, Igor - Université de Picardie Jules Verne, France

Meier, Dennis - Norwegian University of Science and Technology, Norway

Paruch, Patricjya - University of Geneva, Switzerland

Ramesh, Ramamoorthy - UC Berkeley, USA

Rappe, Andrew - University of Pennsylvania, USA

Seidel, Jan - University of New South Wales, Australia

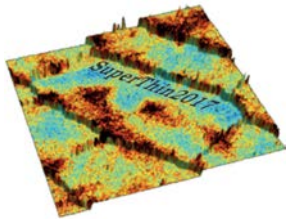
Setter, Nava - Ecole Polytechnique Féderale de Lausanne (EPFL), Switzerland

Stengel, Massimiliano - Institut de Ciencia de Materials de Barcelona (ICMAB), Spain

Vanderbilt, David - Rutgers University, New Brunswick, USA

Zubko, Pavlo - University College London , United Kingdom

Superconductivity in atomically thin materials and heterostructures



Location: CECAM-Lugano, Lugano, Switzerland
Webpage: https://www.cecam.org/workshop-0-1391.html
Dates: November 20, 2017 to November 23, 2017

1 State of the art

Since the discovery of graphene, two-dimensional (2D) materials have become the core of the modern material physics. Tremendous effort has been put into advances to not only fabricate, but also functionalize 2D materials, in order to meet the technological grand challenges in sustainable energy solutions and device miniaturization. In that respect, it is now well established that 2D materials are very susceptible to chemical functionalization by dopant atoms, electric gating, strain, or interface interplay with the substrate, making them far more versatile than their 3D counterparts. In that respect, the corresponding effects on emergent superconductivity, in its different mechanisms and phases, are the least investigated property of 2D materials to date.

Recent observations of superconductivity in graphene (alkali-doped or twisted-bilayer), high-T superconductivity in monolayer FeSe on STO, as well as unconventional and topological superconductivity in 2D systems with strong spin-orbit coupling, raised a serious challenge for the theory to (a) explain the observed features, and (b) make further predictions towards functional alterations of those materials. Unfortunately, while modern experimental techniques are enabling increasingly multifold studies of superconductivity (in-situ synthesis, functionalization, transport and/or scanning-probe measurements), the community has witnessed an increasing gap between the ab initio calculations and those on mean-field levels, and even more to the desired device modelling at the ultrathin limit. This workshop was aimed to change this unsatisfying picture: to bring together some of the experts in the field, on both theoretical and experimental end, and discuss the needed multi-scale characterization of atomically thin superconductors, in order to tackle the main challenges and identify further exploration avenues in this booming field of research, with envisaged applications in ultra-low power and ultra-light electronics.

2 Major outcomes

This workshop was devoted to understanding superconductivity in 2D materials, and its competition with a wealth of other possible quantum phases entailing collective behavior of the electrons (such as charge density wave phase, the Ising state and chiral spin textures due to strong spin-orbit coupling, etc.). It is a great unknown how exactly the interplay of possible phases behaves, how it can be controlled, and what the resulting hybrid states are like. In this workshop, owing to recent advanced experiments and developing theoretical tools, the main routes to control and enrich superconductivity in 2D limit by structural (strain and layer-by-layer addition) and electrochemical means (by gating, impurities and adatoms, etc.) were identified, and thorough discussions took place towards general atomic-scale control of collective quantum phases in 2D materials that opens the route towards highly versatile quantum devices (employing the advantages of the different phases at play).

The first problem to tackle were the shortcomings of the available computational tools. Namely, in the calculations of conventional superconductivity in 2D materials, the first bottle neck is the efficient calculation of the vibrational modes (within DFPT), then the electron-phonon coupling on a dense (k,q) grid and sufficiently high energy cut-offs, and finally the implementation in the full-spectrum anisotropic Eliashberg theory where Coulomb screening is separately addressed for all electronic bands participating in the Cooper-pairing. Different solutions were presented, and limitations of each approach were properly established. For unconventional superconductivity, in the case of spin-triplet pairing, relevant to e.g. iron-based superconductors, the proper ab initio treatment of Cooper-pairing in presence of (anti)ferromagnetic fluctuations was discussed, as well as for topological and Ising superconductivity in 2D limit. Namely, highly interesting physics is achieved by coupling 2D superconductors with magnetic impurities. For instance, as discussed in the workshop, Fe atoms on 2D NbSe2 or Co atoms under Pb monolayer give rise to long-range Yu-Shiba-Rusinov bound states, and chains or clusters of these impurities can yield topological superconductivity with Majorana quasiparticles, applicable in quantum computing. Furthermore, the electron cloud in 2D metals with strong spin-orbit coupling can form a spin texture akin to the Ising model, and thereby strongly influence other collective quantum phases such as superconductivity. This was discussed related to 2D NbSe2, and gated MoS2, as well as monolayer Pb on Si(111) and Pb-Ta mixtures. This discussion promises to be only the tip of the iceberg, as it has indicated that unconventional and topological superconductivity can equally arise in these systems.

Further on 2D transition metal dichalcogenides (TMDs), a lot of attention was given to the instability of the electron liquid known as a charge density wave (CDW). Although also present in bulk TMDs, CDWs change drastically in the 2D limit, where enhancement, depletion and non-monotonic behavior of the CDW strength all have been observed. CDWs are often thought to be in direct competition with superconductivity, however, discussions during this

workshop revealed that the relation between CDWs and superconductivity actually depends on precise influence of the CDW reconstruction on the electronic properties.

Last but not least, the multiband effects in 2D superconductors have been discussed, with respect to dependence of critical temperature on band hybridization, the possibility of crosspairing over different bands, and various novel phenomena stemming from the interplay of multiple coexisting superconducting condensates, with profound changes in the interplay detected with increasing thickness of the sample one monolayer at the time. The conclusions drawn have an outlook to other materials (e.g. MXenes) where experiment should seek similar behavior.

3 Community needs

The needs of the community in terms of computational resources is multi-fold. On coding side, significant improvements are needed for ab initio descriptions of superconductivity in 2D materials, as discussed in the previous section. There are several home-made solvers in Europe, and one publicly available (the EPW package, attached to Quantum Espresso), but none of them is at the level of desired precision, efficiency, or ease of use. Furthermore, to understand the recently-detected Cooper pairing in bilayer graphene twisted at small angles, the unit cells of thousands of atoms are needed, surpassing the ability of any of the available DFT codes.

The available HPC resources in all European countries are much appreciated and heavily used by the community working on 2D superconductivity. However, to obtain the access to HPC infrastructure one usually needs to prove the scalability of the used codes, before parallelizing the calculations on large number of computing nodes. This remains a problem, as available codes do not scale well in at least one stage of the needed calculations.

These and many remaining scientific challenges warrant further support from CECAM, Psi-K, and other European networks, as regular workshops of the kind we just had are the best way of advancing the science in the shortest term possible. The topic is very scientifically advanced, and challenging in terms of needed components in deeply quantum physics, as well as materials science. At present, the experimental progress advances much faster than the theoretical understanding, and this should be rectified as soon as possible. Nearly every month a scientific surprise is found in this field, without theoretical prediction, nor proper subsequent description. Considering the wealth of physics and chemistry involved, on atomistic scale, with advanced experiments at hand (on all continents, but still led by China and USA), one should definitely consider a series of CECAM workshops on the topic.

4 Funding

The participants in the workshop in most cases seek individual funding from the national agencies, within annual calls. Although being regularly available, this funding channel is rather modest, especially considering the employers costs for personnel that quickly deplete the allocated budget. For that reason, all participants of the workshop look at European calls (ERC and other).

Joint research proposal were definitely discussed, particularly between teams performing multiscale simulations of 2D superconductors (from atomistic scale to devices). Two joint proposals were submitted in the first call of the new EU Flagship on Quantum Technology, on topological superconductivity in atomically-thin materials and particularly heterostructures. One project stemming from this workshop was funded within the QUANTERA call, for advanced quantum detectors (superconducting and otherwise) based on 2D materials. Further joint applications for funding are expected in the EU-RIA-NMBP call of 2018.

5 Will these developments bring societal benefits?

The immediate societal and economic benefits were not in the focus of the workshop, as this line of research is primarily fundamental at the present stage. However, it is clear that societal benefits can be found in related proposals for ultrafast, ultralight, ultrasensitive, and scalable electronics, for use in various sensors, THz and satellite technology, and medical applications relying on SQUID technology. We also point out the relevance of all discusses science to quantum technology of second generation (i.e. quantum information and quantum computing) where 2D superconductors will play a notable role, owing to their highly-tunable properties, and versatility under strain, temperature, heterostructuring, etc. that was discussed in detail during the workshop.

Concerning the funding opportunities in this respect, we thoroughly discussed the upcoming calls for funding within the new EU Flagship on Quantum Technology, where projects of higher TRL levels (namely closer to applications) are highly sought. In that respect, we identified several companies in Europe that are interested in testing and developing further devices based on 2D superconductors, specifically for new (cryogenic) probes with single-spin sensitivity, plasmonic applications, THz detectors, and single-photon emitters and detectors.

Finally, significant funding opportunities will be sought in the upcoming calls related to “Adopting materials modelling to challenges in manufacturing processes”, in the part related to Nanotechnologies, Advanced Materials, Biotechnology and Advanced Manufacturing and Processing, where joint applications with industrial beneficiaries are also expected.

6 Participant list

Organizers

Milosevic, Milorad
Universiteit Antwerpen, Belgium

Perali, Andrea
University of Camerino, Italy

Roditchev, Dimitri
Institut des Nanosciences de Paris, Université Paris, France

Aperis, Alex - Uppsala University, Sweden

Bekaert, Jonas - University of Antwerp, Belgium

Bergeal, Nicolas - ESPCI Paris, France

Biscaras, Johan - IMPMC-Paris, France

Black-Schaffer, Annica - Uppsala University, Sweden

Calandra, Matteo - Institut des Nanosciences de Paris, CNRS, France

Capone, Massimo - International School for Advanced Studies (SISSA), Italy

Chen, Qihong - University of Groningen, The Netherlands

Faulkner, Michael - University of Bristol, United Kingdom

Grigorieva, Irina - University of Manchester, United Kingdom

Gruneis, Alexander - University of Cologne, Germany

Hasegawa, Yukio - Division of Nanoscale Science, Institute for Solid State Physics, The University of Tokyo, Japan

Kamlapure, Anand - Universität Hamburg, Germany

Kang, Ning - Key Laboratory for the Physics and Chemistry of Nanodevices, Peking Univeristy, China

Mañas-Valero, Samuel - University of Valencia, Spain

Menard, Gerbold - Niels Bohr Institute, Copenhagen, Denmark

Moreno Ugeda, Miguel - CIC-NanoGUNE, San Sebastian, Spain

Nigge, Pascal - University of British Columbia, Canada

Parab, Pradnya - UM-DAE Center for Excellence in Basic Sciences, University of Mumbai, Kalina Campus, Santacruz (E)-400098, India

Profeta, Gianni - Universita dell''Aquila, Italy, Italy

Qu, Amy - University of British Columbia, Canada

Raychaudhuri, Pratap - Tata Institute of Fundamental Research, Mumbai, India, India

Renner, Christoph - University of Geneva, Switzerland

Robinson, Marianne - CECAM, Switzerland

Saito, Yu - The University of Tokyo, Japan

Seibold, Goetz - \'Physik komplexer Systeme\' BTU Cottbus, Germany

Senkovskiy, Boris - Institute of Physics II, University of Cologne, Germany

Steigemann, Conrad - University of Halle (Saale), Germany

Stornaiuolo, Daniela - Università degli Studi di Napoli Federico II, Italy

Uchihashi, Takashi - NIMS Tsukuba, Japan

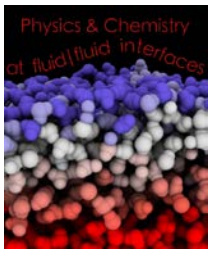
Valentinis, Davide - University of Geneva, Switzerland

Wang, Lili - Tsinghua University, China

Weitering, Hanno - University of Tennessee, USA, USA

Zhang, Lingfeng - University of Antwerp, Belgium

Physics and Chemistry at Fluid/Fluid Interfaces



Location: CECAM-AT
Webpage: https://www.cecam.org/workshop-0-1459.html
Dates: December 11, 2017 to December 13, 2017

1 State of the art

The molecular properties of liquid/liquid interfaces have been studied by computer simulations since the very beginning of the field itself but, differently from the solid/liquid interfaces, fundamental questions such as the shape of the interface itself, as well as the structural and dynamical properties of the molecular layers at the interface are still lively debated: new results on simple liquids, backed by novel theoretical analysis, have recently shown that the widely accepted capillary wave theory has in fact some important limitations, and that lateral correlations are playing an important role; the organization of ions at interfaces is another example of a seemingly simple system, where the fine balance between different effects has a major impact on the structure and properties of charged interfaces, as well as on the deviations from the Hofmeister series; our understanding of chemical reactions in the vicinity of interfaces happens to be sensitive to the surface roughness, requiring novel theoretical approaches; the problems related to the non-locality of the stress have also been studied intensively in recent years. In addition, non-equilibrium phenomena such as Super-and Sub-Maxwellian kinetic distributions, or the formation of interfaces in active matter are examples of active fields of research that are testing the limits of validity and applicability or thermodynamics in our understanding of the physics and chemistry at fluid/fluid interfaces. The focus of the workshop has been on the following aspects of liquid/liquid interfaces: intrinsic properties and molecular layers, partially miscible fluids, interfaces of biological relevance, active matter, evaporation and dissolution, cavitation phenomena.

2 Major outcomes

During the discussion session several topics were debated: Edward Smith proposed an alternative definition of the local pressure tensor through control volumes. The problem of defining and interpreting the local stress was pointed out by several researchers as a relevant and still unsolved one: the absence of an experiment that can probe the local stress with enough resolution, for example at the molecular scale, as discussed by Samuli Ollila is a significant impediment towards identifying an operative definition for this quantity. Likewise, it emerged that the community is very interested in the developments of all kinds of new experimental techniques that can probe interfacial properties, like the 2D sum frequency generation spectroscopy discussed by James Skinner. Patrice Malfreyt reported on recent results on the calculation of the surface tension in different geometrical setups. No clear consensus emerged about the possibility of defining uniquely the surface tension of arbitrarily curved interfaces.

The keynote lecture of Pavel Jungwirth opened the debate on the dramatic impact that the interpretation of experimental and simulation data can have in building our view on the role of interfacial water in biological systems.

Room temperature ionic liquids received a great deal of attention recently, and it turned out that their particularly rich phenomenology also extends to their interfacial properties, as pointed out by Martin Lisal and Miguel Jorge.

The phase behavior of mixtures of water and organic solvents have been discussed by David van der Spoel, Dominik Horinek, and Ilan Benjamin, while Natalia Cordeiro addressed the behavior of more complex interfaces like those formed by the thermoresponsive PNIPAAm.

Christoph Dellago discussed the physics of interfaces at negative pressure, in particular regarding the bubble nucleation of water under tension.

Last, but not least, there has been much interest in the possible analogies between equilibrium thermodynamics and the phase behavior of active fluids with boundaries. Laura Filion has discussed novel approaches to simulation and theory for these systems.

3 Community needs

The community is using an impressively varied set of computational tools. For the production of molecular dynamics trajectories, the majority is either using or developing one or more of the established simulation packages. On the other hand, most of the analyses are performed with in-house code: in some cases, this is highly specialized code, tailored to the need of the specific problem. However, there are also several types of analysis for interfacial systems that

are common to many research lines. The obvious outcome is that a significant amount of duplicated code has been written. The community would surely benefit by a different development strategy, centered on identifying a common set of tools, which could be developed collaboratively, sharing experience and human resources to produce open, more performing and reliable tools. Regarding HPC resources, most of the results discussed during this workshop have been obtained using HPC clusters or GPU computing, which is an increasingly appealing option regarding price/performances for soft matter simulations

4 Funding

The field could undoubtedly benefit from more collaborative efforts between experimentalists, theoreticians, and computer simulators. In this sense, initiatives that are fostering networking would represent a valuable tool for the development of the field. Current H2020 actions like the Marie Skłodowska Curie Innovative Training Networks (in the form of European Training Networks or European Joint Doctorates) would give the opportunity to fund a focused research program, with long-lasting effects in the field.

5 Will these developments bring societal benefits?

The focus of the workshop has been on fundamental aspects of liquid interfaces, and on the methodological issues of their investigation. Given the fundamental nature of this research, the societal benefits might not be immediately evident. However, one has to keep in mind that fluid interfaces are playing a fundamental role in several applied fields, including food production, cleaning agents, personal care products, and pharmaceutics. Faster and more accurate computational approaches and better theoretical modeling are in the long run expected to improve the ability of the industry to tailor the properties of emulsions to improve stability, extend product shelf life, control appearance. Also, obtaining an accurate characterization (at the molecular scale) of the physicochemical changes happening at complex liquid interfaces can lead to a better understanding of the mechanisms underlying, for example, transport through the cellular membrane, which has a clear potential for impact in the development of novel drugs

6 Participant list

Organizers

Jedlovszky, Pal
Eszterházy Károly University, Eger, Hungary, Hungary

Sega, Marcello
University of Vienna, Austria

Aasen, Alio - SINTEF Energy Research, Norway

Andricioaei, Ioan - University of California Irvine, USA

Benjamin, Ilan - University of California Santa Cruz, USA

Cordeiro, Natalia - Faculdade de Ciencias da Universidade do Porto, Portugal

Dellago, Christoph - University of Vienna, Austria

Duboue-Dijon, Elise - Czech Academy of Sciences, Czech Republic

Enders, Sabine - KIT, Germany

Fabian, Balazs - Budapest University of Technology and Economics, Hungary

Filion, Laura - Utrecht University, The Netherlands

Fischer, Johann - University of Natural Resources and Life Sciences, Vienna, Austria

Giri, Amal Kanta - University of Porto, Portugal

Henao Aristizabal, Andres - Universität Paderborn, Germany

Holý, Daniel - IOCB, CAS, Prague, Czech Republic

Horinek, Dominik - University of Regensburg, Germany, Germany

Jorge, Miguel - University of Strathclyde, United Kingdom

Jungwirth, Pavel - Academy of Sciences of the Czech Republic, Prague, Czech Republic

Khedr, Abeer - University College London, United Kingdom

Lbadaoui-Darvas, Maria - EPFL, Switzerland

Lisal, Martin - Academy of Sciences of the Czech Republic, Czech Republic

Lishchuk, Sergey - Sheffield Hallam University, United Kingdom

Malfreyt, Patrice - CNRS- Blaise Pascal University, Aubière, France

Ollila, Samuli - Institute of Organic Chemistry and Biochemistry, Academy of Sciences, Czech Republic

Schoettl, Sebastian - University of Regensburg, Germany

Skinner, James L. - Univ. Wisconsin, Madison, USA

Smith, Edward - Imperial College London, United Kingdom

Steinhauser, Othmar - University of Vienna, Austria

Trick, Jemma - King"s College London, United Kingdom

van der Spoel, David - Dept. Cell & Molec. Biol. Uppsala University, Sweden

Vattulainen, Ilpo - University of Helsinki, Finland

Voroshylova, Iuliia - Faculdade de Ciências da Universidade do Porto, Portugal

Wilhelmsen, Øiwind - SINTEF Energy Research, Norway

Zeiner, Tim - TU Graz, Inffefeldgasse 25 C, Graz, Austria

Expeditious Methods in Electronic Structure Theory and Many Body Techniques

Location: CECAM-ISR
Webpage: https://www.cecam.org/workshop-0-1465.html
Dates: December 17, 2017 to December 20, 2017

1 State of the art

The topic of the workshop was electron dynamics and structure. The motivation is nonequilibrium open quantum system dynamics. For example, photocurrent generation in molecular/nano-junctions, which is an extremely challenging task. Transport is a nonequilibrium problem requiring description of the dynamics of electrons, holes, excitons, coupled to phonons and electromagnetic fields, in an open system. In the language of quantum mechanics, this is a strongly interacting vibronic system in which the Born-Oppenheimer approximation breaks down while at the same time it is driven away from equilibrium by the applications of electromagnetic fields and bias potentials. An exact solution is only available for simple, non-interacting, model systems. Otherwise, approximate techniques and simulation techniques are required. Both nuclear and electronic dynamical processes are involved in these systems and in both types of processes, mean-field treatments are not adequate. Thus, correlations play a key role, both with regard to electronic interactions, electron-phonon and phonon-phonon couplings. In the context of the nano-structured systems at hand, this poses a formidable challenge to practically all of the methods outlined above. Much activity in the field is thus, directed at pushing the limits of the existing techniques. The proposed workshop will provide a snapshot of this very active field and aims to stimulate the development of new directions.

2 Major outcomes

The workshop took place in Tel Aviv University and included 66 participants, of these 27 were invited speakers, 4 Faculty members of various institutions, 8 Postdocs and 27 students. The topics presented were exact factorization methods, GW methods, Time-dependent density functional theory, stochastic density functional theory and GW, Stochastic 2nd order Moller-Plesset Perturbation Theory methods, self-consistent GW+DMFT, GF2 embedding methods, stochastic coupled cluster theory, stochastic methods in machine learning approaches, Tensor networks, Inchworm Monte Carlo, local configuration interaction methods, orbital free density functional theory, beyond Bethe-Salpeter equations, stochastic configuration interactions, Simulated nuclear magnetic resonance results in the superconducting regime of the two-dimensional Hubbard model and their relationship to the cuprate high-temperature superconductors, multiconfiguration wavefunction and reduced density matrix method. driven Liouville von Neumann (DLvN) approach. There was a poster session and prizes were given to the 3 best posters by a committee of scientists. There was an excursion to the Old City of Jerusalem.

4 Funding

- CECAM IL
- CECAM Int.
- School of Chemistry TAU
- Faculty of Exact Sciences TAU
- Chemical Physics Department in School of Chemistry TAU
- Prof. Eran Rabani
- Fritz Haber Center for Molecular Dynamics, The Hebrew University of Jerusalem
- Registration Fees

6 Participant list

Organizers

Baer, Roi
Hebrew University of Jerusalem, Israel

Rabani, Eran
Tel Aviv University and University of California, Berkeley, Israel

Yogev, Yael
Tel Aviv University, Israel

Berkelbach, Timothy - University of Chicago, USA

Booth, George - King"s College London, United Kingdom

Cohen, Guy - Tel Aviv University, Israel

Dieterich, Johannes M. - Princeton University, USA

DiStasio, Robert - Cornell University, USA

Galli, Giulia - University of Chicago, USA

Goerling, Andreas - University of Erlangen-Nuremberg, Germany

Gross, Eberhard K.U. - Max Planck Institute of Microstructure Physics, Halle, Germany

Gull, Emanuel - University of Michigan, USA

Hod, Oded - Tel Aviv University, Israel

Kosloff, Ronnie - The Hebrew University of Jerusalem., Israel

Kronik, Leeor - Weizmann Institute of Science, Rehovoth, Israel

Louie, Steven G. - University of California at Berkeley, USA

Neuhauser, Daniel - University of California, Los Angeles, USA

Neuscamman, Eric - University of California at Berkeley, USA

Reich, Daniel - Universität Kassel, Germany

Reining, Lucia - Ecole Polytechnique, Palaiseau, France

Schapiro, Igor - Hebrew University of Jerusalem, Israel

Shiozaki, Toru - Northwestern University, USA

Sorella, Sandro - International School for Advanced Studies (SISSA) and CNR-IOM DEMOCRITOS, Trieste, Italy

Takeshita, Tyler - University of California, Berkeley, USA

Ten-no, Seiichiro - Kobe University, Japan

Thom, Alex - University of Cambridge, United Kingdom

Thoss, Michael - University of Freiburg, Germany

Vlček, Vojtěch - University of California, Los Angeles, USA

Werner, Philipp - University of Fribourg, Switzerland

Zgid, Dominika - University of Michigan, USA