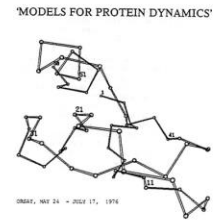
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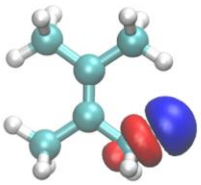
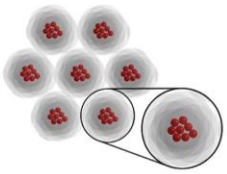
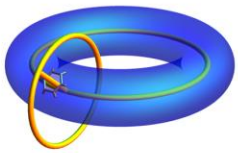
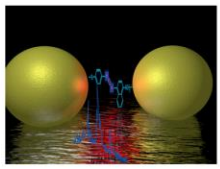
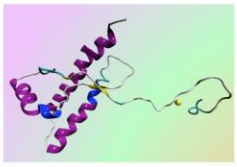
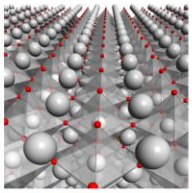
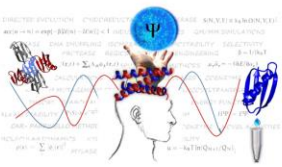
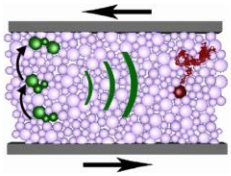
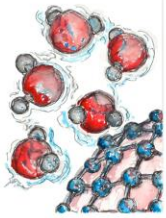
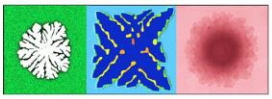
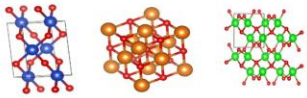
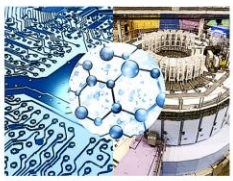
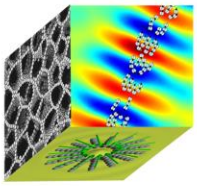
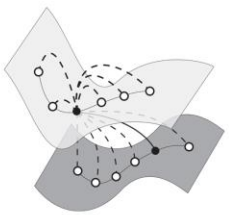


Report of Activities
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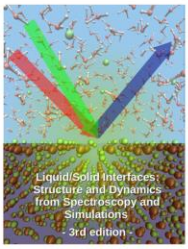
Liquid/Solid Interfaces:
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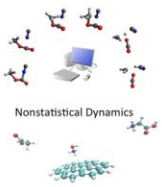
3rd edition

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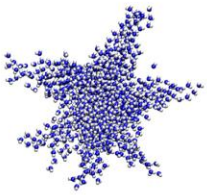

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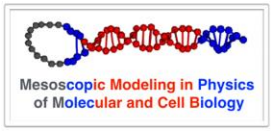
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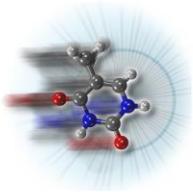
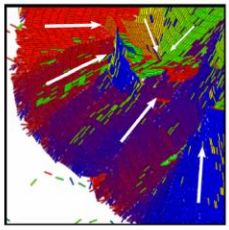


Electronic
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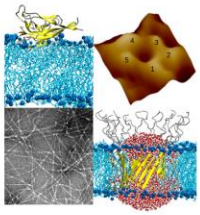
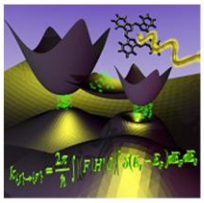
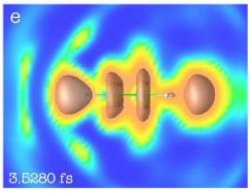
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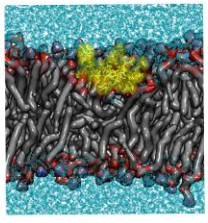
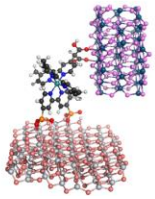

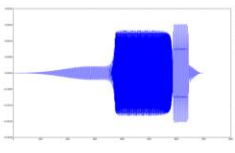

Please address any comments or questions to: director@cecam.org

Carrying on a tradition of almost 50 years, the CECAM program of workshops and schools originates from proposals collected from the community via an open call. For the 2016 program, 85 such proposals were refereed by 2-5 external experts and by the members of our Scientific Advisory Committee, and 69 events were selected by the CECAM Council based on their ranking. The acceptance rate of about 80% reflects the high quality of the submitted proposals, ensures a good balance of activities in HQ and the Nodes, and makes it possible to explore a broad range of scientific topics.

More in detail: 51 workshops were hosted by CECAM in 2016, 17 in Switzerland (15 at EPF-Lausanne, 1 at ETH-Zurich, and 1 at USI Lugano) and 34 in the rest of the Nodes. 21 events focused on materials, 8 discussed biological applications, and 22 centered on new methods and algorithms. Interesting new domains were also explored, most notably big data and machine learning, with one specific workshop and several dedicated sessions in other events. An important novelty in the program was the set of workshops related to the E-CAM Center of Excellence for Computing, a Horizon 2020 funded project coordinated by CECAM HQ and involving 14 Nodes as beneficiaries. A dedicated section of this publication describes E-CAM events that include State-of-the-Art workshops in classical and quantum dynamics, electronic structure and multiscale modeling, Scoping Workshops to foster collaboration with industry, and Software Development Workshops that consolidate and enhance the successful experiment to produce, document, and store software at CECAM, initiated in 2014 with the Electronic Structure Library.

18 schools were also hosted at CECAM HQ and in the Nodes in 2016, reflecting our commitment to basic and advanced training. These schools ranged from broad, introductory schools on statistical mechanics and electronic structure and their connection to computational methods, to more advanced topics such as multiscale approaches or activated events and kinetics, to training on methods and their implementation on specific software packages.

2080 scientists (1649 in the workshops, 431 in schools) from 51 different countries and at different stages of their career participated to the 2016 CECAM program. Female participation was of about 20% to schools and 15% to workshops, and junior scientists were encouraged to take an active role both as organizers and participants.

The scientific reports collected in this publication describe the 2016 CECAM workshops and summarize their main scientific outcomes. They provide a rich overview of the current trends in simulation and modeling, and explore new directions for the field. This collection demonstrates CECAM's continuing quantitative and qualitative output. We hope that it will contribute to inspire the community in its research and foster new initiatives and collaborations.

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Liquid/Solid interfaces: Structure and dynamics from spectroscopy and simulations - 3rd edition

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1168.html
Dates: January 25, 2016 to January 27, 2016

1 State of the art

Interfacial phenomena at solid-water interfaces play important roles in a wide range of natural and industrial processes. At the microscopic level, it is well established that solids and liquids influence their respective structural and chemical properties.

From an experimental point of view, interface selective vibrational spectroscopy, such as nonlinear second harmonic generation (SHG) spectroscopy and sum frequency generation (SFG) spectroscopy techniques, play central roles in addressing the liquid structural properties at interfaces. The wealth of information given by these advanced spectroscopic methods calls for theoretical calculations which provide the underlying atomistic picture and microscopic origin of the interfacial special order and reactivity that occur at interfaces. The aim of our workshop was to bring together the experimental and computational communities which share the common goal of probing the molecular-scale behavior of both liquids (water is certainly the most common liquid present at interfaces) and solids (oxides, semi-conductors, . . .) at liquid-solid interfaces, to advance the microscopic detailed knowledge of the interfacial structures, dynamics and chemical reactivity. We believe we have fully achieved this goal. Indeed, we managed to gather together many active scientists investigating the solid-liquid interfaces within different communities. We had live discussions in a friendly atmosphere where questions could be freely asked. We received positive feedback from many of the participants. In particular, younger participants enjoyed the discussions and profit from the presentations and discussions.

2 Major outcomes

One of the central topic in the workshop centered around charged interfaces and electrochemistry. The community is trying to move on from uncharged interfaces (e.g. the water-vapor interface) to charged interfaces. Knowing the molecular structure of water next to a charged substrate is a prerequisite to the fundamental understanding of many natural phenomena and is of great importance in the development of advanced energy conversion and storage devices. Protein folding, photocatalysis for water splitting, and proton-exchange membrane fuel cells are just a few familiar examples.
At a charged interface, the “bonded interface layer (BIL),” is mainly responsible for electrochemistry at interfaces and directly controls e.g. ion desolvation and charge transfer in chemical reactions. Next to the BIL, the deeper water sub-phase has essentially the bulk H-bonding structure that could be influenced by a long-range electric field set up by surface charges and the screening ions in a region known as the diffuse layer.

Current knowledge on the microscopic structure of the BIL is limited e.g. by the difficulty to experimentally separate between the BIL and the diffuse layer contribution. In his talk, Y.-R. Shen reported on the development of a Phase Sensitive Sum-Frequency Vibrational

Spectroscopy (PSSFVS) scheme which allows to selectively address the BIL of charged water interfaces, assuming the double layer theory in the treatment of the experimental data. Controversy in the interpretation of the localized vs diffuse layer contribution still animates the field as we could see emerging within the multiple discussions during his talk, also involving other experimental speakers, such e.g. S. Roke and E.G.H. Backus also working with interface sensitive spectroscopy experiments. Double layer modelling represents a challenge also for the simulation community. Indeed, in many cases the extent of the diffuse layer is such that it is not so easily included in atomistic models, in particular at the ab initio level of theory. The BIL also represents a challenge for different reasons: the main issue here is how the material chemistry and the solvation physical chemistry can match at an accuracy level
which includes the electronic structure calculations. The double layer description was also central to the talk of M. Sprik who presented an ab initio approach at the insulator-electrolyte interface, and discussed theoretical issues related to the exact calculation of electric fields within simulation boxes typical of ab initio MD simulations.
Interestingly, the modelling of ions in the aqueous solution and the accompanying description of the electric double layer, is common to both electrochemistry and colloids science and geochemistry. This has emerged e.g. from the talks from E. Borguet, from the experimental side, and from the talk of M. Machesky, from the computational perspective. A very interesting question which is still awaiting an answer in the geochemistry community is the extent of charge localization/delocalization at the interface.

3 Community needs

Deeper investigations of the different contributions to interfacial spectroscopy: for example, measures and calculations of the response function associated with the diffuse layer. Can the contribution extracted from interface measurements be compared to that measured from the bulk with other techniques? How far can we go with atomistic models? Is it possible to extend current simulations in order to address the relative importance of the BIL vs diffuse layer? That question is especially crucial for the ab initio MD community, such electronic representation being mandatory for vibrational spectroscopy calculations.
A need for obtaining a 3D resolution of interfaces has also emerged from discussions. In this respect SFG needs to be used in combination with other techniques, such as Atomic Force Microscopy (AFM) in order to gain higher spatial resolution: this is a relevant question to both electrochemical as well as geochemical interfaces. AFM has been facing new exciting developments and has now reached the possibility to address buried solid/liquid interfaces beyond the more traditional surface science approach. In a future follow-up workshop, we aim to invite a few of the developer pioneers of such techniques.
One important aspect of the discussions has shown that the community (experiments and simulations) has to move beyond the characterization of the structure of the solid/liquid interfaces and start to address reactivity in more atomistic details. Incorporating surface reactivity is a common theme to both electrochemistry and geoscience communities. Major advances on the experimental point of view include for example running flow SFG experiments that have been recently developed in the group of M. Bonn and EGH Backus in Germany.
Inhomogeneous catalysis at solid-liquid interfaces is another domain where modeling can be extremely useful for getting a real understanding of the mechanisms at play, and provide more rational design for catalysts to be used more efficiently. The combination of theory and experiments can help to identify reaction mechanisms and rates.

The wealth of information coming from the experiments and simulations on interfacial spectroscopy needs to be more centrally organized and “standardized”. This at least from

what concerns systems which have been now addressed for quite a long time. A suggestion from several attendees was in the direction of establishing some golden standard in the field which can be easily accessed. This emerged for example from the talk of D. Hore and E. Borguet. Is the water/vapor interface already clear enough to be one of these reference systems?
Finally, a further challenge for the community is emerging form the recently developed 2D-SFG spectroscopy experiments, which has opened new questions on structural dynamics of interfacial liquids. What can we understand from experiments and simulations? Multidimensional interface specific spectroscopy poses new challenges for theory/simulations, including combining accuracy and statistically relevant sampling of the necessary time-scale.

4 Funding

No specific funding needs or strategies were discussed.

5 Will these developments bring societal benefits?

The focus of this workshop was to move from the characterization of liquid/solid interfaces with uncharged surfaces to that of charged surfaces. A deeper understanding of interfacial structures, for example of water, will make it possible to devise cost effective and clean progress in crucial fields such as energy conversion and storage devices with clear societal benefits.

6 Participant List

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Towards a Common Format for Computational Materials Science Data

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1290.html
Dates: January 25, 2016 to February 5, 2016

1 State of the art

The development of modern commercial products – be it from the health, environment, clean energy, heavy industry, information or communication technology sector – depends strongly on the development and design of new and improved materials. However, identifying the best material or designing a novel and improved material for a specific task/application is a significant challenge. Of key importance are the characteristics of the materials at the atomic and molecular levels, which determine their properties and behaviors at the macroscopic scale. To aid and guide this search, computational materials science employs complex methods and computing algorithms ('codes') to investigate, characterize and predict material properties. Fueled by the "Materials Genome Initiative for Global Competitiveness", announced by President Obama in June 2011, these computational techniques are increasingly and successfully employed also for the "high-throughput screening" of materials. In conjunction with techniques from big-data analytics and machine learning, such an approach enables to scan many thousands of compositions for the material with the best-suited properties to predict trends, and to identify potentially (technologically) important candidates. So far, however, different technologies and frameworks developed in this context have addressed only very specific aspects, e.g. by focusing on properties relevant to one particular application and/or by supporting only one or very few electronic structure codes.

In practice, this means that computational material scientists produce a huge amount of materials data on their local workstations, computer clusters, and supercomputers using a variety of computer codes that are most commonly developed by European research groups. Though being extremely valuable, this information is mostly unavailable to the community, since most of the data are stored locally or even deleted right away. But even if they are available, a re-use and re-purposing would not be straightforward, given that different codes often use very different file formats and conventions to store the same physical data. Enabling sharing and comparing such data is thus a pressing issue that needs to be addressed to advance this field, as exemplified by multiple European initiatives. For instance, the European Center of Excellence for Novel Materials Discovery (NOMAD-CoE) aims at establishing a unified, code-independent data format, to which the raw data calculated by different electronic structure codes can be converted, so that big-data analytic techniques can then be exploited to obtain unprecedented insight from vast amounts of calculations. In a similar spirit, the Center of Excellence E-CAM, which was recently established by CECAM to build an e-infrastructure for software, training and consultancy in simulation and modeling, is committed to actively support the development and adoption of software libraries and standards within the electronic structure community. One measure aiming at this is CECAM's Electronic Structure Library (ESL) initiative, which drives establishing an Electronic Structure Common Data Format (ESCDF)

2 Major outcomes

There are some differences in the goals of data representations in the two actions:

- The ESCDF provides a standardized data format and an API every code can use. Material science code developers profit from centralizing implementations like efficient parallel IO and hiding file format specific issues. At the same time this allows a certain amount of interchangeability of data, for example for post-processing tools. The data itself is not altered, so that checkpointing and restarting functionalities can be granted without additional data loss.

- The NOMAD-CoE aims at making also the data itself comparable, which involves data transformations ranging from simple unit conversions up to normalizations based on reference calculations and analytics tools.

As both initiatives target the whole electronic structure code community, they are based on the same concepts and codes, thus have a large common ground. So, for a maximal mutual benefit, they jointly organized the present workshop.

Many attempts of standardization fail because initiatives are too small to reach a critical mass or try to impose their solution to a community for which it is not profitable to adapt to it, possibly also because due to shortcomings of the standard. This is avoided by involving all major codes right from the beginning. The workshop attended key experts of ABINIT, BigDFT, CASTEP, CP2k, CPMD, Dmol3, ESPResSo, Exciting, FHI-aims, FHI-98, FLEUR, KKR, LMTO, Octopus, Quantum Espresso, SIESTA, Turbomole, VASP, Wien2k. Each code expresses key magnitudes like wave functions, operators, and density matrices as linear combination of basis functions. There are various types of such “basis” established, some of them of very different character. Some codes describe all electrons in this basis, others use a simplified description of the core electrons. This results on one side in basically different data representation, on the other side also comparing certain magnitudes like energies is not trivial. This is addressed within the NOMAD-CoE, with funding currently granted until October 2018, by developing a conversion layer for normalizing this data and analytics tools for error quantification.

The workshop provided a unique platform to discuss and decide the fundamental paradigms needed to establish a common framework that supports several different electronic structure and force field codes and that is prepared to interface with the newly emerging field of data-driven material discovery in the European research landscape. In this view, a common purpose of the NOMAD-CoE and the CECAM-supported ESL is to integrate the computed results from leading electronic structure codes. Defining a common code-independent representation for all relevant quantities, e.g., structure, energy, electronic wave functions, trajectories of the atoms, etc., is challenging, as the codes differ, for example, in their choice of basis sets and treatment of the core electrons (e.g. usage of pseudopotentials). To tackle these challenges from a technological point of view, an envisioned strategy is to build on the experience gained during previous community projects with somewhat narrower focus but with similar philosophy. For instance, one of the most consistent and successful efforts was the development of the (NetCDF based) ETSF file format by the ETSF. Similar standardization efforts are currently under way within the EUSpec network. In this context, it is also planned to extend and modify the ETSF file format, in particular for greater flexibility for parallel I/O.

The key players in the electronic-structure and force-field code development were thus brought together, in order to discuss and implement the aforementioned code-independent representation of materials science data. The workshop was divided into two parts: a 2.5 days discussion on the file format specifications, followed by an 8.5 days coding effort.

3 Community needs

In the first part, each session was followed by an extended discussion, which led to actual guidelines for the future common-format storage. In the following, we list the topic of the sessions and the decisions taken in the respective discussions:

- A common energy zero for total energies. To make (total) energies stemming from different codes comparable, it is necessary to define a reference energy scale. To achieve this goal, it was concluded that a simple, pragmatic computational prescription viable for all codes is necessary. To bridge the gap between periodic and non-periodic codes both free atoms and simple bulk systems shall be used as reference systems.

- Compact representation of scalar fields: Density, Wavefunction, xc potentials, etc. The comparison of scalar fields across methodologies and codes requires to translate the internal, code and basis set specific representation of these fields into a common format. For such a representation, it was concluded that an all-electron formalism is desirable, since it allows to evaluate additional properties such as electric field gradients and NMR shifts. Which specific all-electron basis set (Numeric Atomic Orbitals, Gaussians, or APW+lo /FLAPW type basis sets) is best suited for this purpose needs to be evaluated in detail.

- Quantities related to excited-state calculations. Advanced many-body perturbation theory (MBPT) calculations (GW, BSE,…) currently output only few properties (spectra, self-energies, etc.) that need to be parsed and stored. To facilitate the analysis of this kind of calculations, it is essential to develop and store a detailed classification of all approximations used in the MBPT calculation in the metadata, given that many different numerical formalisms are implemented in different MBPT codes.

- Molecular dynamics related common format. The fundamental information generated during molecular mechanics' calculations are the geometric configurations and trajectories. Accordingly, these are also the most useful quantities to store. However, trajectories from specific approaches (Metadynamics, Replica Exchange, …) have to be handled with care. It is thus crucial to store respective metadata and settings. If possible, the original submission scripts should be retained as reference.

- Metadata for a code independent format. For the properties desirable for the metadata ontology, it was concluded that both human and machine readable formats are needed. An unambiguous conversion ("translation") script is required for this purpose. Since multiple ontologies are currently under development (NOMAD, TCOD, ESL), discussion among these different communities should be encouraged to establish a common language/wording. Besides having a standardized central definition (reference), customization options for local users are desirable.

- Establishing error bars and uncertainties. Clearly, quantifying the errors and uncertainties of the data included in computational materials' databases is an essential step to make this data useful at all. Challenges in this field arise, since the errors are code, property, and material specific. Also, the dependence of different errors on each other needs to be taken into account. A first step in this direction is to establish unique identifiers for structures through "similarity recognition". Furthermore, a systematic investigation of numerical errors is required across codes for both simple and complex properties, which also requires a clear definition of errors/deviances, e.g., for continuous functions. With respect to errors arising from the use of approximated xc-functionals, (more) test sets are required as a reliable, high-level reference. In this context, using experimental benchmarks can be tricky, since they hardly allow for error analysis.

- The Electronic Structure Common Data Format (ESCDF). A standardized data format for electronic structure calculations must provide a framework for saving and reading data without enforcing a specific physical representation, while providing means to store different types of data. This can be achieved with self-describing formats like HDF5 or NetCDF, which are extendable and allow the inclusion of metadata needed to interpret them. The first version of the ESCDF must include specifications to read/write the following type of data: geometry/structure of the system, basis sets, densities, potentials, and wavefunctions. The associated software library and corresponding API will focus on flexibility, extensibility, and performance in order to maximize its usefulness and adoption by the community of code developers.

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 millions 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.

The NOMAD Project has additional demands on storage and server infrastructure, as besides the raw data also data generated by normalization and analytics tools needs to be stored and provided to the scientific community.

5 Will these developments bring societal benefits?

There are some differences in the goals of data representations in those two actions:

The ESCDF provides a standardized data format and an API every code can use. Material science code developers profit from centralizing implementations like efficient parallel IO and hiding file format specific issues. At the same time this allows a certain amount of interchangeability of data, for example for post-processing tools. The data itself is not altered, so that checkpointing and restarting functionalities can be granted without additional data loss.

The NOMAD-CoE aims at making also the data itself comparable, which involves data transformations ranging from simple unit conversions up to normalizations based on reference calculations and analytics tools.

As both initiatives target the whole electronic structure code community, they are based on the same concepts and codes, thus have a large common ground. So, for a maximal mutual benefit, they jointly organized the present workshop.

Many attempts of standardization fail because initiatives are too small to reach a critical mass or try to impose their solution to a community for which it is not profitable to adapt to it, possibly also because due to shortcomings of the standard. This is avoided by involving all major codes right from the beginning. The workshop attended representatives of of the most important codes (see above). Each code expresses key quantities like wave functions, operators, and density matrices in terms of basis functions. There are various types of such

“basis” established, some of them of very different character. Some codes describe all electrons in this basis, others use a simplified description of the core electrons. This results on one side in basically different data representation, on the other side also comparing certain magnitudes like energies is not trivial. This is addressed within the NOMAD-CoE, with funding currently granted until October 2018, by developing a conversion layer for normalizing this data and analytics tools for error quantification.

The conclusions of the discussion, as reported above, will be implemented in the data format of the NOMAD Archive. A key to success, here, may be that NOMAD is not “ imposing” the common format to code developers, but rather to convert existing output into the common format.

However, a direct standardization of the code outputs would greatly facilitate the maintenance of useful big –data storage. To this end, an API definition, which is directly usable for all represented codes, has been developed in the second part of the workshop, and a library implementation will follow.

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High Throughput materials discovery: Perspectives and Challenges in theory and experiment

Location: CECAM-ISR, University of Tel Aviv, Israel
Webpage: https://www.cecam.org/workshop-0-1204.html
Dates: February 3, 2016 to February 5, 2016

1 State of the art

The design of new materials with specific properties is one of the main challenges of modern materials science. In the last decade, there was great progress of both theoretical and experimental methods that are aimed to find novel materials, with desired physical properties, by design. On the experimental side, combinatorial materials methods became a very powerful tool for the automatic production and characterization of a very large set of possible compounds. On the theoretical and computational side, there is constant improvement in the predictability and scalability of advanced computational chemistry methods such as Density Functional Theory (DFT) and beyond, this progress allows the use of high throughput methods for materials design. Furthermore, the ability to calculate and verify experimentally the properties of many materials allows to apply advanced methods such as data mining, statistical analysis, and machine learning algorithms that enable researchers to draw physical conclusions from the behavior of families of materials and even find new physical trends. The combination of all of the above methods leads to the creation of a new paradigm of materials informatics that resembles the appearance of bioinformatics in biology and biochemistry. To support this progress the US White House has declared in 2011 the "Materials Genome Initiative" (MGI), aimed to accelerate the discovery and industrial exploitation of new materials. On the computational side, this paradigm involves highly multi-disciplinary approaches that combine theoretical chemistry, computer science, informatics, applied mathematics, and thermodynamics. Furthermore, in recent years, there is an ever-increasing synergic collaboration between experimentalists and theoreticians in this field leading to unique mutual feedback circles that result in enhanced capabilities for materials design.

2 Major outcomes

The progress of different experimental and theoretical projects was presented and discussed. Among the many examples that were presented – finding of new oxide based photovoltaic cells with a consistent improvement in efficiency, achieved by experimental high throughput methods. A family of missing oxides that were predicted by computational and verified later by experiment was presented. A high throughput search for novel magnetic materials with a high Currie temperature has demonstrated both the ability to find new materials and the difficulty in finding many of them. The development of new functionals for Density Functional Theory for having better predictions was also presented. Several questions were discussed – the need for better fusion of data coming from experimental and theoretical high throughput efforts is very clear. Another important question is the type of education that is needed for students in this new field of materials informatics. Finally – it seems that impressive efforts were already done in the direction of automatic finding or design of new materials, there are several success stories but the field is still far from fulfilling the high potential and hopes. The creating of large databases and the development of new artificial intelligence methods might give in the future a better fulfillment of the potential and faster finding of new materials. Fusion of data sources can also help in this direction.

3 Community needs

The community of high throughput materials experiment and theory is growing and more databases are being formed for both experimental results and theoretical calculations. There could be several issues that could help faster progress:

- Development of standards that are accepted in all the community, this exists for structure but less for electronic structure and other calculations or measurements. This is already done in many databases (e.g. the AFLOWLIB) but it would help to have an on-going effort of developing universal standards that are accepted by all.

- Checking the idea that publication of results should be supplied with a machine friendly data that can be added to databases or used by others – such an approach was taken in the field of bioinformatics in some of the leading journals.

- Improving the education that is available to students to enter those fields. Currently students are arriving from different disciplines such as physics, chemistry, computer science, materials science and engineering. The education is achieved through on the job training and special workshops, schools and conferences. In some places there are already higher degrees programs in computational materials science. Perhaps there should be also tracks that are dedicated to materials informatics.

All the suggestions should probably be discussed at higher forums of top decision makers.

4 Funding

Funding is needed to support this field in several aspects:

- Research grants that are specifically aimed at promoting high throughput, data assisted, discovery of new materials by experiment and theory. While there are calls for materials modeling there is a place for calls that will specifically promote data assisted methods.

- Funding of leading institutes, which can be government labs or academic to promote standards and to make large amount of information and tools available to researchers.

- 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 Materials Genome Initiative (MGI) are hard to imagine and can be well beyond the current most optimistic view of the field. Like any other new field, the current success stories that are already delivered are lagging behind the long-term potential and vision of this initiative. Again, it is possible to learn from Bioinformatics, initially people thought and promised that it will completely change the worlds of Biology and Medicine, many promises of bioinformatics are still not fulfilled but it has already completely changed biological and medical research and it is very clear that it did not reach yet the full potential. Materials informatics is progressing in a slower pace, there is a less obvious target (e.g. getting the sequence of the full Human Genome, patenting of genes and other initial milestones in bioinformatics) and less specific funding.
Yet, the research of theoreticians and experimentalists in general materials science, computational chemistry and condensed matter physics is already affected by the availability

of larger amounts of data and data analysis tools and this trend is only growing. The progress of artificial intelligence methods such as machine learning and deep learning will also influence the future progress of the MGI. In the long-term future, the methods and databases that are being built today will affect every field were materials engineering is needed and this is practically everything – energy applications, medicine, car and air industries and many others.

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Hydrodynamic Fluctuations in Soft-Matter Simulations

Location: Monash University Prato Centre, Italy
Webpage: https://www.cecam.org/workshop-0-1208.html
Dates: February 9, 2016 to February 12, 2016

1 State of the art

While usual hydrodynamics is a macroscopic (thermodynamic) theory, the small length scales involved in soft-matter systems force us to take thermal fluctuations into account. This is either done via a top-down approach (Langevin noise added to the Navier-Stokes equations, simulated on a lattice or via particles), or bottom-up modeling. In the latter case (Dissipative Particle Dynamics, Multi-Particle Collision Dynamics, Lattice Boltzmann) there are additional (non-hydrodynamic) degrees of freedom, and the noise is applied to those. To successfully apply these methods, one needs not only an efficient computer implementation, but also a thorough understanding of the underlying theory, which is typically fairly complex and advanced. This is the reason why there is clearly a continuous need to foster communication between the various groups who typically are familiar just with one of these approaches, and also to teach the younger generation of researchers. The combined school and workshop took both of these aspects into account.

2 Major outcomes

Firstly, the school comprised a cast of leading international experts who provided a thorough overview over the field. Introductory lectures on basic hydrodynamics, Langevin theory, and Landau-Lifshitz fluctuating hydrodynamics were given by Burkhard Duenweg. Piotr Szymczak then gave a detailed lecture on Brownian Dynamics with hydrodynamic interactions, including a discussion of advanced methods where high-order approximations to the interaction tensors are being used. This was further elaborated by Mike Graham, who put emphasis on the general theory of Stokesian flow and the associated Green's functions, which enables the derivation of new advanced algorithms. Tony Ladd gave an introduction to Lattice Boltzmann methods, while Alexander Wagner discussed thermal fluctuations in this context. Marco Ellero gave a comprehensive lecture on Dissipative Particle Dynamics and Smoothed Dissipative Particle Dynamics, while Thomas Ihle explored the subtleties of Multi-Particle Collision Dynamics. Alejandro Garcia gave an exhaustive lecture on the older (but still useful and successful) Direct Simulation Monte Carlo method. In his lecture, Rafael Delgado-Buscalioni discussed the development of advanced algorithms for fluctuating hydrodynamics (grid-based Navier-Stokes solvers) with emphasis on methods to account for fluid-particle coupling. Finally, this program was complemented by Ravi Prakash Jagadeeshan's lecture on theoretical approaches to the development of closure approximations for the dynamics of polymer solutions with hydrodynamic interactions, highlighting its application to nonlinear rheology. All in all, this program provided a unique chance for graduate students and postdocs to learn about the field from amongst the foremost practitioners of the state of the art.

Secondly, the workshop provided an opportunity for exchange of new ideas and results, in terms of further developments of the methods, their theoretical foundations, as well as of their applications to intricate problems in soft-matter dynamics. A highlight in new method

development was the talk by Robin Ball, who invented an exciting new approach to the calculation of hydrodynamic interactions by means of wavelets. Further methodological advances were provided by Aleks Donev, who discussed the coupling of Brownian Dynamics to on-the-fly Stokes solvers. Theoretical foundations were explored and refined in the talks by Pep Espanol (relation between the theory of Brownian motion and the concept of coarse-graining, with emphasis on interpolation schemes to couple "point" particles to grid solvers), Giovanni Ciccotti (rigorous theory of Non-Equilibrium Molecular Dynamics and its relation to hydrodynamics), and Thomas Ihle (kinetic theory for systems of active particles). There were several talks on the new and emerging field of active particle suspensions (by Suzanne Fielding, Holger Stark, Thomas Ihle), while more traditional but still unresolved questions in the suspension dynamics of colloids, blood cells, star polymers were discussed by Marco Ellero, Mike Graham, and Rafael Delgado-Buscalioni. Alexander Wagner re-visited the topic of Lattice Boltzmann simulations of spinodal decomposition, with an outlook to block copolymer systems, while Alejandro Garcia discussed intricate problems in the field of electrokinetics. Piotr Szymczak presented his recent results on the equilibrium conformations of aggregated chiral filaments, and Tony Ladd investigated the formation of caves and similar geological structures due to water flow. These contributions highlighted the importance of hydrodynamic fluctuations in soft-matter dynamics, and even more the fact that the field of non-equilibrium hydrodynamic phenomena in soft-matter systems is vast and to a large extent poorly understood.

3 Community needs

The community clearly needs access to HPC facilities - these simulations are typically large-scale, involving many degrees of freedom and long-time scales. Most active groups in the field, however, seem to be reasonably supplied. Also, most groups seem to have functioning codes that serve their purpose. However, it may be advisable to maintain the contacts between different groups employing different and complementary approaches, with the view of possible future developments of novel hybrid algorithms, which may be the method of choice for problems that we are presently not even aware of! Contact to experimentalists is vital, since it is they who provide the new challenges and poorly understood phenomena. This was clearly reflected in the workshop, where most investigations were motivated by unresolved experimental results. However, we feel that these contacts are well established and there is no particular need to further foster these. We consider education in the field as very important, given the complexity of the theory on the one hand, and the smallness of the community in this fairly specialized area on the other, which implies that there would be organizational obstacles to establish a suitable course at, say, a university. We therefore feel that CECAM can and should play an important role in this regard. In view of all these considerations, we believe that it is a good idea to have CECAM workshops/schools on the subject on a semi-regular basis.

4 Funding

The event was funded by the CECAM node SMSM, in accord with what the node views to be one of its central missions. We are not aware of external funding sources that could finance an event like ours. Joint research proposals were not discussed at the meeting, at least not on the formal level. We also did not view this to be the purpose of the meeting.

5 Will these developments bring societal benefits?

The benefits of this kind of research are intangible and not quantifiable on a short time scale. Of course, soft-matter systems are fundamental to various industries (e.g. pharmaceuticals, food, oil recovery, plastics, cosmetics, chemicals), but the investigations discussed in the meeting were not driven by immediate applications, but mostly rather by the desire to understand the underlying physics.

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Models for Protein Dynamics 1976-2016

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1116.html
Dates: February 15, 2016 to February 18, 2016

1 State of the art

The workshop “Models for Protein Dynamics 1976-2016” celebrated a field that was nurtured by Carl Moser’s CECAM and the ground-breaking 1976 workshop attended by most of those who led the field of biomolecular simulation in the past 40 years. The first simulation of a protein was actually performed during the two-month workshop.

In the 300-page workshop report are described a 8.8 ps simulation of a 58 amino-acid protein in vacuo (McCammon), and a 1 ps simulation in a crystal (Rahman & Hermans). The increase in computer power since the 1976 workshop, although predicted, has been extraordinary. Yet an improvement of about 10 orders of magnitude in computer power While enormous progress has been made on some issues, remarkably little has been made on others. Thanks to immense advances on the experimental techniques available to investigate biological molecules, and with the crucial contribution of computational methods in the analysis of experimental data, we now have a much broader, and deeper, fundamental understanding of how biological macromolecules behave. Biomolecular simulation has been instrumental in revealing the role of dynamics in biological function, and in directing the development of experimental techniques more suited to understand biological function, such as single molecule ones.

Despite 40 years of remarkable progress, applications of biomolecular simulation still lag behind. The role of simulation in the development of new drugs, for example, is limited relative to what may have been predicted, say, twenty years ago. Simulation has not replaced experimental structure determination of proteins; conversely, the importance of dynamics highlighted by the first simulations is now broadly recognised as crucial to all properties of proteins and the structure–function paradigm, and provides a spotlight on functional disordered protein states, allostery and aggregation. Methods to treat quantum mechanical degrees of freedom or inclusion of polarisability in classical macromolecular models are still evolving but are currently computationally inefficient, while classical potentials, not dissimilar from those used 40 years ago, turn out to be surprisingly accurate and, with a few tweaks they allow ab initio folding of a few proteins to be observed during millisecond long simulations.

2 Major outcomes

The scope of the proposed workshop was to gather those who participated to the 1976 workshop “Models for Protein Dynamics” and current key players in the field of biomolecular simulation to discuss successes, failures and future challenges. What will computational studies of biomolecules deliver in the next 40 years? And what should we focus on now for that progress to occur faster?

This workshop has been an exceptional occasion for leaders in the field to present their vision, suggest goals that are within reach and those that require collective effort.

Some of the participant to the 1976 workshop who could not attend this workshop contributed with memories and thoughts that have been published with the programme of the workshop, and are reported at the end of this report.

The first talk, by Herman Berendsen (and delivered by Sievert-Jan Marrink since Herman was not able to travel) evoked the pioneering times of biomolecular simulation (and simulation of complex chemical systems in general) when CECAM's workshop contributed enormously to the development of the field.

The workshop was dominated by discussion. The main focus was assessing the achievements and the failures of 40 years of biomolecular simulation and propose a roadmap to address the full complexity of biological systems in the next 40 years.

Much longer simulations and advanced sampling methods have made exploration of free-energy landscapes possible, but the large barriers, for example, between side-chain conformations, cannot be crossed during even long simulations.

To what extent can we freeze degrees of freedom and reproduce experimental properties? Coarse-graining, still considered by many as a necessity if systems that reproduce the complexity of the cellular environment are to be studied, yet there is little consensus on how this can be done rigorously.

Force fields remain a hot topic. Although atomistic force fields, developed independently during the past 40 years are converging, in the sense that mostly the same results are obtained using different ones, and agreement with experimental results is better than ever, improvements have been obtained by adding a huge number of parameters. During the workshop consensus has been reached on the fact that time has come to stop tweaking old (if not dead) force fields by modifying and adding new parameters, and novel ones, based on alternative functional forms, should be determined from scratch.

One proof of the reliability of simulations in biomolecular sciences is that, while simulations have been considered a curiosity for decades, and unable to address the experimental hypotheses, now experiments are routinely complemented with simulation, even if sometimes only to illustrate in real space and time, at atomistic resolution, conclusions that could have been drawn directly from the experiment.

In these past forty years simulation has not solved all the questions, but has certainly become a field of interdisciplinary science. We have now computational tool and understanding of the physical principles and of the biological complexity that we did not have previously. Or, to quote Michael Levitt, we have now the chance to do things better.

3 Community needs

Since 1976 computers have evolved enormously. The fastest computer available to date (Anton) is about 10 orders of magnitude faster than the faster computer available in 1976, while for a few hundred Euros one can buy a GPU that is roughly 108 times faster than that. The field has developed and progressed, but the expectation of gaining ability to predict all molecular phenomena related to life and disease through models and numerical simulations is still not clearly within reach. It was observed that in nowhere the increase in computer power has brought proportional progress (think airplanes design or public administration!).

In the context of biomolecular simulation, the reasons of this "apparent failure" was extensively discussed during the workshop, although some pointed out the successes,

including those that were not predicted in 1976, and the importance of simulation in fundamentally understanding the physics behind complex molecular systems.
Indeed, we now understand the importance of entropy in determining the stability of specific molecular conformations and complexes, even if determination of free-energy differences still, in general, lacks accuracy; the ability of obtaining precise estimation of free energy of binding, for example, is crucial in the design of new drugs.

4 Funding

No funding needs or strategies were discussed.

5 Will these developments bring societal benefits?

The ability to simulate correctly and efficiently proteins, and in general biological systems, will have an obvious and crucial impact in drug design and on other aspects of the pharmaceutical production.

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Entanglement in Strongly Correlated Systems

Location: Centro de Ciencias de Benasque (Spain)
Webpage: https://www.cecam.org/workshop-0-1275.html
Dates: February 15, 2016 to February 27, 2016

1 State of the art

In recent years we have lived a series of important advances in the study of systems with strong correlations, both from a numerical and analytical perspective. From the point of view of numerical calculations, new methods based on tensor networks are pushing the boundaries of simulation algorithms in unprecedented directions (such as MPS, PEPS, MERA, and related techniques extending the Density Matrix Renormalization Group method). Equally important are recent advances in quantum Monte Carlo (e.g. to compute topological entanglement entropies) and exact diagonalization (in e.g. numerical calculations of the entanglement spectra). From the point of view of analytical methods, important developments have also taken place recently. Examples of these are continuous unitary transformations to assess topological phases, AdS/CFT methods to describe superconducting states of matter, the analysis of boundary Hamiltonians in PEPS, string-net models for doubled topological phases and its connection to loop quantum gravity, and the tensor network description of chiral topological phases in terms of 2d PEPS.

2 Major outcomes

The workshop has fully accomplished its major goal to favor the advance in the field of strongly correlated systems. On the one hand, it has host numerous discussions of current developments in the field among the leading researchers in the area with specialized talks focusing on recent results. On the other hand, it has provided long "perspective" lectures on advanced topics, with the aim of being understandable by the whole audience (specially to many young postdocs and graduate students who participated), in order to promote a common scientific basis for researchers in the field.

3 Community needs

The necessity for such a specialized meeting in the area of strongly correlated systems was clear given its fast development and the critical mass acquired by the community. This workshop offered a dedicated forum for the presentation of recent progress in the field, the discussion among experts and the exchange of new ideas. Regarding the second objective, we have obtained the participation of well-known experts who provided lectures with a broad perspective. The exchange of ideas will plant the seed for many future international collaborations.

Examples of specific topics treated in the workshop are:

• New tensor network numerical methods

• Advances in topological order

• Tensor network description of chiral topological states

• Entanglement Hamiltonians, AdS/CFT, and Holographic Principle

• Simulation of lattice guage theories

4 Funding

The workshop benefited from the CECAM funding (13 kEuros) and ~5 kEuros from the MAINZ graduate school of excellence. No specific funding strategies for research in this area were discussed.

5 Will these developments bring societal benefits?

The field sf strongly correlated systems, especially topological phases, etc... is still very much an area of fundamental research. While applications to the design of quantum computers have been proposed and are being pursued by research groups funded by Microsoft Corporation, it will be several years before this field and the research presented at the workshop will be of more immediate interest for commercial exploitation by European industry.

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Beyond point charges: novel electrostatic developments in force fields

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1263.html
Dates: April 4, 2016 to April 7, 2016

1 State of the art

Point-charge based force fields have been, and still are, widely used in molecular simulations for many years. This is particularly true in the modelling of biological systems where force field families such as and AMBER and CHARMM have now been parameterised to the point where accuracies of less than 1 kcal mol-1 can be achieved in blind challenges of, for example, small molecule free energies of hydration. However, it is recognised that the accuracy of the common, empirical, pair-wise additive fixed point change model is very limiting for many applications. It is known to give a poor representation of the electrostatic potential around many molecules, and to be incapable of capturing environment-dependent polarisation effects.

To address these known limitations, more sophisticated functional forms to capture electrostatic interactions have been proposed. These include the use of distributed multipoles to provide a better representation of the molecular electrostatic potential, and induced dipole and Drude models to capture explicit polarisation. While the improved representation of the underlying physics should of course yield improved accuracy, the use of more elaborate functional forms introduces additional costs in terms of more parameters to optimise, and longer calculation times. This workshop examined the current state of the art with these new potentials, considered the likely advances over the next few years, and the issues which stand in the way of more widespread adoption of these methods.

2 Major outcomes

The workshop focused on five main themes:

- The deficiencies of conventional fixed charge force fields.

  It is recognised that fixed charge force fields have their limitations, and a number of examples were discussed where extensions beyond fixed charges were required to give agreement with experiment. Notable examples included crystal structure prediction and calculation of IR spectra. Interestingly, simple scaling of charges in charged systems was shown to give improved results in some cases.

- The hierarchies of methodologies for moving beyond this approximation, including multipole-based methods and polarisable potentials.

  In terms of permanent electrostatic interactions, approaches to move beyond atom-centred point charges including the addition of off-site partial charges and multipole methods, were discussed. It was expected, and preliminary results demonstrated, that the correct incorporation of charge penetration effects in this context would be helpful for overall

accuracy and force field transferability.
The two main approaches to including polarisation – Drude models and inducible dipoles – were presented, without a clear view as to which was to be preferred. Having a plurality of models under development was felt to be advantageous in this context.

- Issues of parameterisation of advanced electrostatic models.

  A number of issues with the stability of multipoles derived using a distributed multipole analysis were discussed, and it was felt that an alternative approach based on Iterative Stakeholder Atoms was to be preferred. The multipoles derived through this route appear more robust and transferable. An interesting method to reduce the overall number of multipoles without a significant loss of accuracy was described, and it was noted that this could have immediate impact in the area of crystal structure prediction. Finally, to address the difficulty of the simultaneous optimisation of many parameters, the consensus was that automated fitting methods such as “Force Balance” should solve this problem, particularly since experimental and theoretical data are combined as targets in the fitting process. Multipoles derived from the analysis of high-resolution crystal structures may prove useful in this context, as will the electric fields in proteins derived from Stark effect experiments, to provide restraints to the fitting process.

- Issues of implementation of these advanced potential energy functions.

  Algorithmic improvements were discussed, particularly in the context of inducible dipole models, including extended Lagrangian methods to improve convergence. In terms of new implementations of these models, domain decomposition software exploiting these advanced potential energy functions is becoming available, as are GPU implementations. It is to be hoped that the combination of better algorithms with more efficient codes will extend the number and scale of simulations that can be performed. This is turn will allow for proper, large-scale, testing of the simulation parameters, something that has hitherto proved impossible.

- Applications of these methods, in particular the contexts in which the expense of these new force fields is rewarded with improved scientific insight.

  A number of target systems were identified where moving beyond atom-centred point charges will prove advantageous. These include crystal structure prediction, calculations of the Stark effect due to electric fields inside protein systems, and DNA compaction by cations.

3 Community needs

Overall it was felt that the field was at a turning in terms of its potential impact. A number of approaches to include a more rigorous description of electrostatics and polarisation are in development, and it was felt that this should be encouraged. The combination of new algorithms and better optimised software will increase the scope and scale of the scientific problems that can be tackled. The use of automated parameterisation procedures combined with the capability of performing the sort of large scale testing hitherto seen only in the context of fixed-charge force fields, will allow force field performance to be unambiguously assessed, and areas for improvement identified. In terms of identifying the most fruitful application area for applying these potentials, crystal structure prediction was felt to be particularly ripe. It is a mature discipline with an established programme of large-scale blind challenges. As a result, large amounts of experimental and simulation data are available, allowing not only for the experimentally observed structure to be identified, but for the energies of possible decoy structures to be calculated and ranked. Combining simulation

with the experimental multipoles that may be derived from high-resolution crystal structures may prove advantageous in terms of force field functional form and parameter optimisation.

4 Funding

In terms of the implications of this work for funding bodies, we have some specific recommendations. The important developments described here are being undertaken in research groups spread across at least two continents, and often independently. A multidisciplinary approach is required. Algorithm development may be taking place in a comparatively inefficient, but familiar code, such that its advantages will not be properly realised without the algorithm being deployed in a faster, domain decomposition code, for example. As such, funding is needed for two purposes. First, collaboration networks need to be funded to allow the exchange of scientists within and outside the EU. This will help foster the cooperation needed. Second, funding to support research based directly on these collaborations needs to be available. Thus, funding schemes across countries and continents need to be developed, through funding agencies supporting joint-funding schemes.

5 Will these developments bring societal benefits?

The potential impacts of developing and applying more accurate potential energy functions are significant. Accurate crystal structure prediction, for example, allows for the optimisation of the solid phase in pharmaceutical development, giving improved bioavailability and hence biological response. Ultimately, more accurate potentials will deliver more accurate predictions.

The next few years will be particularly exciting. New codes and methodologies are becoming available, allowing robust validation and more widespread use of these new energy functions. It is therefore planned to repeat this workshop in three years' time, to review our success and look further ahead.

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Chemical Energy at the Nanoscale: Simulation Meets Experiment

Location: CECAM-ES
Webpage: https://www.cecam.org/workshop-0-1287.html
Dates: April 5, 2016 to April 7, 2016

1 State of the art

The manipulation and control of chemical energy over molecular and mesoscopic length scales underpins much of our current efforts to understand and design the building blocks of next-generation energy materials for catalysts, batteries, supercapacitors, or gas stores. Particle-scattering techniques at intense sources offer the exciting prospects of providing unprecedented insights into the mechanisms of chemical binding, energy transport, conversion, and storage, particularly under nanoscale confinement. Confined spaces are readily available, e.g., in nanostructured materials such as zeolites, Metal-Organic Frameworks (MOFs) or graphene-based substrates. State-of-the-art muon, neutron and synchrotron techniques provide an excellent route to interrogate these confined systems, but the interpretation of experimental data still remains challenging beyond the use of simplified and heuristic physical models, or a (rather sporadic) use of first-principles calculations. Computer Simulation (CS) offers a yet-to-be-exploited bridge across these and other experimental techniques. Recent successes in this direction include Inelastic Neutron Scattering (INS) and Synchrotron-based Spectroscopy (SS) in conjunction with Density Functional Theory (DFT) to establish how THz modes are linked to anomalous elastic properties in MOFs and how these may affect molecular uptake. Experimental efforts in the field of charge storage under realistic conditions are also on the rise. This is an area where CS can play a pivotal role in the design and interpretation of scattering experiments, including operando studies of proton conduction and charge-discharge kinetics & dynamics in nanostructured media. Neutron scattering provides a unique means of accessing the dynamic structure factor (particularly at low energy transfers), to quantify transport coefficients or the vibrational density states, links that remain to be fully explored and exploited. A combination of scattering experiments and computational methods (e.g., classical molecular dynamics and Grand Canonical Monte Carlo and molecular dynamics, as well as electronic-structure methods, particularly using DFT) provide a sound framework for the rational design of energy materials. Computation can be used to inform, guide, and interpret complex scattering experiments where the link between the 'raw observable' (e.g., a differential scattering cross section) and the physico-chemical property of interest (e.g., binding energy, ionic or thermal conductivity) may not be a direct or obvious one, or has not been explored at all to date. All of these aspects led to lively discussions during workshop.

2 Major outcomes

Much of the current approaches to store chemical fuels such as molecular hydrogen or hydrocarbons rely on the use of nanoporous media - over 50% of all catalysts used by the chemical industry currently involve the use of zeolites. Neutrons provide an ideal probe to analyse light species and, in concert with computational modelling, they can address key questions such as the rational design materials with pores that match molecular diameters, as well as the desired binding energies. In the case of molecular hydrogen, these requirements are relatively well understood, yet we are not there yet in terms of finding useful materials for mobile applications. CS has and can still play an important role in narrowing the search for suitable materials both in terms of adsorption energies, pore size, and adsorption-desorption kinetics. On the experimental front, SS provides a route to study electronic structure and binding as well as local atomic structure around heavier (i.e., metallic) species, all of which go hand-in-hand with the use of neutron techniques to probe light adsorbates. CS provides a good complement to these experiments, by assisting in the interpretation of X-ray spectra, which are very sensitive to small structural changes (as illustrated in MOFs), or by computing dynamic structure factors. Total scattering techniques and INS also constitute superb routes to explore disordered materials (e.g. polymers) and their dynamical response, including metastability and kinetic trapping. The study of the latter in realistic materials still represents a challenge to computational methods. Further work in the area of Nuclear Quantum Dynamics (NQD) is also needed, particularly in the context of light atomic species and the computation of dynamical observables in real time. This area has witnessed some recent successes driven by the combination of neutron experiments and cutting-edge computational methods – see, e.g., the forthcoming CECAM event http://www.cecam.org/workshop-0-1314.html). Atomic mean-kinetic energies are sensitive to the chemical environment, with important implications to the study of disordered and complex structures (amorphous ices, graphite oxide, etc). The implementation and development of computational methods (thermostats, quantum Monte Carlo, path integral molecular dynamics, ring-polymer molecular dynamics, instanton theory, etc) is desirable, as it would provide a rapid development in the area of light-weight media for energy applications.

On the theoretical and computational fronts, the area of supercapacitors has evolved significantly in the last few years. Dynamic-charge models provide an essential ingredient to model carbon-based electrodes. Mean-field theories have been used to predict superionic states, which speed up charge-discharge dynamics, a key feature required for next-generation supercapacitors. Also, spatial confinement can also give rise to entropic barriers that influence in an unexpected way molecular transport at the nanometer scale. These theoretical efforts have not been followed up yet by systematic experimental studies. At this juncture, the use of experimental strategies to sample the dynamics of charged liquids under nanoscale confinement would be very both interesting and timely.

Rare-event sampling techniques in combination with first-principles methodologies also provide a powerful tool to investigate catalytic and energy-storage media, to explore the role of the surrounding confining environment or the solvent (water). Ab-initio computations of these (unavoidably large) systems should also provide entirely new insights in catalysis, including biological and biomimetic media. Relative to the use of force fields, an immediate advantage of DFT lies in its ability to interrogate the underlying electronic density and bonding in the material, although this is still accompanied by a relatively high computational cost. The use of linear-scaling techniques expands significantly the capabilities of DFT methods, making it possible the study of 103 -104 atoms over timescales of tens of picoseconds. Recent advances on this front pave the way for the study of intrinsically disordered media ubiquitous in practical applications.

Likewise, the computational investigation of porous materials over longer length and timescales will benefit from the further development and use of polarization methods that build and take us beyond the "image-charge" approach. The advent of novel "soft" porous structures, characterized by the presence of low-frequency modes, brings also new challenges, as well as opportunities. Future force-field developments should consider benchmarking themselves against dynamic features as well as structural ones, which are already the main focus of existing strategies. Experimental studies also remain a key ingredient to benchmark these new approaches, including the study of yet-to-be-established correlations between storage capacities and pore structure & dynamics. The osmotic ensemble provides an interesting technique to investigate flexible nanoporous solids.

The investigation of pores in rocks is also of particular interest for gas storage. Computational approaches based on hybrid Reverse-Monte-Carlo techniques and its variants can be used in conjunction with experimental data obtained from, e.g., neutron diffraction, to reconstruct the pore structure on a computer. These computational techniques have proven quite valuable to date yet their extension to the dynamical domain remains an outstanding challenge to both theory and computation. Another major bottleneck is the accuracy of the force-fields, either classical or reactive, which still provide contrasting results, particularly in dynamical properties.

Although full agreement with experimental data is the ultimate goal, it was noted at the workshop that this is not always possible, since physico-chemical phenomena in nanostructured media inevitably involve kinetic effects, which may sometimes not be captured by current computational approaches. This aspect should be taken into account in future computational work, as well as in force-field development.

3 Community needs

Our community would benefit from the development of robust computational methods and tools for the interpretation of experimental data. Current efforts in this direction exist, e.g., the nMOLDYN software package to link molecular dynamics simulations to neutron-scattering data. Further development, integration, and dissemination of these computational tools as part of wider research programmes would offer much-added value. These efforts would also enable the implementation of databases containing experimental and computational results for further data-mining, and a direct assessment of the latter, including the accuracy of the corresponding force-fields (in classical simulations) or functionals (in DFT computations). Establishing such a database would be of enormous benefit to our community.

4 Funding

The further development of the aforementioned methods will certainly benefit from a more integrated approach across experiment, computer simulators, and theory. Current initiatives within the European Materials Modelling Council (EMMC) can serve as an initial forum to connect all relevant players, as well as to target H2020 actions such as ITN or FETOpen in the foreseeable future. Europe is in a privileged position to lead these developments, as it hosts leading particle-scattering sources, as well as internationally renowned groups in computational materials chemistry.

5 Will these developments bring societal benefits?

The control and manipulation of chemical energy at the nanoscale will lead to more efficient materials, and possibly uncover hitherto-unveiled energy-conversion mechanisms or new catalytic processes. In the short term, it will allow the optimization of materials for gas storage and catalysis, with a direct impact on energy applications. Our ability to design new materials for fuel storage, or improve the charge-discharge dynamics of supercapacitors, will impact the development of greener routes to power cars, and the use of efficient wearable devices. An increased synergy between experiment and simulation provides new avenues to develop accurate computational methods to predict adsorption and transport in carbonaceous materials, or the stability of clathrates, of direct relevance to the gas and oil industries.

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Probing Potential-Energy Surfaces

Location: Zermatt
Webpage: https://www.cecam.org/workshop-0-1253.html
Dates: April 10, 2016 to April 15, 2016

1 State of the art

The potential energy surface (PES) is a fundamental mathematical concept in physics, chemistry, and materials science. The PES relates the potential energy of a given system, for example a material or a molecule, to its structural parameters, i.e. the positions of the atomic nuclei. Stationary points, i.e. minima and saddle points, of a PES represent stable conformations/configurations and the transitions between them. Probing potential energy surfaces (PPES), finding these points and describing their relative energetics is key to understand molecular structure and dynamics, chemical reaction mechanisms and catalysis, or material properties.

The most fundamental PPES is the accuracy of the energy function that is used. The applied methods range from simple empirical potentials to density-functional approximations and up to very accurate benchmark methods like coupled cluster or quantum Monte Carlo. In practice, one has to balance accuracy and computational cost. Realistic problems are often characterized by a substantial number of degrees of freedom. As a consequence, a large search space results that has to be sampled appropriately. Subsequently, descriptive coordinates of the PES have to be selected or combined to create an understandable representation.

2 Major outcomes

After successful meetings in 1994, 1999, and 2005, the workshop stayed within the interdisciplinary tradition of the PPES series and brought together scientists with different back-grounds, e.g. in condensed matter physics, materials science, computational physics, chemistry, and industry. Experts of the field of total-energy calculations, scientists who develop or enhance methods, and those who apply the information gained by these techniques had the possibility to exchange ideas and experiences.

A special focus of the PPES-IV workshop was on big-data-driven materials science, e.g. the Materials Encyclopedia and the development of Big-Data Analytics tools for materials science of the NOMAD Center of Excellence.

Deliberately, the session “Materials big data the concepts, infrastructure and applications” was set to the very beginning of the workshop as the major future challenge of the field lies in the utilization of large-scale electronic-structure calculations and machine learning to solve the pressing questions of mankind like developing a carbon-neutral and energy efficient industry. PESs can be input to, as well as output of, machine learning approaches. Machine learning can also be used to reduce the dimensionality by predicting collective variables for both, sampling and plotting of a PES. The speakers Matthias Scheffler, Fawzi Mohamed, Emre Ahmetcik, Georg Huhs, Johan M. Carlsson, and Hagen-Henrik Kowalski covered a variety of different topics and open questions of the field.

It followed two sessions on “Electron-phonon coupling” and “Semiconductor / photovoltaics and excited states” respectively. In realistic materials, like catalysts or also in semiconductors and photovoltaics, excited states and the coupling between electronic and nuclear motion (electron-phonon coupling) play an important role, for example in electronic spectroscopy or in thermal transport. Methods to incorporate such effects were covered by the speakers Stefan K. Estreicher, Christian Carbogno, Claudia Draxl, Friedhelm Bechstedt, and Axel Groß.

During the session on “(Bio)molecules and water”, ways to sample the structure space of biomolecules and the pitfalls when it comes to a sufficiently accurate description of their energetics were discussed, as well as the peculiarities of describing “water”. Speakers were Roberto Car, Carsten Baldauf, and Mariana Rossi.

After having examined current challenges, the talks in the “basic concepts” sessions of the speakers Xiangyue Liu, Björn Bieniek, Karsten Reuter, Niklas Menzel, Matthias Rupp, Sebastian Kokott, Igor Ying Zhang, Tonghao Shen, and Christopher Sutton dealt with the underlying concept of probing potential energy surface, namely the energy function.

The final session was dedicated to “Surfaces: nanostructures and catalysis”. Heterogeneous catalysis is a classical example for the usefulness of a PES point of view. A particular focus of this session was the realistic treatment of catalysts by incorporating defects and the assessment of alternative reaction pathways by means of the topology of minima, transition states, and bifurcations. The speakers Harald Brune, Christian Ratsch, Bryan Goldsmith, Karl-Heinz Ernst, Hong Li, Weiqi Wang and Sergey Levchenko covered a wide variety of questions in different systems.

The entire program of the workshop, including the titles of the presentations can be found here:
http://th.fhi-berlin.mpg.de/meetings/PPES2016/index.php?n=Meeting.Program

3 Funding

For workshop funding, besides CECAM and psi-k, the NOMAD center of excellence is a relevant funding opportunity for us.

Joint research proposals were discussed during the meeting.

4 Will these developments bring societal benefits?

Yes

5 Participant List

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Theoretical and Computational Studies of Non-Equilibrium and Non-Statistical Dynamics in Gas-Phase, Condensed-Phase, and Interfacial Reactions

Location: CECAM-FR-IDF, Institut Heny Poincaré (salle 314), Paris, France
Webpage: https://www.cecam.org/workshop-0-1241.html
Dates: April 11, 2016 to April 13, 2016

1 State of the art

Whether chemical reactions proceed through statistical or non-statistical mechanisms is a long-standing problem. One of the most reliable and widely used models in reaction dynamics is transition state theory (TST). However, advances in experimental and theoretical methods reveal the existence of non-statistical effects in a number of chemical reactions. These effects cannot be taken into account by TST, and although they can usually be neglected in the calculation of highly averaged macroscopic coefficients, as the thermal rate constants, they are of key importance in the analysis of the reaction from a microscopic point of view.

We can distinguish two classes of non-statistical effects: (i) non-RRKM, where IVR is not complete; (ii) non-IRC, when the reaction does not follow the intrinsic reaction coordinate (IRC). Their borders are not always sharp and other classifications were suggested. A close interplay between theory and simulations is necessary to understand these phenomena and to set up a well-defined approach to study and predict chemical selectivity.

Direct dynamics simulations can be employed to study and identify non-statistical phenomena. Thanks to the increasing computer power, direct dynamics can nowadays be applied to relatively large systems in gas phase, condensed phase or in vacuum/solid interfaces. These simulations can help improving the existing theoretical models, which in general are based on statistical assumptions and on a reduced dimensionality potential energy surface.

In the gas phase, there are examples of non-RRKM and non-IRC behavior for both unimolecular and bimolecular reactions. In condensed phase, post-TS dynamics simulations can help to understand the selectivity in organic reactions.

2 Major outcomes

An important conclusion from the workshop is that a new theory has yet to be developed to describe both the statistical and non-statistical limits of chemical reactions. That theory cannot rely on previous models like RRKM. By way of example, an emergent strategy is to study phase space structure rather than configurational space. This methodology was already successfully applied to the study of non-statistical “roaming” mechanisms in small molecules with reduced dimensionality potential energy surfaces.

Regarding the well-known ZPE problem that affects classical trajectories, a simple and promising method was proposed at the workshop. The method was successfully tested on a system that behaves according to RRKM theory.

It will be of interest to extend the methodology to non-statistical reactions and to compare the results with accurate QM methods.

On the other hand, it will be important to design new QM/MM methodologies for condensed phase dynamics. In particular, there is a need for accurate strategies to include a significant number of solvent molecules into the QM part. One way to do it would be to generalize methods for constraining the configuration space (like Boxed Molecular Dynamics, BXD, developed by participants of the Workshop) of the first solvation shell without significantly perturbing the dynamics of the reaction event.

A themed issue of “Philosophical Transaction of the Royal Society A” will be edited by the organized on the topic of the workshop with contributions from the invited speakers. This issue should be ready for beginning of 2017.

3 Community needs

In terms of hardware, it would be interesting to explore the possible use of GPUs to carry out dynamics simulations. This would entail the adaptation of some of the programs. At present, a drawback of this architecture is the relatively modest memory resources, which makes it difficult to apply non-adiabatic direct dynamics techniques based on wave function theory.

The Workshop has facilitated the collaboration between several research groups to implement/interface different algorithms/codes. For example, the transition state search algorithm developed by one of the participants will be interfaced with TeraChem, which uses GPUs for first principles molecular dynamics. Also the possibility of using Tight Binding DFT (DFTB) when studying large systems was proposed. Additionally, the suitability of various strategies to construct potential energy surfaces like Empirical Valence Bond, the highly accurate Permutational Invariant Polynomials, or the use of direct dynamics will be tested on several systems of different sizes.

The community would benefit from a centralized web platform providing access to quantum dynamics software, potential energy surfaces, benchmark results, and description of the underlying algorithms.

We plan to organize in the near future a training workshop on nonstatistical dynamics for graduate students and postdocs.

Finally, it was suggested to design a web portal to host the various computer programs developed by the participants of the workshop as well as a database with the trajectory snapshots of the simulations carried out by the different teams for further analyses. That web site would be available to the scientific community.

4 Funding

Several researchers that attended the Workshop have funding through COST actions. One goal of the meeting is to incorporate more researchers in existing COST actions of mutual interest.

Additionally, some work packages of the H2020 Center of Excellence for Computation E-CAM are closely related to the topics covered in the workshop and it would be worth exploring our involvement in this project.

5 Will these developments bring societal benefits?

Accurate treatment of nonstatistical effects is becoming increasingly important in predicting the outcome of catalyzed organic reactions and in simulating mass spectra (MS) of molecules. In recent years, theory has proven to be of paramount importance in these areas, and it has come to a point where it is nowadays an indispensable tool that helps design experiments.

From this perspective, our field is expected to be of great value in the effective synthesis of new drugs with potential use in medicine, and in the development of more accurate protocols of analysis through MS experiments.

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Ultra-fast phenomena in quantum physics: a challenge for theory & experiment

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1257.html
Dates: April 11, 2016 to April 15, 2016

1 State of the art

With the advent of nanoscale physics and ultrafast lasers it is now possible to directly probe real-time the correlation between particles in excited quantum states. In addition, it is now possible to control and manipulate the opto-electronic properties of a wide range of materials by tuning the properties of the external laser field.

Nevertheless, despite the massive number of available experimental results there are still scarce numerical and theoretical methods in use of the scientific community. The fast development of new characterization techniques and the production of stable nanoscale materials have not been followed by a similar evolution of the theoretical tools.

Experiments are usually carried on systems, such as nanostructures and biological systems, that are formed by hundreds/thousands of atoms, and their peculiar properties are related to their reduced dimensionality and extended surface. Any reliable theory is inevitably linked to a detailed knowledge of their structural and dynamical properties. Due to the complexity of these systems, however, state-of-the art methods are either confined to simple models with empirical parameters, thus depriving the theory of its predictive aspiration.

An alternative to simple models are Density Functional Theory and the Green's function formalism. These formalisms are two of the most powerful and versatile in physics, and have already been proved to be extremely useful in several other contexts. Still the communities working with different methods remain fragmented and, often, not in contact among themselves and with the experimentalists. In this way, theoretical advances are slowed down and the possibility of inspiring new experiments and practical applications is jeopardized. This situation is unavoidably creating a gap between theory and experiment.

2 Major outcomes

The goal of the workshop was to gather together several prominent theoretical and experimental scientists working on ultrafast phenomena. The talks have stimulated several discussions during the coffee-breaks, lunches and the round table.

We found the necessity of advancing state-of-the-art techniques in the following sectors:

1. Functional design: The use of time-dependent density functional theory is most welcome in materials science due to the favourable scaling with system size. However, in the nonlinear transient regime the commonly used adiabatic local density approximation suffers from some drawbacks. We identified the features that a TDDFT functional should include for the description of important correlation effects in transient spectroscopy. We also discussed the possibility of building nonadiabatic functionals from recently proposed schemes based on non-equilibrium Green's functions (NEGF). Another thing we discussed is nonadiabatic effects in finite systems. Here quantum chemistry methods offer accurate benchmark results to assess the importance of non-adiabaticity and possibly suggest which scattering

mechanisms to include in the NEGF approach.

2. Strong-correlation: Another topic of discussion has been how to export to the time-domain strong-correlation approaches and how to use them in a first-principles manner. The discussion was mainly focussed on nonequilibrium dynamical mean-field simulation of inhomogeneous systems.

3. Nuclear motion: The interaction between electrons and nuclear vibrations is ubiquitous and it plays a crucial (a not yet fully understood) role in out-of-equilibrium situations. There have been several talks and discussions about successes and failures of different methods (and implementations), namely the diagrammatic approach based on the second-Born approximation, Ehrenfest dynamics and the surface hopping method. In particular the focus has been on dissipation and decoherence effects in bulk systems, and in charge transfer processes in finite systems.

4. Finally we briefly discussed the more complicated dynamics of magnetic systems (again which approximations for different systems and for different regimes) as well as how to find and eventually how to design the shape, duration and intensity of a laser pulse to steer the dynamics of electrons (optimal control theory)

3 Community needs

On the basis of the discussions during the workshop it was possible to identify several potential fields of common interest that reflect the main needs of the community:

1. Need for a virtual infrastructure to ease the communication and the knowledge transfer among the scientists working with similar techniques but on different systems. A possibility could be the expansion of the collaboration team within the European Spectroscopy Facility or within the existing European centers of research like the Deutsches Elektronen-Synchrotron or the Italian Free Electron Laser facility.

2. Need of reliable and well-tested numerical toolbox available to theoreticians to interact with experimentalists for the interpretation of the transient spectra. These tools should be based on a well established knowledge database.

3. Need of periodic workshops to gather theoretical and experimental advances and open new field of research and collaborations. The invited speakers of the workshop expressed great enthusiasm for the idea of repeating similar workshops. This confirmed the importance of the topic and the need of these kind of meetings for the ultrafast physics community. We have been strongly encouraged by the participants to organize a second event on this topic.

We have also noticed that the interaction between theoreticians and experimentalists is of utmost importance to promote the progress in the field. The main reason being that the ultra-fast community is relatively new and a close and continuous contact between theoreticians and experimentalists represent the key aspect for a successful success and expansion of the ultra-fast science in the physics community.

4 Funding

The community of ultrafast phenomena is currently quite fragmented and diversified. At this stage, it is still difficult to put up a self-contained network for writing grant applications. A preliminary classification of the various subdisciplines would be extremely useful for this purpose. This meeting had the main purpose of bringing together for the first time several prominent scientists working in the field of ultrafast phenomena and of favouring the contacts

between them.

On the basis of this current situation the organization of a sequence of CECAM workshops to tight the collaborations and to form an organized network on this topic would be most welcome, especially considering the enthusiasm of the attendees and the interest in contributing to a successful workshop by all speakers we originally contacted.

EU funding for a network focused on ultrafast phenomena would be definitely appropriate. CECAM funding for another workshop, and later, a tutorial might be appropriate.

5 Will these developments bring societal benefits?

The interdisciplinary collaboration between theoretical and experimental groups will have impacts in many fields, such as energy sources and health. The ever-growing energy demand has fuelled the expansion of research on renewable energy sources. One area of interest is photovoltaic energy: organic and hybrid materials offer great potential for production of low cost, large area solar cells. Despite relevant advances in the synthesis and optimization of novel nanomaterials, much less has been done in the challenging task of understanding fundamental phenomena of the photon-energy conversion. For this reason it is relevant to build a synergic experimental and theoretical program aimed at understanding the behaviour of several materials, contributing to the development of photovoltaic and optoelectronic fields.

This collaboration will also have impacts on health and wellbeing. In particular, light-matter interaction plays a crucial role in biological processes: solar light, the fuel of life, also contains harmful UV radiation, which can induce significant photodamage to biomolecules. Skin cells, for example, are prone to cancer if overexposed to sunlight; and in DNA UV light could initiate photoreactions corrupting genetic information, the pillar of life. Luckily DNA dissipates this energy very efficiently. Spectroscopic setups to probe these process in DNA and other biomolecules have hence been developed in various labs; however, their complexity prevents from a univocal interpretation of the experimental data. This intricate scenario calls for a great effort from the theoretical and computational community to develop tools to shed light on the photoprotection mechanisms.

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Emergent dynamics of out-of-equilibrium colloidal systems at nano- to microscales

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1325.html
Dates: April 18, 2016 to April 20, 2016

1 State of the art

The focus of the workshop was on emergent dynamics in driven out-of-equilibrium colloidal systems. This is a rapidly growing area of research aiming towards prediction and discovery of novel multifunctional dynamic architectures that are not generally available at equilibrium conditions.

We particularly focused the program to three main sub-topics:

- emergent dynamics in magnetic colloids in external time-dependent fields
- dynamics and self-assembly in electrorheological fluids and liquid crystals
- collective phenomena nanoconfinement and under mechanical stress

The common question in most of the contributions was how the external driving and collective particle interactions coupled to the fluid flow determine colloidal emergent behavior. We had a perfect mixture of experimentalists, theoreticians and simulators in the meeting, which proved to be very productive in terms of discussions and future collaborative projects.

We tested an innovative workshop structure: having only a few formal lectures and extended discussion sessions with sound-bite presentations and poster discussions. It turned out to be a good model for promoting open discussions and we suggest to keep such structure in the future.

2 Major outcomes

A) Electric fields

Crossed magnetic fields have produced several wonderful phenomena that are difficult to understand from a fundamental perspective. Realizing the same with crossed electric fields might allow 3d position determination and at the single particle level, since dielectrics are often transparent, while magnetic materials are not. This would enable more detailed comparisons of experiment with simulation. In electric and magnetic field driven systems, the high-frequency behavior should be similar, while the double-layer polarization makes the behavior fundamentally different at low frequencies. Low frequency effects (electrohydrodynamics, polarization charge electrokinetic effects) are to date poorly explored both experimentally and theoretically and represent a wide-open area where novel emergent behavior can be expected.

B) Magnetic colloids

Several presentations on periodically driven paramagnetic and ferromagnetic colloids have revealed a great potential of magnetic systems to assemble into non-trivial structures including dynamic steady states. A question for theoretical consideration is how to correctly deal with the complex interplay of time-dependent magnetic forces, elastic (or visco-elastic) response of the system, and hydrodynamics. This is a challenging task but has been partially attempted recently and should be addressable in the next 3-4 years.

C) Shear and nanoconfnement

There was quite some discussion about systems under mechanical stress and in nanoconfinement. Some emerging interesting questions that deserve future attention from the community are:

- Crystal-to-crystal transitions in colloidal systems
- Mechanisms of stress release in out-of equilibrium systems under shear
- Role of soft matter and nanoscale processes in setting of the cement (to what extent can we design the dynamic assembly pathway in order to improve the final cement properties and engineer novel green formulations?)

3 Community needs

A) Emerging new areas

One possible new area is field driven colloidal assembly in non-Newtonian media. Colloids in a liquid crystal medium experience localized forces, due to the complexity of the elastic deformation field. This in fact might be another direction - "coherent electric fields in complex fluid medium" that might mimic swarming.

B) Computational Challenges

The study of hydrodynamics in 3 dimensions (3-dimensional electromagnetic fields, active colloids, fields in emulsions, colloids in anistropic liquid-crystalline media) will require large-scale computer simulations.

4 Funding

We are strongly convinced that all the topics mentioned above are suitable to be funded by the Horizon 2020 programme. Some initiatives are already substantiated in form of proposals (e.g. NANOTRANS ITN on transport of soft matter at the nanoscale, NANOPHLOW FET on similar topic, COLLDENSE ITN on complex colloids...). We suggest that another collaborative proposal on Emergent Phenomena in Soft Matter is put together, either as a training network (ITN) or as a research collaboration (FET).

5 Will these developments bring societal benefits?

The progress in the areas discussed on our workshop is of a definite importance for the industry since it can potentially provide access to a new class of materials (active materials and structures) that are not available through conventional techniques.

Industrial partners that first come to mind are Unilever, Saint Gobain, BASF, Solvay, Schlumberger.

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Marrying continuum and molecular physics: the Andersen-Parrinello-Rahman method revised into a scale bridging device

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1347.html
Dates: May 23, 2016 to May 26, 2016

1 State of the art

Multi-scale modelling has become a hot topic in computational physics. In terms of solid results, however, its success has not been overwhelming. It is regrettable, in particular, that concurrent multi-scale methods coupling molecular dynamics with continuum mechanics are even less developed and less well understood that methods linking Newtonian molecular dynamics with some viable approximation of the underlying quantum structure.

In partitioned-domain methods, the atomistic and continuum models are completely and independently defined in different space regions, partially overlapping. Sophisticated smoothing and filtering techniques may painfully mitigate, but not eradicate, severe interface artefacts. Moreover, typical numerical experiments feature a finite element mesh size as small as 5–10 atomic spacings, i.e., of nanometre order.

In hierarchical multi-scale methods, the whole domain is covered by a macroscopic grid on which a continuum model is computed. The molecular model enters as a local refinement for obtaining the information purposely left out from the continuum formulation. This approach holds a far better promise than the previous one. Its current implementations, however, suffer from the feeble coupling between molecular and continuum degrees of freedom.

A definite boost to hierarchical multi-scale methods would be given by the adoption of the Andersen-Parrinello-Rahman method of MD, revised with a view to concurrent molecular-continuum simulations. This method is characterised by the decomposition of particle velocity into the sum of a spatially tidy streaming velocity, parameterised by the cell deformation rate, and a disordered thermal velocity. The introduction of collective degrees of freedom affecting simultaneously all of the particles within a cell lends itself naturally to a seamless coupling with continuum mechanics, hinging on the idea of identifying the deforming MD cell with an infinitesimally small piece of a continuous medium.

2 Major outcomes

The size of the meeting was deliberately quite small (13 participants, organisers included). Only two speakers (one of the organisers and one participant) introduced the method and highlighted its features in five half-day sessions out of six. These presentations were done in a lecture format, leaving plenty of space for in-depth discussions, intended to be the key element of each session. In fact, more that half of the overall session time was occupied by lively – at times fierce – discussion.

This work method, while strenuous and demanding, proved to be very effective. We were able to achieve a common understanding of the revised Andersen-Parrinello-Rahman method and of the issues involved, in spite of the different backgrounds of the participants – or better, capitalising on their complementarity. Without the stimulus provided by the harsh criticisms, the passionate discussions and the impromptu ingenuity experienced all along the workshop, most errors and deficiencies in the preliminary notes (drawn up by one of the organisers and made available to participants) would have not been detected, let alone put right.

As an immediate follow-up to the workshop, the writing of a comprehensive report on the revised Andersen-Parrinello-Rahman method and its application to concurrent molecular-continuum simulations is underway. In this report, a complete and univocal identification of the basic constructs of continuum mechanics in terms of molecular quantities is explicitly obtained, and the fundamental elements of a multi-scale algorithm for hybrid continuum-atomistic simulations of macroscopic molecular systems are presented. This algorithm is based on the idea – keenly discussed in the last session of the workshop – of modelling the macroscopic system by sampling it with widely scattered mesoscopic MD cells that interact with each other via their collective degrees of freedom, linked by the balance and compatibility equations of the continuum theory.

Building on the success of this workshop, Eliot Fried, Giovanni Ciccotti and Paolo Podio-Guidugli have co-organised the course “Hierarchical multi-scale methods using the Andersen-Parrinello-Rahman formulation of molecular dynamics” to be held at OIST (Okinawa Institute of Science and Technology Graduate University) on April 3–8, 2017. This OIST-funded course will offer us a major opportunity to gain further experience with the method, while making it more widely known.

3 Community needs

In the near future – say, from now to the OIST course in April 2017 – our limited computational workforce will concentrate on code development, designing and performing various small-scale numerical tests both on single-cell algorithmic variants and on a few, relatively simple benchmark continuum-atomistic simulations. Therefore, no massive recourse to computational infrastructures is envisaged on this time scale.

On the contrary, we have a strong and urgent need to reach other communities – in particular, scientists and engineers interested in the mechanics of materials at intermediate scales – to convince them of the potential of the revised Andersen-Parrinello-Rahman method for upscaling molecular information by more orders of magnitude than hitherto possible. Success in this direction could provide us, at the same time, with stimulating technological applications, keen collaborators and access to industrial funding.

A new CECAM workshop on this topic next year would be untimely. Local activities on related topics will likely be taken by the CECAM–IT–SIMUL Node. A new CECAM workshop could possibly be envisaged for 2018 or 2019, but it is definitely too early to consider this opportunity.

4 Funding

Our endeavour is still essentially methodological in nature. As a consequence, in the near future we will not be able to produce strong applications for funding. At the same time, our need for financial resources will be minor. If our effort to get in touch with scientists and

engineers interested in the mechanics of materials at intermediate scales will be successful, we shall be in a much better condition for identifying funding channels and producing joint research proposals.

In the last session of the meeting we agreed on joint research programme, to be developed by nearly one half of the participants immediately after the workshop (and which is in fact under development). We hope that by the end of the OIST course in April next year we will be in better conditions to upgrade this joint research programme into a joint research proposal.

5 Will these developments bring societal benefits?

For the same reasons presented under the previous item, there are no societal benefits of our research topic foreseeable for the near future. However, if the method discussed at the workshop holds its promise to boost by orders of magnitude the range of scales encompassed by hybrid continuum-atomistic simulations, in the long run it will prove one of the most beneficial developments in computational sciences, with an enormous range of applications.

Just as an example, consider the potential benefits in the field of engineering mechanics, where the traditional analytical framework has been that of a continuum. However, the mechanical deformation and failure of many engineering systems are inherently multi-scale. Indeed, the observed macroscopic (continuum scale) response is governed by physical processes that occur at a hierarchy of finer scales. The current challenge in several solid mechanics applications is to incorporate micro-structural and atomic details to improve model predictions. However, approximations need to be done since the explicit representation of an Avogadro number of atoms is out of reach even for the most powerful computers (and, even if such a representation were within reach, it would be unmanageable and unintelligible).

However, we do not want to count our chickens before they're hatched.

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Structural and Functional Annotation of Bioinorganic Systems: Perspectives and Challenges from Theory and Experiments

Location: CECAM-IT-SNS
Webpage: https://www.cecam.org/workshop-0-1283.html
Dates: May 23, 2016 to May 25, 2016

1 State of the art

Transition metal ions play essential roles for protein structure and function. They pose a biological threat when improperly handled, often resulting in early cell death. These phenomena underlie neurodegenerative disorders that are of a progressive nature. The contribution of metal to life and evolution but also to disease resides at the interface between metal ions such as iron and copper and various proteins. How has evolution coped with optimizing the chemical nature of metal-protein interfaces so as to render it "efficient and safe" ? And under which condition does it fail ensuing in disease and early death? How can computational analysis of the above interfaces shed new light into possible mechanisms of diseases that are strongly age-related, such as neurodegeneration or cancer? Can quantum mechanics provide some clues as to an issue of apparently insurmountable nature? This workshop has been an excellent forum to attempt to answer these highly challenging questions and to discuss key aspects of the role of metal ions in medicine and of the contribution that molecular simulation can give to those.

2 Major outcomes

The workshop showed several examples in which molecular simulation provides atomistic understanding of the process at a spatial and temporal resolution, inaccessible to experiments. This information may help develop new drugs. However, although our understanding of the role of metal ions in several pathological states (cancer, neurodegeneration among others) has greatly improved in the last years, leveraging this knowledge to create novel therapeutics remains highly challenging. Trying to integrate experiment and theory synergistically is also a challenge. Several participants suggested that joint meetings between theoreticians and experimentalists might sprout new scientific research if they succeed in integrating highly diverse chemical and biophysical tools and approaches present in the community. Some of them even suggested a larger participation of experimentalists in similar meetings in the future. They finally suggested to allocate more time dedicated to discussions and brain storming to facilitate the integration between the two fields.

The workshop focused on several aspects, including:

1. Metal-ion trafficking, transport, folding. Metal transporters regulate metals intracellular uptake and/or efflux, and direct their trafficking inside the cell. Here, the interplay between experimental biophysics (especially NMR), bioinformatics and molecular simulation was emphasized.

2. Simulations are instrumental for the investigation of novel targets based on transition metals. These include iron-sulfur proteins, recently related with Parkinson’s disease,

cancer and diabetes, metabolic, genetic and biogenesis-related diseases.

3. Metallo-proteins or metal-dependent RNA filaments perform/enhance the efficiency of specific chemical reactions. Atomistic understanding of these processes may lead to engineered biological systems for technological and medical applications.

4. Theoretical challenges. Challenges of simulations techniques to treat transition metal-based biomolecules have been addressed during the conference. It was noted that approaches typically used in condensed matter physics, such as quantum Montecarlo, along with advanced quantum chemistry methods, lead to very exciting results in the field.

3 Community needs

1. The very large computational infrastructures available in Europe and USA allow to address high performance computing (HPC) -based investigations of metal dependent biological phenomena with molecular simulations techniques. However, understanding the mechanism of a complex bioinorganic process usually requires the integration of several different computational techniques and not all of them perform equally well in supercomputing centers. Hence, local resources (e.g. at Universities) need to be tightly integrated with supercomputing center. Unfortunately, this is not always the case.

2. We strongly need shared archives across Europe and USA reporting computational techniques to treat metal ions in biological systems (e.g. new ways to develop force fields for classical MD simulations)

3. The participants have underlined the success of this workshop. Prompted by this, a biannual series of workshops on experimental/computational approaches to metals in medicine has been strongly auspicated by the participants.

4 Funding

Typical channels to organize these future conferences would be CECAM, Psi-K. Our workshop was also sponsored by an EU program dedicated to HPC applications in biological systems (the HPC-LEAP Joint Doctorate: http://hpc-leap.eu). We will seek in the future contributions of this kind. Specific cost actions on ‘structural and functional annotations of bioinorganic systems’ can also help in the organization of focused meetings. Funding for this kind of biological problems is available from the National Institute of Health and National Science Foundation in USA. While in Europe they are provided by European Program Horizon2020, In Italy by Telethon, Italian Cancer Research Association (AIRC), Italian Ministry for Education and Research (MIUR), and in Germany by the DFG.

5 Will these developments bring societal benefits?

Increasing our knowledge on metals ions in biomedicine, from understanding how metal ions are transported into and within the cell, to the action of metal-containing drugs, to the reactivity of enzymes based on transition metal ions, may greatly help develop new drugs and identify new metal-based targets. This is of course of great significant societal benefit. It may reduce costs associated to health care treatments and to third persons taking care of ill people (relatives).
Novel drugs may also largely help slow down the progress of the diseases and/or decrease side-effects, such as, for instance, the pain associated with neuroinflammation. This research is also obviously highly connected to pharmaceutical industries. Funding opportunities for these topics can be sought from the latter, or by EU agencies, such as, for instance, the H2020 grants. Other sources of funding include national funding agencies such as the DFG-

Deutsche Forschungsgemeinschaft in Germany and in funding agencies for world-wide projects such as the Human Frontier Science Program.

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Exploring Chemical Space with Machine Learning and Quantum Mechanics

Location: CECAM-ETHZ, Zurich, Switzerland
Webpage: https://www.cecam.org/workshop-0-1256.html
Dates: May 30, 2016 to June 3, 2016

1 State of the art

The goal of this workshop was to bring together the main scientific players who are likely to deepen our understanding of chemical compound space using quantum mechanics and machine learning. Many participants came together to benefit from the mutual exchange of ideas in this upcoming field of atomistic simulation and computation. Specific scientific domains included statistical mechanics, liquid and solid state physics, quantum chemistry, graph theory, molecular physics, condensed matter physics, optimization algorithms, data mining, and statistical learning. Invited speakers and oral contributors represented a broad and strongly diverse spectrum of scientific disciplines which all dealt with the question of how to cope with chemical space. Current methods and topics include the definition of representative sets of molecules as chemical libraries, the generation of huge data sets with billions of molecules for near comprehensive explorations, the application of discrete optimization procedures, statistical learning, molecular and atomic and crystal representations, as well as implications for exchange-correlation potentials used within density functional theory. Molecular design problems were discussed as well. Younger participants presented posters. There was ample opportunity for discussion after presentations, during poster sessions or coffee-breaks, or at the social dinner.

2 Major outcomes

Specific ideas, topics, problems, and solutions which were discussed included:

- Efficient exploration schemes which search CCS to rapidly identify compounds with target properties. This included point-wise and iterative modifications of compounds, evolutionary algorithms to optimize materials as well as training sets for machine learning models, filtering of large sets of candidates (top-down) as well as construction of candidates (bottom-up).

- Libraries of molecules, either large or representative, were presented and justified.

- Machine learning models of properties of molecules, polymers, and crystals. Machine learning models of atomic forces for molecular dynamics applications in crack propagation were discussed. Outstanding problems include the optimal way of representing materials or molecules. One suggestion (by Stephane Mallat) to use wavelets has attracted particular interest.

- The link between conceptual density functional theory and chemical compound space was discussed, in particular with respect to higher order derivatives including nuclear hardness and molecular Fukui functions (both second order derivatives). The link to the linear response kernel, enabling the calculation of perturbed electron densities was made and discussed. It was also shown to be useful for the prediction of doped fullerene compounds.

- Estimating changes in stability using first order derivatives in nuclear charges of binary metal clusters was also discussed in combination with genetic algorithms for structural searches.

- Molecular dynamics based free energy estimates of optimal drug-candidates for ligand binding using alchemical interpolations were also discussed.

- Strict bounds and inequalities in chemical compound space, independent of molecular geometry, were presented.

- The problem of many density functionals with fractional electron number is well known, similarly, problems also occur when considering fracitonal nuclear charges. The exact functional must resolve these problems, and has been derived and presented for 2 electron systems.

3 Community needs

This event largely dealt with theoretical and computational efforts in the atomistic simulation sciences. As such, little experimental input is available. It would be highly desirable to create an outreach effort for automated synthesis and characterization in the future. For the moment, however, further theoretical developments are required to get a better grasp on (i) the nature of chemical space, (ii) the methods which enable robust and reliable routine exploration campaigns, and (iii) algorithms that are computationally sufficiently efficient to cover representative property and compound domains.

Most alchemical interpolations were implemented in well-known and established community codes, such as Quantum Espresso, CPMD, Turbomole, or HORTON. For machine learning models, no widely spread software has emerged yet. Because of its relative simplicity (when compared to quantum chemistry codes) it remains to be seen if this is actually necessary. It might be helpful to grow the community and to decrease entry barriers to newcomers.

In the opinion of the organizers, it would be helpful to regularly organize follow-up workshops on chemical space. This is still a young and emerging field-yet it is poised to grow. It might prove helpful to organize separate events for the machine learning and the alchemy parts since there was relatively little mutual overlap between participants from these two groups. Generation of quantum data for training machine learning models will certainly require substantial HPC resources. The alchemy group, by contrast, requires minimal hardware resources since the approach is basically routed in an aggressive extension of perturbation theory involving all sorts of perturbations in the external potential. Many legacy quantum codes already have extensive perturbation modules integrated. As such, minor modifications enable them to seamlessly include perturbations in chemical composition.

4 Funding

Typical funding channels in this line of research include the US Materials Genome Initiative as implemented by the US department of energy, the US national institute of standards, the US national science foundation, the US Navy, the US army, or the US air force. In Europe, many participants had funding from the European commission, or from national funding agencies, such as the Deutsche Forschungsemeinschaft or the Swiss National Science Foundation. Senior participants also relied on funding from their home institutions.

5 Will these developments bring societal benefits?

The virtual design of novel molecules and materials with predefined properties holds promise to revolutionize chemistry as we know it. Potential applications leading to societal benefits abound and include, among others, new materials for harvesting energy, storing energy, cleaning water, improving energy efficiency, obtaining improved drug candidates, and others.

Furthermore, there is a more fundamental aspect to the goal of exploring chemical space from first principles: A deepened understanding of the chemical universe humans inhabit offers immense opportunities for atomistic control of matter. Eventually, these ideas and methods will become part of chemical engineering where they can have substantial impact on society on a global scale. Since we are aware of only a tiny fraction of all the chemicals that one could possibly synthesize, chances are that we are still far from fully exploiting what chemistry has in store for humanity as a whole. These developments are likely to have lasting and beneficial effects for all of humanity.

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The flow of amorphous solids: from atomistic simulations to Earth Science applications

Location: Centre Blaise Pascal - ENS de Lyon
46, allée d'Italie
Lyon - FRANCE
Webpage: https://www.cecam.org/workshop-0-1260.html
Dates: June 15, 2016 to June 17, 2016

1 State of the art

The ambition of this workshop was to set the path towards a unified description of the flow of amorphous solids, bridging the gap between the atomic, mesoscole and continuous descriptions. We believe that such a multiscale framework is highly relevant to addressing a wide range of challenges in a number of applications in the Earth sciences.

Our aim was to bring together a group of leading experts in the field of computational modeling of amorphous plasticity at all scales (molecular dynamics, discrete element model, granular dynamics, mesoscopic elastoplastic models, finite element models) with leading experts in the relevant fields of Earth sciences.

This confrontation was intended to help: (i) identify the concept of amorphous solid as a useful paradigm for several Earth science systems; (ii) popularize in the Earth science community the numerical methods used in material sciences; (iii) offer a consistent multi-scale approach of the flow of amorphous solids combining the micro, meso and macro scales; (iv) understand the mechanisms controlling the localization of the deformation; and (v) Define the specific challenges posed by geophysical amorphous flows in terms of rheology, strain localization, instabilities and numerical modelling.

2 Major outcomes

The workshop was structured into five half-day sessions that addressed five well identified questions. The poster session was accessible throughout the duration of the workshop to facilitate the transfer of knowledge and interactions between the material science and physics communities and the Earth science community. An important place was given to discussion during each session. All abstracts with one selected image were provided in the ‘book of abstracts'.

The **session 1** on day 1 – Examples of flowing amorphous solids in Earth Sciences – was aimed at identifying a class of natural systems that can be represented by an amorphous paradigm. The five talks were:

1. Jérome Weiss: Examples of flowing amorphous solids in Earth Sciences - A focus on sea ice
2. Michael Zaiser: A simple model of plasticity in amorphous materials and its application to rock failure
3. Nicolas Brantut: Shear localisation and dynamic weakening during earthquakes
4. Anne Mangeney: Simulation and detection of granular flows using numerical modelling and seismic data
5. Pierre Dublanchet: Fault creep and earthquake interaction

The **session 2** on day 1 – Numerical approaches – was intended to give an overview of the methods that are currently used in the material science and statistical physics community to represent the flow and plasticity of amorphous material. The six talks were:

1. Jean-Louis Barrat: Review of elastoplastic and related models
2. Anael Lemaître: Analysis of flow and relaxation events in sheared and quiescent liquids
3. Bruno Andreotti: Rheology vs dynamical mechanisms
4. Damien Vandembroucq: Lattice models of amorphous plasticity from depinning to shear-banding
5. Sylvain Bouillon: A Lagrangian FE model for sea ice to deal with discontinuities in a continuous framework
6. Guillaume Kermouche: Plastic flow of silicate glasses at the micro-scale

The **session 3** on day 2 – Strain localisation – looked at the processes controlling the degree of localization in various natural systems based on our advanced understanding of localization in a variety of amorphous materials. The five talks were:

1. Alexandre Nicolas: On general mechanism leading to strain localisation in amorphous solids
2. Kamran Karimi: Role of inertia in the role of amorphous systems: a finite element based elasto-plastic model
3. Pinaki Chaudhuri: Transient heterogeneities during onset of flow in glassy systems
4. Pierre Saramito: Smooth or abrupt localization: numerical modeling and comparison with suspensions and liquid foams
5. Eduardo Jagal: Strain localization in the limit of extremely low strain rates

The **session 4** on day 2 – Physical phenomena: relevant for Earth Sciences? – looked at a variety of experimental and numerical evidence of deformation in amorphous systems and the possibility to draw analogies with Earth Science applications were discussed. The five talks were:

1. Francois Landes: Scaling laws in earthquake occurence
2. Ezequiel Ferrero: Spatio-temporal patterns in ultra-slow domain wall creep dynamics
3. David Rodney: Energy dissipation in oxide glasses at the atomic-scale
4. Guilhem Mollon: Simulation of debris flow inside a contact using a multibody meshfree strategy
5. Mathieu Leocmach: Yoghurt under stress

The **session 5** on day 3 – From atomic to continuous via mesoscopic descriptions – described how a multi-scale framework can be successfully used in the material science or micro-fluidic community and how such a multi-scale framework can be adapted to the needs of the Earth science community. The five talks were:

1. Michael Falk: Bridging from atoms to continua in the mechanics of amorphous solids

2. Tristan Albaret: Informing mesoscopic models from atomistic results to simulate plasticity in amorphous solids

3. Francesco Puosi: Modeling the flow of athermal disordered media: shear transformation dynamics and mean-field concepts

4. Craig Maloney: Elasto-plastic automata with realistic near field interactions: avalanches and diffusion

5. Jean-François Molinari: A critical length scale predicts transition in adhesive wear mechanisms

In addition to the oral session a poster session was running throughout the duration of the workshop and three time slots were specifically allocated the posters. A list of the posters is given below

1. Francesca Boioli: Mapping between atomistic simulations and Eshelby inclusions in the shear deformation of amorphous Silicon
2. Ezequiel Ferrero: A display of GPU implementations in Condensed Matter Physics: four distinctive cases
3. Mathieu Leocmach: Hierarchical wrinkling in a confined permeable biogel
4. Chen Liu: Driving rate dependence of avalanche statistics and shapes at the yielding transition
5. Alexandre Nicolas: Towards a Finite-Element based model for the flow of amorphous solids
6. Francesco Puosi: Flow of athermal disordered media: microscopic consideration on a mean-field model

3 Community needs

The workshop was successful in that it attracted ~ 40 researchers at different stages of their careers and from different communities (Earth Sciences, Materials, Physics).

While this first attempt to bring together the Material/Physics and Earth Science communities was slightly biased towards the former in number of participants (ratio ~70%-30%), the quality of the presentations and the active discussions that took place during the talks and the discussion sessions made this event a rare occasion to share very different sets of knowledge and techniques between the two communities.

The large variety of numerical methods introduced illustrated the wealth of methods available but also the need to further popularise these within the Earth Science community. A useful complement to this workshop would be to organise a summer school with leading experts introducing these methods via tutorials and hands on sessions.

Also while the first contact was achieved a second workshop should be organised in a few years (2-3 years) to tackle the specific problems that Earth Science is facing. A session at

EGU could be a good platform to advertise our first conclusions. Also we intend to use our website as a platform to promote the outcomes of this proposal (via the presentations, videos and report) but also to store some useful links to existing software, tutorials, publications, etc.

4 Funding

It would be good to allow different nodes to use the CECAM umbrella and be able to organise workshops even if funding is not allocated. It is indeed possible to organise a workshop by raising money from the participants.

Also, it is important to make the funding of the different nodes a bit more transparent. For example, how much money is allocated to each node, what workshops are funded on what basis, etc.

One aspect that we need to discuss further is the road map in terms of future research priorities and funding (Horizon 2020, etc)

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Density- and response density-based models for Intermolecular Interactions in Molecular Assemblies and in Solids

Location: Nancy - France
Webpage: https://www.cecam.org/workshop-0-1266.html
Dates: June 20, 2016 to June 23, 2016

1 State of the art

Models for the intermolecular interaction energy are usually much more powerful and versatile than the often computationally expensive ab initio methods on which they are based. While many accurate models for intermolecular interactions include physical terms such as the electrostatic, dispersion and short-range repulsive effects, a number of contributions of quantum mechanical nature are often omitted: polarization, charge-transfer, charge-penetration, and more generally, subtle anisotropic effects.

Better success can be obtained with models based on the electronic density and the density-response rather than fitted atomic parameters only. In principle, such models can account for the electrostatic interaction exactly and the exchange-repulsion fairly accurately, additionally, through the density response, they can also be used to construct plausibly accurate, but simplified models for quantities that involve excited states such as polarizabilities and dispersion coefficients.

Response-based models have recently seen successes in systems where van der Waals (dispersion) interactions are significant. These interactions are important in the modeling of several problems in materials science, including the study of the stability of molecular crystals or the adsorption of molecules on surfaces. The poor description of this kind of interactions by traditional approximations employed in density functional theory (DFT) has long limited the applicability of this methodology to systems where vdW forces play an important role. This problem has been to a certain extent overcome by empirically adding pairwise corrections to include van der Waals (vdW) interactions in DFT. However, recent more sophisticated approaches which take into account both density and response effects, e.g. the MBD (many-body-dispersion) model or the LRD (local density response) model, have been shown to describe intermolecular interactions with a higher accuracy.

2 Major outcomes

All of the talks contained some highly interesting results and many raised open problems. Relatively few talks had density modeling as main topic; mostly various aspects of the response density modeling were discussed.

Concerning density modeling it has been pointed out that high-resolution X-ray diffraction may allow us to access to precise experimental charge density models, based on contained wave function optimization techniques. Such models include various many-body effects, like induction and electron correlation and therefore it is far from being trivial to use them in conventional force field parameterization, which is usually based on the non-interacting subunit properties (functional groups, molecular or ionic subsystems).

Response charge densities played a central role in most of the talks. Several talks concerned directly by the evaluation of the atomic or subsystem responses, most frequently in a dipolar form, based on time dependent DFT in the time or in the frequency domain. It has been shown that for benchmark purposes, coupled cluster level correlated densities and charge density susceptibilities can be calculated as an efficient means to take into account intra-monomer electron correlation in the symmetry-adapted perturbation theory (SAPT) framework.

Modeling density response can be done for various purposes. Perhaps the most fundamental one is to use the charge density susceptibility (CDS) of the entire system in view of calculating the electronic correlation energy. FDCDS (fluctuation-dissipation CDS) of the subsystems enter naturally in the generalized Casimir-Polder formula for the dispersion energy. A more sophisticated object is the first order density matrix response, which is useful to evaluate the exchange correction to dispersion and induction interaction energies. Response functions have been used in various embedding methods too. One possibility is to apply them to represent a polarizable environment for a small embedded subsystem, another one is to use a polarizable solute in order to interpolate between two explicit wave function optimizations in order to reduce computational costs.

A common property shared by all interaction energy (contribution) models was the description of the various types of interactions in terms of local quantities such as the "local response density", the "exchange-hole dipole moment" or the dipole moments from a local harmonic oscillator description of the response function. It has become obvious that via this approach the different models may also be applied to extended molecular systems for which ab initio quantum chemistry methods are not feasible anymore. Phenomena which play a role in large-scale simulations have also been addressed, e.g., environmental effects, polarisation screening effects or charge transport.

It is clear, however, that the calibration of interaction energy models against results from standard ab initio methods rather than experimental observables may be the most promising route towards the development of accurate and transferable models. Standard ab initio wave function methods have become feasible for fairly large systems in recent years so that this methodology will become an important approach for the advancement of interaction energy models in the future.

Collaborations catalysed by workshop:

- Rocca & Scherrer : response functions
- Verstraelen & Misquitta : charge transfer
- Piquemal & Misquitta : charge/polarizable models in TINKER-HP
- Verstraelen & Tkatchenko : charge fluctuation models
- Sherrill & Hesselmann : Psi4 and SAPT-DFT
- Rocca & Tkatchenko : molecular crystals
- Hedegard & Dobson : RPA and long-range dispersion models
- Lu & Misquitta & Rocca : embedding/partitioning of response

3 Community needs

Code interoperability: A number of the methods presented have been implemented in Open Source programs like Psi4, CamCASP, Horton, SAPT2015 & TINKER-HP. It was felt that these methods, or a sub-set of them, should be implemented in the more commonly used codes so as to make them more widely available to the community. There is already a degree of collaboration in the community that will make this possible, but a dedicated meeting/discussion under CECAM may be useful.

Themed Discussions: Some of the more contentious issues that arose in this workshop (charge-transfer, density/response partitioning methods) need to be clarified in a systematic and scientific manner. The possibility of using CECAM discussion sessions for this arose, but with the novel idea of combining the discussion with a "Blind test"-like selection of systems that the participants will have to study in preparation for the discussion. The results of these calculations would then be used to focus and critically evaluate the competing methods in a manner that is next to impossible using traditional means. There is the possibility of writing a joined paper on the subject at the end of the discussion session. This would make the results of the discussion available to the general scientific community.

Follow-up meeting: The intermolecular interactions community is a small, but very active community that has traditionally made use of very successful meetings at Telluride, USA that are held biennially. This meeting was meant to complement the Telluride workshops, by (1) introducing a different emphasis to the science, (2) allowing much more time for discussions, and (3) being substantially cheaper for European participants, and also for those from overseas. We largely succeeded in all respects as there was significant enthusiasm for a follow-up meeting, to be held in two years.

4 Funding

The workshop was financed by the 12000 euros support of the CECAM. All participants - including those not presenting talks - were offered accommodation in the same hotel, within a few minutes walk of the conference site. In addition a banquet and a cold buffet with drinks during the poster session was offered to all participants. In accordance with the CECAM traditions no participation fee was required. Coffee breaks, badges and a booklet of abstracts were provided as well. Mainly for practical reasons (administrative simplicity) the book of abstracts and the badges were paid on the research fund of one of the local organizers. Our budget was insufficient to offer travel or other types of financial aid to speakers or participants and none of the speakers or of the participants reclaimed such extra aid.

We note that the financial success of the workshop was largely due to the lower costs incurred in Nancy compared with larger cities. This allowed a good price-quality ratio.

5 Will these developments bring societal benefits?

Intermolecular interaction models lie at the heart of simulation methods used in materials design, bio-molecular systems, drug design, organic molecular crystals (energy, devices, displays). The last decade or so has seen a significant increase in our capacity to theoretically model these interactions, and also in the techniques needed to take these developments to the force-fields that are used by the main-stream simulation programs used in the fields listed above. Many of the researchers responsible for these developments were present at this meeting: both theorists, and those working more on the development of force-fields. Consequently, the scientific ideas, collaborations that were sparked at this meeting

(and fuelled by other such meetings) will eventually lead to real benefits to our society in the fields listed above, and no doubt in other areas we have not considered.

Further, one of the themes of this meeting was to see where our current theories are not adequate enough to meet some of the challenges posed by the technological applications we seek to solve (how to handle systems with excited states in photovoltaics is one of these), and in this meeting, we have made steps to highlight these problems, and suggest research avenues that we need to consider in the next few years so as to be able to solve these problems.

Although we did not have a direct participation from industry, some of the participants have strong collaborations with industry, through which the novel ideas that emerged, particularly in the scientific discussions, will find direct application to research areas in health and energy that are tremendously important to our society.

Finally, at meetings like this where we bring experts from around the world together with graduate students and post-docs, we, as a community, participate in the scientific development of the next generation of researchers and build our new scientists and industrialists.

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Atomistic simulations in prebiotic chemistry – a dialog between experiment and theory

Location: CECAM-FR-IDF, University Pierre and Marie Curie, Paris, France
Webpage: https://www.cecam.org/workshop-0-1301.html
Dates: June 20, 2016 to June 22, 2016

1 State of the art

The chemical origins of life on Earth date back approximately 3.5 billion years. During this time period in Earth's history, a process of prebiotic chemical evolution was sparked, where small biologically inactive molecules reacted to form biologically active polymers and, eventually, the simple cell. In 1924, A. I. Oparin published his primordial soup theory proposing that life originates from simple nonliving organic compounds through gradual chemical evolution. In 1953, Miller and Urey reported the surprising results he had achieved by the application of an electric discharge on a mixture of the gases CH4, NH3, H2O, and H2. The result of this experiment was a substantial yield of a mixture of aminoacids. Similarly, Orò demonstrated the spontaneous formation of nucleic acids bases from aqueous hydrogen cyanide subject to heating.

The last couple of years witnessed an unprecedented development in the research of the origin of the first genetic materials. Recent experimental papers published in 2015 point to formamide as a prebiotic hub. Self-organization of nucleotide precursors leading to RNA-like molecules has also been addressed recently.

Theory and modeling have generally provided considerable insight into prebiotic chemistry. Significant new insight has been obtained through AIMD studies on the mechanisms and barriers for the synthesis of simple organic molecules on substrates such as ice or minerals, the simulation of the effect of the pressure/temperature shock waves induced by the impact of bolides in the early Earth, the recent first in silico Miller-Urey experiment, the simulation of peptide oligomerization at hydrothermal conditions, or the determination of chemical paths leading to the formation of sugars and nucleotides.

The purpose of this workshop was to bring together experimentalists and theorists together.

2 Major outcomes

The workshop has been aimed at establishing connections between scientists working in theoretical modelling and leading experimentalists from the field of the origin of life research. Theoretical chemistry was represented by high-level electronic structure calculations, quantum molecular dynamics as well as classical force-field-based molecular dynamics simulations.

On this two-days-long event 27 talks were presented covering almost all areas of the origin of life research starting from astrobiological aspects up to the modelling of oligonucleotides and simple proteins. The workshop was started by a historical overview on the development of the origin of life field given by Antonio Lazcano, who served as the president of the ISSOL (International Society for the Study of the Origin of Life) for two terms. He welcomed the initiative to bring together researchers working on theoretical as well as experimental investigation of the origin of life and stressed the importance of the molecular level understanding of these chemistries, in which atomistic simulations might play a dominant

role.

John Sutherland presented a “Pierre et Marie Curie Colloquium” talk in which he has outlined several subjects in which future computational studies could aid experiments at reconstructing the prebiotic synthesis of nucleic acid precursors on the primordial Earth.

The conference overviewed the main topics where computations have already been demonstrated to be a useful complement of experimental investigations. In particular, the following topics have been addressed. Several talks have been devoted to the synthesis of biomolecular building blocks, like nucleobases, nucleosides as well as amino-acids. A particular attention was payed to the role of various energy sources, like heat, UV-light, proton irradiation and high-energy impacts, which expanded the covered research areas to an extraterrestrial context. Likewise, modelling of prebiotic reactions catalyzed by mineral surfaces or interstellar ices was addressed by several talks. A special emphasis was put on the self-assembling and oligomerization processes leading to the first biopolymers.

Based on the surprisingly rich repertoire of examples demonstrating the success of computational chemistry tools at addressing chemical problems related to the origin of life, we concluded that ”in silico” experiments represent perhaps the most accurate method to address energetics of these complex chemical transformations. Thus, they are especially well-suited to evaluate plausibility of various prebiotic scenarios.

The conference fostered intense interactions between several research areas. Application of theoretical modelling tools to impact chemistry on mineral surfaces represents a highly perspective area of cooperation between experimental and theoretical groups. Such collaboration could significantly facilitate the interpretation of impact experiments performed in the presence of various meteoritic materials or minerals. Likewise, a very promising area of experimental-theoretical collaboration is the investigation of chemistries taking place in reductive atmospheres, which might give a clue to the question what kind of small organic and inorganic molecules other than the popular HCN and formamide could accumulate and kick-start life in a prebiotic environment. Likewise, prebiotic photochemistry is an area where computations could significantly contribute to the progress of the origin of life research.

3 Community needs

During the workshop the pertinence of ab initio modelling in the field of prebiotic chemistry was demonstrated and recognized by the experimentalists present. Even in this very complex field, theory can bring useful insight on the chemical mechanisms in a given environment. To advance the field through a cross-feeding of experiment and theory to build reaction networks and explain with them the formation of biomolecules and the role of building blocks such as cyanic acid and formamide, what is needed from theory is the possibility to provide accurate thermodynamics in complex, prebiotic, environments and related rate constants. As of thermodynamics, methods such as metadynamics have made this a reachable goal. What is needed is then the access to large scale facilities, not so much for performing heroic simulations of extremely large systems, but to be able to efficiently explore chemical and physical (temperature, pressure) space.

As of rate constants, further theoretical developments are needed to reach a similar situation and is an active field of research in the simulation community at large, not just limited to prebiotic chemistry.

4 Funding

Research on the origin of life is typically funded by two private foundations, like Templeton and Simon's foundations. However, these two institutions typically support experimental projects and not theory. Other, more popular founding resources are NASA or ESA, which mainly concentrate on the astrobiological aspects of this research. Human Frontiers Science program is another potential funding channel.

5 Will these developments bring societal benefits?

The origin of life on our planet belongs to one of the most basic questions mankind ever raised. Hence is its general interest, which is exemplified by regular topic-related press-releases in leading newspapers and scientific magazines all over the world. In the last couple of years several press releases appeared related to computational studies in prebiotic chemistry as well illustrating that achievements made by modern computational tools are becoming recognized not only among researchers but also by the general public. Indeed, the press conference organized in the frame of the meeting reflected this success as well: the French press and media were represented by numerous newspapers. The public interest of the topic is further exemplified by the numerous private funds (Simons Foundation, Templeton Foundation) traditionally sponsoring the origin of life research. Among the world-wide associations supporting the origin of life research the Human Frontiers Science Program deserves attention.

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Enzyme Engineering: Bright Strategies from Theory and Experiments

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1336.html
Dates: June 27, 2016 to June 29, 2016

1 State of the art

One of the promising areas of genetic engineering is protein engineering. In this field, chemists, biochemists, biologists, and engineers alike are engaged in e.g. tailoring enzymes for specific purposes. Enzymes as Nature's catalysts find many potential applications in chemical industry, biotechnology and medicine. Using enzymes or biomimetic compounds and strategies is often more advantageous than non-enzymatic counterparts due to their exquisite specificity, high catalytic rates, selectivity and environmental friendliness. Nonetheless, to meet the requirements of industrial biotechnology the enzymes need to be optimized by protein engineering.

In the last two decades, enzyme engineering, received considerable attention from both computational and experimental disciplines. In the US the use of enzyme technology in biocatalysis has received as many as 16 Presidential Green Chemistry Awards since the year 2000.

State-of-the-art computational approaches are able to provide direct insight into the structural, dynamic and mechanistic aspects of enzymatic catalysis. Computational protein design has gained momentum in enzyme engineering and first proof-of-principles studies for the full de novo design of enzymes have recently been achieved.

The understanding of the underlying physical and chemical guiding principles of enzyme engineering is key for the discovery and the development of new capabilities and the improvement of desired functions. However, fully predictive computational enzyme engineering is still in its infancy and many theoretical challenges are as yet unsolved. Integration of different experimental and computational approaches is crucial to build new ideas and strategies for the successful design of biocatalysts. Hence, this workshop brought together leading theoreticians and experimentalists in protein and enzyme engineering to highlight recent advances, identify crucial remaining challenges and build effective strategies for the development of improve

2 Major outcomes

a. Industrial Oxidoreductases
   In her talk, Dr. Maria F. Lucas presented a combined experimental and computational study on improvement of oxidoreductases, which are industrially important enzymes. She also briefly mentioned a new simulation protocol called the PELE algorithm. PELE is based on Monte Carlo sampling and decreases the computational cost for the screening of single point mutations.

b. Computational Enzyme Design: "inside-out" approach
   Dr. Nihan Celebi Olcum described the working principles of the "inside-out" approach to create catalysts which are capable of performing reactions not found in Nature. It was clear that this method usually leads to only low enzymatic activities and needs to be combined with directed evolution.

c. Functional Motions of Proteins
   Dr. Turkan Haliloglu highlighted the relationship between protein motions and their functions. It was shown that elastic network models (ENMs) could enhance our understanding how the protein of interest binds a specific ligand and open new ways to design powerful scaffolds. Another related talk on this topic was given by Dr. Luciano Abriata. He also presented accompanying NMR experiments in his talk.

d. Fluorescent and Bioluminescent Sensor Proteins
   Dr. Kai Johnsson focused on the design of fluorescent and bioluminescent sensor proteins, which are important to visualize and manipulate proteins in living cells. Incorporation of non-natural amino acids was used in his study and considered as a promising strategy for the future of protein engineering.

e. Design of Functional Proteins
   Dr. Bruno Correira showed the design of small, thermally and conformationally stable protein scaffolds in his presentation. These scaffolds fall into the class of promising epitope-focused vaccines. A computational approach called Fold From Loops (FFL) was used to allow de novo folding and design.

f. Functional Mimics: Efficient catalysts for energy storage
   The talk of Simone Raugei was centered around molecular electrocatalysts. The speaker focused on the synergistic approach taken between experimental and computational chemists working together and the most important reactive species involved in the process were addressed together.

3 Community needs

In the future, it would be promising to organize a series of CECAM workshops on this topic. In the past, many events were organized in USA on enzyme engineering. There are almost 4000+ people from 75 universities in USA working in enzyme engineering. Nonetheless, in Europe the number of such events is still limited. To stimulate networking and to accelerate the creation of powerful biocatalysts such gatherings are highly stimulating. The form of the workshop(s) could be designed in a different way to encourage useful discussions and collaborations. Including more experimentalists and scientists from industry could be helpful to increase the number of collaborations. In this respect, obtaining co-funding from well-known enzyme companies (such as Lonza, Novozymes) might increase the number of participants from this side as well.

4 Funding

Various funding sources are available to support the organization of local congresses or to contribute to the travel costs of researchers.

a. The SNSF (http://www.snf.ch/en/funding/science-communication/scientific-conferences/Pages/default.aspx)

b. Scientific Conferences

c. International Exploratory Workshops

d. The Company of Biologists (http://www.biologists.com/grants/)

e. Swiss Academies

f. UNIGE – Administrative Commission

g. SCOPES – Conference Grants

h. EMBO

i. Biochemical Society

Events Sponsorship

The Society will provide sponsorship of up to £500 to assist with the organization of single lectures or small events at an institution of Higher Education

Conference Proposals

The Society offers support to a wide range of national and international events.

5 Will these developments bring societal benefits?

A wide range of protein engineering applications are present in the literature:

1. Food and detergent industry applications

   Food and detergent industry cover a broad range of enzymes. For instance, amylases and lipases are common food-processing enzymes. Stability and high activity of these enzymes at alkaline pH and at high temperatures are some of the design goals.

2. Environmental applications

   Another important field of protein engineering are environmental applications. In order to monitor or treat pollutants, enzymes can be used. For example, peroxidases and laccases fall into this category. Chemical modification or protein engineering of oxidative enzymes is a possible route to advance the properties of such enzymes.

3. Medical Applications

   Medical applications of protein engineering are also diverse. For instance, the use of protein engineering for cancer treatment studies has drawn a lot of recent attention. The use of novel antibodies as anticancer agents is a popular approach in this field.

4. Applications with redox proteins and enzymes

   The electrochemistry of redox proteins finds numerous applications in biofuel cells, chemical synthesis and biosensors.

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Interactions and Transport of Charged Species in Bulk and at Interfaces

Location: CECAM-AT
Webpage: https://www.cecam.org/workshop-0-1280.html
Dates: July 4, 2016 to July 7, 2016

1 State of the art

The workshop has been dedicated to the interactions and transport properties of charged species that are essential for both soft-matter materials science as well as the understanding of biological processes. The charged species range from small ions, electrons, protons, and intermediate sized colloids, synthetic macromolecules, proteins and DNA, up to living cells. The interactions between relatively simple charged species (like homogeneously charged colloids and linear electrolytes) have been studied over the last decades and are by now quite well understood. The much more complex charged species that play a role in the development of soft-matter functional materials (like ionic microgels, bio-hydrogels, dispersions in ionic liquids, zwitter-ion like polymers) and in biological processes (like ligand-protein complexes, ion channels, F-actin, DNA) are much more complex, and their interactions are not yet fully understood. These species are often highly charged, so that non-linear Poisson-Boltzmann theory is required, condensation may play a role, dissociation/association to surrounding molecules may occur, and finite ion-size effects can be important.

The transport properties, as well as the response to external electric fields of these complex charged species are equally vivid fields-of-research, where electrostatic interactions are a necessary input. For the complex species mentioned above, very little is known. Transport properties play an important role in the construction of soft-matter functional materials, and in the activity of biological systems. In fact, it has become evident during the workshop that electrostatics in the description of many biological processes (like muscle contraction) are essentially neglected, whereas such interactions most probably do play an important role. Especially challenging topics are mixtures and complex structured systems, like for example bio-sensors, systems with interfaces, ion channels, nerve cells, and crowded media.

2 Major outcomes

During the workshop, a number of topics were discussed: (i) the validity of Poisson-Boltzmann theory and possible extensions, (ii) the interplay between hydrophobic/hydrophilic and electrostatics, (iii) charged interfaces (both between two immiscible liquids with large differences in dielectric constants and lipid membranes, also in connection with counterion condensation), (iii) electrostatics in biological processes (with an emphasis on muscle contraction), (iv) ionic liquids, (v) ionic microgels, (vi) electrostatics in apolar media, (vii) self-assembly patchy colloids, proteins, and polar liquid crystals, and (viii) applications of various types of charged species in the formulation of functional materials (hydrogel-based circuits, biomimetic devices, soft robotic actuators, and porous materials).

The importance of electrosctatic interactions and ion-condensation were discussed in connection to muscle contraction, where actin filaments serve as anionic polyelectrolytes surrounded by a sheet of condensed counterions. Properties of the technologically important ionic microgels, microcapsules, and inverse micelles have been addressed, where electrostatics plays a major role. The inverse-micelles experiments led to an alternative determination of the charge of a single electron, as micelles carry typically a single elementary charge.

The presentations on applications of these types of systems revealed that, in order to optimize the properties of functional materials with respect to the many controllable parameters, requires a better fundamental understanding. Theories and simulations that go beyond the classic Poisson–Boltzmann theory were presented, amongst them proton diffusion along lipid membranes, and structure formation on neighbouring charged interfaces. Contrary to salt solutions, finite size effects play an essential role in ionic liquids. Experiments were discussed, and models have been introduced to include packing effects. Protein interactions and the resulting self assembly have been discussed, where dimerization is shown to lead to screening of charge interactions, while the combination of long-ranged electrostatic interactions and short-ranged hydrophobic/van der Waals interactions give rise to various kinds of phases and microstructural order. Electrostatic effects due to interfaces have been a topic of interest. The interaction between charges on either side of a charged interface between fluids with a very different dielectric constant was discussed, as well as the role of electrostatics in the self assembly of charged colloids in interfaces, including the effect of a magnetic field. Simulations revealed that protein diffusion turned out to be faster near a lipid membrane as compared to bulk, which is due to the water structure near the interface. Besides presentations directly concerned to electrostatics, there was a presentation related to protein-structure determination by electron microscopy, and a presentation on super-resolution human brain tractography. Both of these techniques study systems where electrostatics plays an important role (protein structure and functioning of nerve cells).

On the basis of this workshop and the many lively discussions, we identified three main themes of interest:

- Fundamental theoretical and simulation problems in macromolecular electrostatics.
- The role of electrostatics in biological processes/systems.
- Self assembly and transport in complex synthetic charged macromolecules ,used to create soft-matter functional materials

In a possible successive CECAM workshop we would like to address these themes in a more focused manner. Beyond making progress in each specific field-of-research, we want to foster cross-fertilization between scientists from the three different research fields corresponding to the three above mentioned themes.

3 Community needs

In most processes where electrostatics plays an important role, other types of physical mechanisms also come into play (like combinations of electrostatic interactions and hydrophobic interactions, transport in the presence of crowding, structural properties of water, …). In order to connect to scientists in these related fields, contacts with SoftComp and ESMI will be of importance. One of the organizers (JKGD) of this workshop is a board member of SoftComp (which stands for “Soft Matter Composites), and is actively involved in the organization of workshops that originate from this network. SoftComp is a former FP-6 Network of Excellence which is now running self-sustained without EU-funding. The intention is to connect the participants of the CECAM workshop more closely to SoftComp, in order to achieve the additional knowledge and contacts with other scientists, which is necessary to enhance progress of the CECAM workshop. In addition, JKGD is the coordinator of ESMI (standing for “European Soft Matter Infrastructure”), which is a network of scientists who offer access of European scientists to their infrastructure. ESMI now runs one year without EU funding, and we hope for the approval of a similar network in Horizon2020 this year. One of the members of ESMI is the Forschungszentrum Juelich, offering, amongst other

infrastructure, access to the super-computers and support from simulation-dedicated scientists.
This will allow participants of the CECAM workshop to extend their computer capabilities (in terms of CPU time and support in the design of simulation algorithms). The ESMI infra-structure network also offers access to a wide range of soft-matter characterization and synthesis facilities, from which the experimental participants will profit. To bring the attention towards an integrative understanding on this topic, we propose an innovative two-yearly CECAM workshop that is focused on charged species in bulk and at functional interfaces in various systems.

4 Funding

Potential joint proposals were discussed during the workshop amongst the participants, theoreticians and simulators, as well as the experimentalists. Joint additional workshops may be organized through SoftComp (see the discussion in “Community needs”). Such so-called “topical workshops” should be quite focused, and are, at least in part, financed by SoftComp once approved. Common proposals for experiments and simulations can be submitted to ESMI (see “Community needs”), which will also be financed through ESMI once approved. In addition, the Forschungszentrum Juelich is ready to, spend 5000 Euro from its own budget to finance the possible future CECAM workshops.

5 Will these developments bring societal benefits?

The benefit to the community of this workshop is that the foreseen cooperation between scientists from the three communities of fundamental research, biophysics, and soft-matter functional materials, will ultimately lead to an enhanced progress towards a better understanding of biological processes and/or systems (with possible applications in the rational design of medicine), as well as the design and manufacturing of soft-matter functional materials. This workshop is ultimately beneficiary to bring the impact of solidary grounds to improve the understanding of the charged species that are ambient for our daily lives in bigger scales, such as reducing the aviation clouding in the climate in future, as well as increasing the fuel efficient in the automobile and other portable human transport facilities. Functional soft matter can also provide environmental and human-friendly bio-medical devices to detect early diagnosis of human-brain diseases.

Future innovation in the field of smart soft-materials and biophysics, that are of increasing importance in daily life (like in medicine, self-healing materials, coatings, bio-mass fuel, medicine, and sensors), requires a physics based, quantitative understanding of their properties. Innovative and integrative sciences and technology are urgently needed to formulate the driving mechanisms underlying efficient transport as well as networking of common grounds for their complexities. Interactions between charged species determine in many cases the behaviour of these quite diverse types of complex systems. In synthetic as well as biological systems, the same types of electrostatic interactions play a very important role. The central tasks are then how this complexity of various systems can be probed by appropriate shared protocols.

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Mathematical and numerical analysis of electronic structure models

Location: Station biologique de Roscoff (UMPC/CNRS)
Webpage: https://www.cecam.org/workshop-0-1294.html
Dates: July 4, 2016 to July 8, 2016

1 State of the art

First-principle molecular simulation makes use of more and more complex mathematical models, numerical algorithms and computer architectures. Many successful knowledge transfers from applied mathematics and scientific computing to computational chemistry and physics have occurred in the past 20 years: optimized linear algebra packages, efficient and robust optimization methods, fast multipole algorithms, ... Specific, dedicated numerical methods for molecular simulation have also been developed by applied mathematicians, or by multidisciplinary teams involving applied mathematicians, and successfully implemented in production codes.

Such interdisciplinary collaborations are fostered by many research programs and institutes all around the world (Institut du Calcul et de la Simulation at UMPC, Labex MMCD at Université Paris Est, Maison de la Simulation at CEA Saclay, just to name a few in France related to the organization of this workshop).

These examples show that a better understanding of the mathematical structures of the models, based on a theoretical analysis of the equations, can lead to new ideas for developing more efficient numerical methods. It is also a mandatory step to design certified numerical methods providing not only a numerical approximation of the exact solution of the model, but also error bars allowing one to estimate the quality of the obtained numerical results. The latter point is crucial to assess the reliability of first-principle calculations.

The purpose of this workshop was to gather the small but growing community of applied mathematicians working on electronic structure models, in order to discuss some of the key mathematical and numerical problems arising in the field with a few prominent experts and bright young researchers from the chemistry and physics community.

This event was part of the series of workshops and conferences on "Mathematical and numerical analysis of electronic structure models".

2 Major outcomes

The major scientific points discussed in the meeting were the following:

1. Mathematical formulation, discretization methods, and algorithms for electronic structure calculation
    - rigorous formulation of extended coupled-cluster, GW, and Bethe-Salpeter models (R. Klein, S. Kvaal)
    - h-P discontinuous Galerkin discretization schemes for Kohn-Sham (C. Marcati)
    - compression and acceleration techniques, linear scaling methods, massively parallel algorithms for Kohn-Sham (X. Dai, F. Gygi, X. Liu, D. O'Regan)
    - fast algorithms for linear response eigenvalue problems (Z. Bai)
    - low-rank tensor methods, for ground state calculation, but also for GW and Bethe-Salpeter equations (J. Eisert, V. Khoromskaia, B. Khoromskij, I. Oseledets, C. Yang)

2. Error analysis: certification and extrapolation of computational results

- cross-validation of a variety of softwares for Kohn-Sham calculations, thorough a thorough analysis of benchmark calculation results (F. Jollet)
- a priori and a posteriori error analysis for molecules and solids (G. Dusson, D. Gontier)
- extrapolation techniques (A. Savin)

3. Extended systems and multiscale models

- embedding methods for Kohn-Sham models (L. Lin)
- locality results for tight-binding models (C. Ortner)
- algorithms for Wannier function construction (A. Levitt)
- mathematical modeling and simulation of multilayer aperiodic 2D materials (P. Cazeaux)
- multiscale QM/MM, QM/QM, QM/PCM models ((H. Chen, B. Stamm)
- quantum Monte Carlo methods for Hubbard models (C. Mendl)
- spin dynamics in multilayered ferromagnetic materials (C. Garcia Cervera)

The number of talk was kept limited to 25 (for a 4.5 day workshop) in order to save time for discussions and work in small groups. In particular, each talk was 40' long, followed by 20' of discussion. This format was very much appreciated by the participants. The workshop gave rise to very fruitful discussions, and several collaboration projects have been initiated. It is to be noted that most of the speakers really made a pedagogical effort to be understood by the participants of the other scientific communities, which is obviously an absolutely necessity for the success of a multidisciplinary workshop.

3 Community needs

Among the very numerous codes developed and used by the chemist community, some of them are open, free and/or easily accessible. It would be interesting to organize a session where developers of the various comparable code would present their approach and discuss these with applied mathematicians and computer scientist. It is indeed our experience that some basic ingredients well known in the applied math community are not known or not optimally implemented leading to loss of efficiency in the implementation. Conversely, as is the case e.g. for the DIIS method, classical methods in the theoretical chemistry community are not known and/or not enough analyzed.

The codes that would be presented should be grouped corresponding to similar properties or applications they target. They should also be selected regarding the level of mathematical aspect they contain. Applied mathematicians proposing approaches that are not fully developed would be invited to deliver presentations associated with the software presentations.

4 Funding

The FETHPC-02-2017 (RIA) call for proposal (deadline Sep 2017) of the European H2020 program, is concerned with transition to exascale computing in chemistry and physics.

Specific Challenge: Take advantage of the full capabilities of exascale computing, in particular through high-productivity programming environments, system software and management, exascale I/O and storage in the presence of multiple tiers of data storage, supercomputing for extreme data and emerging HPC use modes, mathematics and algorithms for extreme scale HPC systems for existing or visionary applications, including data-intensive and extreme data applications in scientific areas such as physics, chemistry, biology, life sciences, materials, climate, geosciences, etc.

We believe that this is an opportunity for European participants to the workshop to submit, together with other colleagues, a joint interdisciplinary research project in this area.

5 Will these developments bring societal benefits?

The workshop we have organized was rather upstream with respect to direct societal benefits.

Nevertheless, as this is the case for many applied mathematics contributions, the implementation in application codes appears instrumental.

Some of the numerical methods which were presented and discussed during the workshop have already been implemented, either in Matlab or in production codes used in the chemistry (e.g. Gaussian) or materials science (e.g. Abinit) communities, and have been proved to lead to major gains, in terms of CPU times and/or accuracy.

Developing more efficient numerical methods in the area of first-principle molecular simulation, is key to allow one to simulate larger systems and obtain more reliable results (ideally with controlled error bars).

In this respect, the contributions that have been presented during the workshop are expected to lead to potential large benefits for the chemistry, material science, nano sciences, and molecular biology communities.

A follow-up workshop in the spirit of what has been proposed above would facilitate the development of these improvement and benefits for the user communities.

6 Participant List

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Structure prediction of nanoclusters from global optimization techniques: computational strategies and connection to experiments

Location: IPREM, Technopole Helioparc, Pau, France
Webpage: https://www.cecam.org/workshop-0-1332.html
Dates: July 5, 2016 to July 8, 2016

1 State of the art

This workshop was focused on the determination of clusters, nanoclusters and nanoparticle structure. The workshop gathered researchers from several fields, namely theoretical chemistry, theoretical molecular physics and condensed matter physics working essentially in a bottom-up strategy (from atoms to bulk) at the atomistic scale. The scope of the workshop intended to be (i) methodological, namely report/prospect progresses and new routes in global optimisation algorithm and global exploration of the configurational landscapes, among which the Genetic/Evolutionnary algorithms, Parallel Tempering, Basin hopping, Minima hopping, Particle Swarm based algorithms, Cookos'nest algorithms, etc.... as well as methods to explore other aspects of the landscape, involving the role of temperature on the properties and dynamics on the PES. (ii) state of the art report about recent advances in solving pending problems in the field of cluster structure resolution, and (iii) address new applications, increasing the complexity of the systems in terms of size and composition. Moreover a few experimentalist experts developing techniques to probe the structure had been invited to interplay with the theoreticians. Lively and fruitful discussion took place after each presentation.

2 Major outcomes

The methodological advances concerned the performance of global optimization methods (see state of the Art section). Combinations of algorithms such as Basing-Hopping/Parallel Tempering is quite efficient. Beyond the current algorithms, specific approaches to chemical order, guiding fields, specific algorithms for 2D systems were analysed. The question of the combination of these demanding algorithms with energy/gradient determination of the PES was strongly discussed. Global optimization was shown to be feasable directly with DFT now up to a few tens atoms. Beyond this size, one may use multi-methods schemes combining classical potentials for the exhaustive search of structures and subsequent check with DFT (up to roughly a hundred atoms). Memory algorithms to avoid repetition/revisiting basins were discussed. For dedicated systems (molecular clusters), use of coarse-grained potentials was also adressed. New techniques to optimize the free energy at finite temperature were introduced. Extensions were developed in particular with the use of basin-hopping algorithm in the grand canonical ensemble, opening a route to a thermodynamical picture of nucleation with all atomics degrees of freedom. The workshop also revealed a significant evolution in the type and complexity of systems and applications: size up to nanoparticles of 100-300 atoms, composition (mixed clusters, non stochiometric species) inducing chemical order/disorder (bi- or tri-metallic nanoalloys), chemical structural transitions induced by inhomogeneities, topological mismatch and internal pressure. A quite important outcome is that in a number of cases, the range size under study now allows for the investigation critical sizes of of structural transitions and convergence to the structural properties of bulk systems (using force fields). Special algorithms were developed to deal

with the complexity brought by the environment (supported or solvated nanoparticles). In order to analyse this increased complexity, new analyses and descriptors were proposed, using graph theory, definition of new topological distances, allowing for structure classification but also to a global analysis of the relevant areas of the PES (minima, barriers, paths, funnels). Finally, the significance of equilibrium structures in the nanoparticle size range vs the role of temperature on structural/thermodynamical chemical order was discussed. The interplay between theory and experiment is compulsory since experimentalists have (almost) no direct access to structure of free nanaoparticles. The discussion with the experimentalists was very fruitful, namely about (i) the relevance of structures and the identification of isomers and the advance brought in structure recognition via assignments of IR or electronic spectroscopy, action spectroscopy(IRMPD), photoemission spectra, electron diffraction, chemical reactivity (ii) the role of anharmonicities in the observables associated with either quantum delocalization and/or temperature, (iii) the experimental control of size and composition, the influence of the external parameters (iv) adressing single nanoparticles vs ensembles. There is a need for free energy calculations and theoretical spectroscopy beyond harmonic approximation, which cannot yet be achieved with DFT for systems sizes>100, but with simpler potentials. Two significant questions can be stressed: (i) the definition of ab initio references because of problems met by DFT with the fluctuation of the results upon the functionals, its difficulties in open-shell cases (magnetism) (ii) the need for transferable and versatile approximations (DFTB, force fields). However, within a multi-approach framework, advances in both size (targetting the range 100-1000) and composition can be expected. This progress will be due both to algorithmic advances together with specific adaptation of the algorithms to massive HPC (centralized or distributed).

3 Community needs

Due to the increasing size generating more and more numerous isomers, to the need of benchmarking extended, combined or new algorithms, and to the development of the applications (size and diversity), data storage and available repositories for structural data become an option, which could be reached however based on a distributed and networking hardware or in some dedicated centers having the material power and the manpower to maintain such data with web open access to the scientific field community and convivial interface for storing/retrieving data and the softwares that were used to produce those data. A series of CECAM workshops would be a nice tool to further structure the community, maybe also involving audience of other related workshops organized recently (metal nanoparticles...) with a strong overlap. Also links with techniques developed in biophysics or biochemistry/biology to investigate and analyse the structure and dynamics of biological complex systems at the atomic scale could be developed.

4 Funding

Typical funding for this research can be obtained from classical national or european calls, using either calls dedicated to fundamental research, but also joint calls dedicated to applications in which nanoparticles are of interest and need theoretical support. Although official joint proposals were not directly worked out during the meeting, a number of collaborations concerning common needs of theoreticians, and collaborations on various applications were discussed, putting forward bases for more formal proposals.

5 Will these developments bring societal benefits?

The main scope of the workshop remained essentially fundamental. However, solving and better understanding of structural aspects in the gas phase or/solvants or of deposited nanoparticles has some direct applications in various fields such as nanotherapy vectors, biomarkers, non-invasive cancer cell elimination, theranostics, catalysis, and nano cluster-based nanodevices for information storage, photocatylisis for pollution control, energy conversion and storage (fuel cells). With the size of nanoparticles now realistically addressable by theory and in combination with experiment, real applications become a reachable target. Also, not only the minima but the full landscape generated by the PES, including determination of reaction barriers and of funnels, opens a route the description/understanding processes in the range 100-1000 atoms. Some contributions were directed to this search: reverse design and automatic identification of good candidates for properties using similar algorithms to optimize absorption wavelengths or band gaps, as those developed for energy, in order to obtain properties dedicated to specific applications. Also scaling-up perspectives for nanoscale integration were now experimentally demonstrated in the case of supported metal clusters, with control/video monitoring of structural transitions and properties on temperature (electron-spectroscopy analysis and e-beam heating) for size selected clusters. This raises the level of challenge to overcome for theoreticians.

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Computational methods for modelling multiply-charged droplets

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1333.html
Dates: July 6, 2016 to July 8, 2016

1 State of the art

Charged liquid droplets are ubiquitous in both nature and technology; aerosols, thunder clouds and electrospray are just a few prominent examples. The composition of the droplets varies with the context, but typically a droplet is composed of solvent and charge carriers such as simple ions or macroions. This workshop brought together scientists who study different aspects of the physics and chemistry of charged droplets via both experiments and computations.

The chemical and physical processes that take place within a droplet are complex, compared to vapour/solvent phase chemistry, and determine the outcome of the experimental measurements. A major cause of the complexity is that the droplet environment is dynamic. Droplets generated by electrospray ionization undergo evaporation, fragmentation and develop charge-induced instabilities. These factors affect the

charge state of a macromolecule and the stability of a macromolecular complex (such as nucleic acids, proteins), which is the outcome of electrospray mass spectrometry. In atmospheric aerosols, the charged droplets undergo condensation and may attain unique morphologies that in turn may affect the nucleation barrier in the formation of ice crystals or rain drops.

Currently, several aspects in the physical and chemical behaviour of charged droplets have been understood. The solvation of simple ions in clusters and vapor-liquid bulk interfaces may provide insight into the solvation of these ions in droplets. An important process that charged droplets undergo is fragmentation. In this area, considerable progress has been made in developing theoretical and computational methodologies starting from the studies of metal and model argon clusters and progressing into the studies of aqueous droplets with simple ions. The charge-induced instabilities in droplets due to various charge distributions caused by the presence of simple ions or charged macromolecules have been determined by simulations and theory.

2 Major outcomes

The participants identified several directions to be pursued:

1. Currently, charged droplets of up to a few thousands of solvent molecules are modeled at the atomistic level. The linear dimensions of these droplets are of a few nanometers. However, in practical applications droplets of tens of nanometers up to approximately 100 nanometers appear in atmospheric aerosols or in electrospray ionization applications. Bridging the length-scale gap covered by the entire electrospray ionization process calls for multiscale modelling.

2. Many applications in electrospray ionization processes involve sampling of the conformations of macromolecules either in the droplet environment or in the gaseous phase. Advanced sampling techniques are required and these may benefit by transferring

the experience already developed in the polymer community.

3. Force-fields are generally parametrised for infinite dilution, but are relatively untested at the high droplet concentration limits that are relevant to applications in electrospray ionization and atmospheric aerosols. Polarizability is probably important for calculating certain quantities such as reaction rates and rates of fragmentation accurately.

4. There is a need in experimental/simulation groups who perform simulations that attempt to reproduce particular experiments to have access to codes and software for sampling conformations of macromolecules in the gas phase. Therefore, there is a need for development, optimisation, maintenance and sharing (open source) of codes for modeling the processes of macromolecules in the gas phase. Moreover, the force-fields for macromolecules from solution are not necessarily appropriate for the gas phase. AMBER16 may have started on this, but only for proteins.

5. Simulators should start with realistic potential or actual experimental conditions so that the results are predictive for experiments. Conversely, are there better experimental structural probes that can make closer contact with the predictions of the simulations?

6. Simulators should educate themselves on realistic instrument set-ups, bearing in mind that the designs of different vendors may differ considerably.

7. One of the questions to be examined is whether the notion of hydrophilicity/hydrophobicity of a macroion in a droplet is the same as that in the bulk solution. A droplet with macroions is characterized by many interfaces that play a significant role in the manner that a macromolecule is solvated, therefore, the notion of the hydrophilicity may be altered in the finite-sized systems relative to that in the bulk solution.

8. Even though new methodologies are being developed to study computationally the effect of charging coupled to the mechanism by which macromolecules emerge from droplets, this is still an area of research that needs to be explored further. Prominent question is the treatment of the protonation of the macroions in the constantly changing droplet environment. Even though there are suggested methodologies so far there are still methods to be developed and borrow ideas from quantum mechanics-molecular mechanics modeling.

3 Community needs

The computational community will benefit from the following:

1. Outreach to the experimental community (in atmospheric aerosols and electrospray ionization) with which there is going to be mutual benefit by transfer of knowledge.

2. The participants identified the need for open source software that includes advanced sampling techniques of the conformations of macromolecules in the gas phase.

3. We think that future CECAM workshops will benefit both the computational and experimental communities for the following reasons: (a) Currently many experimental groups in electrospray ionization mass spectrometry use computations to understand the processes that take place during droplet desolvation. Sometimes in experimental groups the computations are performed by personnel that may not be well trained in theory/computations. The transfer of knowledge in the CECAM workshops can assist scientists who may lack certain background. (b) The understanding by molecular simulations of the factors that determine the droplet stability, the charge state of the macromolecules as well as the stability of weakly bound non-covalent complexes grows rapidly. The community grows as well. Discussion of the cutting-edge research in the workshops and setting new goals towards the understanding of fundamental processes

occurring in those systems helps the progress in the field.

4 Funding

Different funding sources were identified:

1. Electrospray mass spectrometry and chemical analysis companies such as Agilent Technologies, Waters, Bruker, SCIEX, MassTech to name only a few fund the mass spectrometry conferences. These companies are also potential sponsors of a future CECAM workshop on charged droplets.

2. The Royal Society of London operates an International Exchange Scheme that provides a mechanism for seeding new collaborations between groups in different countries. New interactions between computation and experiment, where the complementarity of the partners is clear, could benefit here.

3. In the UK, the EPSRC renewed its "Software for the Future" call in 2014, recognising the importance of developing and maintaining sustainable codes, as well as associated training.

5 Will these developments bring societal benefits?

Possible societal benefits include:

- Electrospray mass spectrometry and chemical analysis companies such as Agilent Technologies, Waters, Bruker, SCIEX, MassTech (to name only a few) benefit from research in improving their technologies. These improvements in turn enable the further development of any commercial applications that use such techniques.

- Molecular insight into the mechanisms of droplet desolvation, obtained by computational means, may improve the efficiency and quality of measurements, which in turn may lead to societal benefits, which may ultimately include for instance lower costs of drugs or improved security at airports because of more efficient chemical analysis.

- A sound understanding of charged droplets in all their complexity also underpins advances in the field of atmospheric aerosols. The molecular physics of such aerosols plays a major role in determining climates and environmental conditions. Hence, computational studies of charged droplets are an area of fundamental research that lies on a path towards informing major political decisions with profound societal impact.

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Multiscale modeling of biomolecular aggregation and protein-membrane interactions in amyloid diseases

Location: CECAM-Lugano, Lugano, Switzerland
Venue: USI University of Swiss Italy
Webpage: https://www.cecam.org/workshop-0-1337.html
Dates: July 11, 2016 to July 13, 2016

1 State of the art

Amyloid protein aggregates are formed by normally soluble proteins that assemble into insoluble fibrils. Amyloid formation is often a pathological fingerprint of a number of devastating diseases, such as Alzheimer's. Characterizing the mechanisms of formation of toxic amyloid aggregates from soluble, monomeric proteins is of major importance in amyloid disease research. In recent years, attention has shifted towards oligomers formed in the early stages of the amyloid aggregation pathway, with several studies showing that oligomers rather than the fully formed fibrils are the most toxic molecular species. Furthermore, growing evidence suggests that cytotoxicity in Alzheimer's disease may be due to multiple causes, including membrane disruption and interactions with other amyloid proteins or protein receptors.

While there are obvious challenges involving the molecular simulation of amyloid aggregation, due primarily to the large sizes and time scales associated with amyloid systems, recent computational and experimental studies have successfully overcome some of these barriers bringing experiment and theory ever closer. Nevertheless, direct comparison with experiment is difficult due to the large length and time scales involved in aggregation. Furthermore, little-to-no direct structural data is available for smaller oligomeric species, as these are difficult to experimentally isolate. It is also challenging to compare results between simulations due to the wide range of potentials and methods used. In addition, there is a critical need for simulations to include more realistic environmental effects, such as the role of lipid membranes, metal ions, and other proteins including receptors and other amyloid proteins.

This workshop provided a timely and critically needed opportunity to identify and discuss the main challenges in this active research field and to propose novel approaches that will enhance future theoretical and experimental studies in the field.

2 Major outcomes

This workshop brought together top and also emerging researchers studying amyloid aggregation, with emphasis on the amyloid-beta peptide involved in the pathology of Alzheimer's disease. We benefitted from the participation of leading experimentalists in the field of amyloid aggregation—more than 1/3 of the talks were given by experimentalists—in order to tackle the crucial question of how to strengthen the connection between molecular simulations and experiments. Our program included both research presentations and open discussions.
A central topic of this workshop was the exploration of novel simulation approaches addressing critical questions relevant to our understanding of amyloid aggregation on different length and time scales. Our goal was to identify enhanced methods and biologically relevant models. A second focus of this workshop was to relate simulation and experiment in

order to identify joint, collaborative approaches for the future.
More precisely, the presentations were organized in the following topical sections including 3 to 4 talks each:

1. Amyloid aggregation: thermodynamics, kinetics and intermediates (2 sections)
2. The influence of metal ions on amyloid aggregation
3. Amyloid aggregation: environmental influences and intermediates
4. The influence of membrane on amyloid aggregation (2sections)
5. Various aspects of amyloid aggregation

The speakers had significant research expertise in more than one of these topics, allowing for rich exchanges. Experimentalists were included in almost all sections, which helped to strengthen the connection between simulation and experiment. Each talk was followed by 10 minutes of discussion time where participants could ask their questions regarding the talk in question. These 10 minutes were always made full use of and lively discussions developed. In addition, each session in the program included a highly productive, moderated panel discussion of key questions identified in each session.

The talks and the posters presented addressed a variety of topics, including: (i) classical approaches to model the assembly and structure of early amyloid oligomers, (ii) in vivo effects in simulation approaches: metal ions, membranes, surfaces, molecular crowding, (iii) coarse-grained approaches to study amyloid aggregation on larger length and time scales, from the formation of protofibril-like oligomers to amyloid fibrils and filaments, and (iv) new simulation and experimental approaches to quantify and control the mechanism of protein and peptide aggregation, and the formation of oligomers and fibrils.

In the discussions, the participants emphasized the increased need for networking, in particular for bridging the gap (including in vocabulary and methods) between the experimental and computational communities. For example, some experimentalists noted that it is difficult to read a simulation paper and know whether the results are valid, or whether the methods are appropriate. There are controversies among simulators regarding force fields, parameterization, validity of implicit solvent models, among other simulation parameters. Without deeper knowledge of simulation tools, it can be difficult for experimentalists to appreciate the limitations and underlying assumptions in a given computational study, which would affect the results or interpretation. In a similar manner, it was noted that experimentalists could help the simulation community by understanding their vocabulary and explaining their experimental systems in those terms. It can be challenging for computational scientists to determine under what conditions an experiment was conducted.

The major outcomes of this CECAM meeting will be summarized in a perspective and submitted as a Viewpoint to the The Journal of Physical Chemistry B.

3 Community needs

Based on the presentations of research involving molecular modeling, it it is clear that high performance computing resources will play an increasingly important role in enabling molecular simulation studies of large molecular systems such as amyloid aggregates. The atomistic level studies benefit from relatively mature source codes and relatively good force fields. Nevertheless, due to the shear size of the problem, new algorithmic developments are needed to enable systematic studies of the formation and stability of amyloid aggregates, which would rely heavily on modern enhanced sampling methods.

In general, it was noted that experimentalists and simulationists should collaborate even more closely with each other than they already do. A joint effort should be to clarify how simulation results could be fed back to experiments, or how the design of experiments could be guided by simulation. For example, some simulations indicate the presence of kinetic traps for oligomer growth that potentially extend oligomer lifetimes. How could this result from simulation be tested experimentally, or used to influence the design of experiments? An important challenge that needs to be overcome here is that simulations and experiments often test different time and length scales, hampering the direct comparability of the results.

Finally, it should be noted that there was a general agreement that ideally, students would be educated in both simulation and experiment. In Germany, for instance, this could be implemented by establishing graduate schools for PhD students where the curriculum would require that the PhD students have to perform always both experiments and simulations for the (amlyoid) system under study. This would be possible with two PhD supervisors per student, one simulation expert and one who is experienced in doing experiments, who agree to join forces and collaborate on a common research question.

4 Funding

CECAM was crucial in providing the majority of funds needed to hold this workshop. A majority of speakers were offered partial or those from overseas even full coverage for their hotel stay, including younger participants, and the poster session and social dinner were also covered from CECAM funds. However, most participants secured their own funding from their own institutions or grants for transportation, accommodation and other expenses. For future meetings, it was noted that it would be helpful to apply for additional funding through organizations such as ECAM in the US, SFI in Ireland, and DFG in Germany. However, one has to bear in mind that in case of applying for funding from DFG one has to submit the proposal at least 6 months before the workshop date. And of course one can only apply for extra funding once CECAM has approved the workshop.

5 Will these developments bring societal benefits?

The outcomes of our workshop stand to provide societal benefits on the long term, through the development of adetailed understanding of basic molecular aggregation processes involved in amyloid formation. This fundamental knowledge may play a central role in understanding, treating and possibly preventing many devastating diseases, such as Alzheimer’s disease, Parkinson’s disease, or type 2 diabetes, to mention only a few. It is our belief that this field of research, both experimental and computational, will lead to health benefits through the development of new drugs that may prevent or treat symptoms of amyloid disease, as well as new biomarkers that may improve disease-related diagnostics. Short term impact includes enhancements in our understanding of basic molecular processes involved in amyloid formations, and the training of new generations of scientists with a multidisciplinary background necessary to tackle problems at the interface of biology, chemistry, physics and computer science.

6 Participant List

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Electronic Structure Theory with Numeric Atom-Centered Basis Functions

Location: CECAM-mm1p, held at TU Munich
Webpage: https://www.cecam.org/workshop-0-1317.html
Dates: July 20, 2016 to July 22, 2016

1 State of the art

Electronic structure theory including density-functional, wave-function, and many-body perturbation theory based methods continues to grow in reach and importance across computational molecular and materials science. For non-periodic and periodic models up to thousands of atoms in size, this first-principles, i.e., quantum mechanics based approach offers unbiased predictions and understanding that meets basic science, materials engineering, and industrial needs. Application examples include electronic materials, energy related materials for photovoltaics or photocatalysis, biomolecular phenomena and reactions, etc. A key methodological choice that distinguishes different successful implementations of electronic structure theory is the choice of the quantum-mechanical basis set used to discretize the underlying mathematical equations. This workshop focused on methods that leverage localized, numeric atom-centered orbital (NAO) basis functions, a choice upon which a number of the strongest available electronic structure developments are founded. Examples include the Siesta code, the FPLO code, DMol3, ADF, PLATO, the FHI-aims code, and many others. In addition, key concepts in NAO codes are closely related to formalisms employed with other types of basis sets, such as Gaussian-type orbitals, linearized augmented plane waves, etc. Specific advantages of NAO-based electronic structure codes include the fairly straightforward modeling of non-periodic and periodic systems on equal footing, suitability for order-N scaling numerical algorithms, efficient scaling towards large systems, efficient algorithms for exact exchange and many-body approaches based on the two-electron Coulomb operator, and the proven potential for simulations from fast qualitative models up to high-accuracy calculations that match the best available benchmark codes.

2 Major outcomes

The workshop featured 22 keynote talks covering:

1. New algorithmic developments for simulations based on numeric atom-centered orbitals (e.g., embedding formalisms (Oberhofer), meta-GGA implementation and performance (Logsdail), many-body perturbation theory (Ren, Rinke and Ying Zhang), friction and non-adiabaticity (Maurer), electron-phonon coupling (Carbogno), charge constraints (Schober), efficient spin-orbit coupling (Huhn)),

2. new developments of broad general relevance to the electronic structure community, including advanced exchange and correlation descriptions (Perdew, Ruszinzsky, Tkatchenko), the structure prediction challenge for complex systems (Marom, Neumann), restoring nuclear quantum effects (Rossi), efficient coarse graining of first-principles predicted data towards larger scale predictions (Ghiringhelli),

3. community-wide initiatives that benefit both electronic structure developers across very different codes, as well as specialists for different application areas, including the CECAM Electronic Structure Library (Corsetti, Oliveira), reference data sets for materials science

and the NoMaD repository (Scheffler),

4. and new trends and paradigms in high-performance computing hardware and associated software development strategies (Vazquez-Mayagoitia, Rampp, Merz).

Notably, two speakers from industry were among those giving keynotes (Neumann, Merz), offering and emphasizing insights into usability and application needs for electronic structure methods that add to those of a purely academic audience; the reality is that time and efficiency matter for industrial applications, even when addressing questions that lie arguably at the forefront of what can be scientifically achieved today (correct prediction of equilibrium structure and polymorphism in molecular crystals for industry applications). A dedicated tutorial of a genetic algorithm structure search algorithm GAtor focused on this very topic was also included as part of the workshop, given by Marom and her students Patrick Liu and Farren Curtis. The “hands-on discussion” format used in the afternoons to discuss focus areas of specific interest in small dedicated groups of participants to be an immensely effective forum to deepen these insights. Insights achieved range from “simple” but subtle bug fixes (platform dependence) of codes common to the developers, to algorithmic strategies for greater efficiency, to the development of new formalisms for many-body theory and to formalisms that extend the quantitative reach of electronic structure theory into new application scenarios. Among the many important aspects of these discussions, raising awareness of common software and algorithmic development strategies and tools is perhaps most noteworthy. CECAM’s Electronic Structure Library is accomplishing the otherwise difficult task of convening developers from distinct code projects who would not normally have an incentive to discuss parallel but separate development strategies and code for similar problems in their respective frameworks. In addition to collecting libraries (libxc as a flagship, solver libraries like ELPA, the orbital minimization method, and the pole expansion and selective inversion (PEXSI) library through the U.S. led infrastructure component ELSI (Blum)), Cecam's ESL has become a forum where developers actually identify new directions and synergistic strategies. Highlighting this effort, and also discussions among the subset of ESL-related developers present, were a key outcome of our own workshop in addition to the numerous science-related advances discussed.

3 Community needs

The community convened at this particular workshop (which, in fact, is now effectively a successful series) continues to be a source of significant scientific innovation with contributions to the wider field. Specific code developments within the FHI-aims code are one area that, through the mere availability of code, benefits a much wider community of users in simulation, experiment, and industry than could be assembled within the confines of this event. Beyond code-specific developments, some significant developments that have a direct effect on the wider community include solution strategies for the Kohn-Sham eigenvalue problem (the ELPA library) and on existing and upcoming massively parallel platforms, as well as new developments in many-body theory. Among the past successes that originated directly from the community assembled at this workshop, we note the translation of many-body approaches from the solid state community, based on GW, to molecular applications, the traditional domain of quantum chemistry. In this series of workshops, we continue to see a strong need and make strong efforts to reach out to a broader developer community, especially centered around library components; again, we stress the importance of CECAM’s ESL on multiple levels (including as a communication channel, in addition to developments of actual code). New high-performance computing architectures continue to form a core need of our activity, and our workshops attempt to play a leading role in this area as well. We believe that our workshops serve an ongoing need in the community and are grateful for past and, hopefully, future funding dedicated to them.

4 Funding

Typical funding channels for our line of research continues to come predominantly from national and transnational academic funding bodies such as the Max Planck Society, European efforts (Horizon 2020), German Research Foundation, Alexander von Humboldt Foundation, the U.K. EPSRC, the U.S National Science Foundation (the fully open-source infrastructure ELSI received major funding from NSF as an initiative benefiting multiple electronic structure codes and other committed stakeholders), etc. We continue to see industry as an opportunity for scientific stimulation and for funding, and in fact as a key to beneficial societal outcomes from our work (see below). Industry is a growing area of attention for us, in addition to the traditional (and central) need to pursue the scientific priorities that are among the foremost intellectual challenges of our field.

5 Will these developments bring societal benefits?

Yes. The core principle of our field is simple. We have an exact equation that would allow computational predictions to understand and improve essentially any chemical, biological, electronic, etc. materials and molecular application around us, but we can only solve the exact equation approximately, and only for a small subset of the real and pressing problems that are of interest to us. We can, for instance, now successfully predict viable new candidate materials for improved photovoltaics. We are on the cusp of predicting molecular crystal structures correctly that are critical for manufacturing in the pharmaceutical industry. We would love to be able to use molecular-scale insights that reveal the underpinnings of Alzheimer's disease, to name just one particular example that seems possible but still significantly out of our present reach. In this case, starting guesses exist for the molecular players (peptides) and suspected chemical agents altering them (transition metal ions), but for meaningful first-principles simulations, we lack sufficient statistical sampling, the accuracy of state of the art density-functional theory is still too limited, and a reliable description of the impact of the exact chemical environment (a brain - not just water!) is difficult at best. Numeric atom-centered orbital based all-electron methods, in fact, hold several specific advantages across all the listed application areas, building predominantly on (i) their intrinsic numerical accuracy near the nucleus, and on (ii) their intrinsically good scalability to large system sizes, by spatial separation of basis functions that already take advantage of the specific numerical form (chemistry) of the partial differential equation at hand. We will continue to build on this simple but effective recipe to address the challenges in chemistry and materials science that are, ultimately, our shared goal.

6 Participant List

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International Workshop on Biomembranes: The consequences of complexity

Location: CECAM-FI, Finnish IT Center for Science, Espoo, Finland.
Webpage: https://www.cecam.org/workshop-0-1330.html
Dates: August 16, 2016 to August 19, 2016

1 State of the art

The plasma membrane of eukaryotic cells comprises some 800 varieties of lipids, a significant area fraction of transmembrane proteins, and is anchored to the actin cytoskeleton. It is clear that the membrane is a complex, heterogeneous environment, but its functional role has elicited debate since the introduction of the raft hypothesis nearly 20 years ago. A major challenge has been to develop experimental techniques that report on the spatiotemporal dynamics of the membrane in live cells on time and length scales that matter for signaling.

This challenge is rapidly being met by new experimental methods that provide information on much shorter time and length scales than previously possible — scales which approach the molecular encounter scale that underlies cellular signaling. Examples include advanced particle tracking, either based on analysis of fluorescence fluctuations by localization microscopy, or interferometric scattering; fluorescence correlation spectroscopy with subdiffraction excitation volumes; neutron scattering from heterogeneous membrane mimetics; and direct nanoscale imaging of composition by secondary ion mass spectroscopy.

The emergence of new experimental techniques presents exciting new opportunities and challenges for computational modeling of membranes. Our goal is to catalyze productive new directions in computational modeling, motivated by new experimental data. Though we expect a new consensus to emerge from the meeting regarding specific challenges, a few clear challenges are listed below.

2 Major outcomes

1. Reconciling simple lipid mixtures and the complexity of the plasma membrane. In experiments and simulations alike, it is common to adopt relative simple lipid mixtures as models of cell membranes. These simple mixtures typically comprise 3 or 4 lipid components and have a symmetric composition with respect to the two leaflets. In contrast, the plasma membranes of animal cells are asymmetric in composition and contain upwards of 800 lipid species. Recent advances in preparing asymmetric model membranes and extracting lipid samples from cells for biochemical and biophysical characterization allow direct comparison to simulations and experiments on simple model membranes.

   Several key discrepancies were identified as targets for future simulation and experiment. First, it is clear from measurements of membrane order and partitioning of integral membrane proteins that the molecular organization of complex mixtures differs from simpler mixtures, but it is unclear exactly how. A better picture of the molecular scale organization of complex mixtures would aid in the development of models to interpret experimental data. Second, the role of asymmetry in plasma membrane organization is only just emerging. It appears that domain formation in the outer leaflet may couple to/induce domain formation on the inner leaflet, but the mechanism needs to be resolved.

Finally, these two issues inform the longstanding question of the nanoscale organization in living cell membranes — are there regions of differing lipid composition and chain order in live cell membranes?

2. Developing a complete picture of lipid and protein diffusion in cell membranes. It is clear that cell membranes are complex and heterogeneous systems, and therefore complex diffusion is expected. However, the presence of spatiotemporal organization over a broad range of scales makes the problem challenging. This meeting therefore brought together several experimentalists, simulators, and theorists at the leading edge of this area. Results from two cutting edge experimental techniques (fluorescence correlation spectroscopy with nanometer detection by stimulated emission depletion, and single particle tracking detected by interferometric scattering) were presented which give different results on the same system — STED FCS observes ordinary lipid diffusion, while iSCAT SPT observes subdiffusion up to msec timescales. Theoretical descriptions for subdiffusive processes were discussed, and simulations proposed to reconcile the results.

3. Understanding the interplay of composition, membrane deformation energetics, and membrane reshaping processes. Recent advances in numerical methods for obtaining curvature properties of lipid mixtures reveal a surprising, non-additive dependence of curvature on lipid composition. Results were also presented for protein-induced membrane deformation, obtained both by simulations and experimental methods. The ways in which cells might exploit composition (both protein and lipid) to drive reshaping processes was identified as an important area for future work.

3 Community needs

A series of workshops is likely on this topic, as this was already the second meeting in Helsinki on membrane biophysics generally. Holding the meeting in Helsinki was from the outset (3 years ago) a strategic choice, designed to draw the Finnish, American, and European membrane simulation communities closer together, to develop collaborations and shared objectives. In this goal, the meeting has been very successful. In the future, it will be important to continue the conversation, and share progress on the outstanding problems identified above.

4 Funding

The funding situation is quite difficult overall and the financial burden in many countries renders the situation even more difficult. Meanwhile, the competition for the available science funding becomes more and more tough. These issues are constantly being discussed among the scientists but there are no easy solutions. First, most of the science funding is based on national sources and limited to teams in a given country. Second, as a related matter, there are only limited sources supporting joint proposals by teams in different countries, meaning that the idea to consider joint research proposals as concerted actions is appealing but not realistic. In this context, the EU, e.g., supports joint research proposals in principle, but in practice those projects focus on industry-dependent actions instead of the basic science that is supported by the ERC for individual principal investigators.

5 Will these developments bring societal benefits?

The benefits are mainly in the area of human health. A key development in recent years is high throughput, “shotgun” lipidomics, which allows parsing of the chemistry of membrane lipids in unprecendented detail. Now that we know what lipids comprise our membranes, we can now ask how the composition of membranes changes with, e.g., diet, and can begin to ask how the biophysical properties of membranes depend on composition. This effort will enlist a range of techniques — experiments on live cells, biophysical characterization of both plasma and model membranes, and simulations to probe molecular level organization and mechanism.

This effort raises a crucial question for the membrane simulation community: What is the minimal lipidomic complexity required to capture the key biophysical properties of real cell membranes?

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Controlling Food Protein Folding and Aggregation: Challenges and Perspectives in Industry, Experiments and Simulation

Location: O´Brien Centre for Science, University College Dublin, Ireland
Webpage: https://www.cecam.org/workshop-0-1346.html
Dates: August 18, 2016 to August 20, 2016

1 State of the art

That molecular mechanisms play a central role in food, from nutrition and taste perception, to food structure, by molecular interaction or processing has long been known, and exploited experimentally and industrially.

Food scientists have striven for years to elucidate these molecular mechanisms that eventually define the macroscopic food product, yet despite enormous advances, including lately with technical innovations in the field of new equipment facilitating the observation at ever smaller scales, food remains a complex mixture of multiple ingredients, subjected to heat, shear and other harsh treatments so that only putative theories can be brought forward to explain the macroscopic observations due to changes at an atomistic or molecular level.

A deeper understanding of how tastants interact with the various classes of G-protein coupled receptors may yield to the design of new and exciting savours. A better knowledge of the conformational changes of taste molecules with temperature could yield to adapting the choice of say sweeteners to specific foods. At a molecular level, the effects of pH and salt on protein structure and interaction with other polymers, including carbohydrates and peptides is restricted to macroscale theories and we still lack refined explanations at the nanoscale. At a mesoscale level, the interaction between proteins and surfaces, be they hard surfaces of processing equipment where fouling is a major industrial issue or oil droplet surfaces where proteins are responsible for the physical stability of a wide range of food emulsions is still lacking.

The objective of the workshop was to give complementary perspectives on five themes: 1. effect of pH and salt on protein structure; 2. the effect of sugars on protein structure; 3. transport and storage of biomolecules and inorganic molecules in microgels or through and within interfaces; 4. macromolecular properties and their simulation; 5. Simulation of tastants and GPCR proteins.

2 Major outcomes

Barroso da Silva & Donnini focused on the effect of changes of solvent pH and salt on protein structure through simulations of titration from two simulation perspectives, the first mesoscale allows the simulation of very large complexes indicates that electrostatic interactions are their main driving forces of complexation, and permits quantitative insights into the relevant molecular mechanisms. The second, constant pH molecular dynamics simulation, allows the correlation between protonation, conformation and pH to be studied in atomic detail.

Gulzar and Cottone focused on the effect of sugars on protein structure. Two perspectives were given. The first explored the role of lactose on dry heating of proteins, as it constitutes a powerful means for improving the food protein functionality (gelling, foaming, emulsifying etc.) by modifying their structure. The second was on the properties of biomolecules embedded into glassy matrices and/or highly concentrated solutions of saccharides discovered through in vivo, in vitro, and in silico studies. These systems show an outstanding ability to protect biostructures against stress conditions. Some sugars, in particular trehalose, are peculiarly effective. The practical uses of treloahose includes long term storage of biomolecules as food or bio-pharmaceuticals.

Three perspectives were given related to transport and storage of biomolecules and inorganic molecules in microgels or through and within interfaces by Jacquier, Lobaskin and Cheung. In the first, the ability of cold-set whey protein microgels to function as pH-sensitive immobilisation matrices for charged bioactives such as amino acids and peptides was presented, highlighting the capabilities of food-grade whey based microgels as matrices that enable the immobilisation of a variety of bioactives by a charge interaction. In particular, it shows the potential for these matrices to function as smart delivery systems, in which uptake and release of bioactives is facilitated by environmental pH change. The second perspective focused on the adsorption of biomolecules on inorganic surfaces, and is of relevance to their purification, the response of the body to implants, food processing, the fate of nanomaterials in vivo, including their toxicology. A computational scheme was presented for the fast assessment of the likelihood of an arbitrary protein adsorbing or changing the conformation of a surface which relates advanced protein descriptors with basic molecular interactions at the interface. The third perspective concerns the adsorption and conformational change of proteins at liquid interfaces using coarse-grained simulations.

Radhakrishnan, Payne, Shell, Ferguson presented work on macromolecular properties and their simulation.

The first addressed the construction of top-down multiscale models for the design of functionalized nanocarriers in cellular targeting, and their predictive value in vitro, ex vivo, and in vivo.

The second perspective explored the properties of Carbohydrate binding modules (CBMs), which are non-catalytic protein domains attached by linker peptides to carbohydrate active enzymes. The third perspective posed the question are there theoretically intuitive and numerically robust strategies for turning all-atom simulations into coarse models that preserve sequence-specific physics? The fourth perspective presents an approach to compute single-molecule free energy surfaces from experimentally-measurable time series in a single molecular observable.

Two perspectives on the simulation of tastants, and G coupled protein receptors were presented. Carloni predicated the pose of bitter taste receptors' agonists by mesoscale simulation and bioinformatics. Santiso ingeniously sidestepped a detailed description of the receptor by focusing instead on conformational properties of a sweet tastant real taster sensory data to explain unusual temperature properties of the tastant.

3 Community needs

The focus of the workshop was on food and pharmaceutical proteins and their interactions with sugar, salt, water and protonation/deprotonation. The md engines GROMACS, NAMD and LAMMPS are the most relevant for md - where system size varies between about 50k to 1M atoms - and typically about 500k atoms. A 500k system will typically run efficiently using

between 100 to 400 cores.

Modelling of pH at atomistic level is much more challenging, and for large systems would need ten fold more core. Mesoscale modelling is also extensively performed using in-house codes and main stream codes such as Expresso. There the system size varies between about 5k to 500k atoms , with the HPC demands from a few core to 200 core.

Collaborating with experimentalists is very important in this field, both in the definition of problems to simulate, in the extraction of data (for instance machine learning and bio-informatics) that is essential in the preparation of initial conditions, and the identification of useful order parameters/descriptors. As this field is very close to industry, and bridges bio-pharma, health science and food science, organizing joint activities is immensely valuable.

4 Funding

Finding channels are available at a national and European level, as well as from industry. However, to produce credible proposals, it is essential to work with experimentalists, both because they tend to know the key scientific/industrial problems in the field, and are much closer to industry than simulators are. In this regard, we would highlight the contributions from Jacquier, who demonstrated the ability of cold-set whey protein microgels to function as pH-sensitive immobilisation matrices for charged bioactives such as amino acids and peptides, and from Gulzar, who focused on the Controll of lactose contents in food processing to avoid variability in protein denaturation/aggregation during dry heating. Jacquier and Gulzar have strong interactions with the food industry, in particular the large multinational Kerry Group.

5 Will these developments bring societal benefits?

Proteins play a major role in the food arena, and controlling protein functionality in food is tipped to become one of the main challenge and also possibly the main driving force for product innovation of the next decades. That molecular mechanisms play a central role in food, from nutrition and taste perception, to food structure, by molecular interaction or processing has long been known, and exploited experimentally and industrially. In this context, it is only in the last decade or so that molecular and atomistic simulation, associated statistical methods and computer hardware have become powerful enough to begin to elucidate many of these mechanisms in detail. That such simulations are difficult, even with massively parallel computer platforms, can be appreciated if one considers two archetypal problems: the modelling of effect of changes of solvent pH and salt on protein structure, and the physico-chemical nature of taste. For the former, the availability of protons in solution, and their transfer to and from titratable sites on a protein involves at a fundamental level quanta mechanisms such as bond breaking and bond formation – and transfer of protons and hydroxyls through water to acids and bases. Such charge transfers can also trigger protein folding/unfolding and the formation or dissolution of protein complexes. The modelling of taste and the interaction of agonist and antagonist ligands on the corresponding receptors is in some respects even more challenging due to their size of the proteins involved and interfacial nature, and equally important, not least because at a molecular level, there really is no real distinction between a ligand imparting taste or a drug acting on a receptor as a therapeutic.

The societal benefits of having a molecular understanding of key process in food and bio-pharma are huge, ranging from new protein systems to replace meat, new tastants that avoid use of sugar, better storage, and better purification methods

6 Participant List

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Quantum Plasmonics

Location: CECAM-UK-JCMAXWELL
Webpage: https://www.cecam.org/workshop-0-1338.html
Dates: August 24, 2016 to August 26, 2016

1 State of the art

Plasmonics is a recent discipline focused on the study of the interaction of light with matter, such as metal nanoparticles or metallic surfaces, where surface plasmons polaritons (SPPs) play a fundamental role. SPPs are mixed states between collective electron density excitations and light that are confined to the interface between a metal and an insulator. These excitations are extremely important because of their potential for nanotechnological applications. In fact, SPPs have a nanometric spatial confinement that is crucial for the development of devices smaller than 100 nm. For example, an important goal of plasmonics is to replace electronics technology with plasmonics offering faster responses resulting from the light properties of SPPs.

In the last few years, mainly because of advances in nanofabrication, interest in plasmonics moved towards the properties of very small nanoparticles systems. In such systems, a new challenge arises, the appearance of quantum effects. In fact, until now, plasmonics has been mainly based on classical physics concepts.

2 Major outcomes

The major outcome of this workshop was the strong interaction between two different scientific communities that works in the same problem but from different point of view, i.e. the plasmonics and electronic structure communities.

The most pointed topic was the difference between the various plasmon family (localized, propagating or bulk plasmons) and how to simulate it, a concept a bit unclear in the electronic structure community. From other hand, several discussions followed on how to attack the quantum computation problem of many electrons, when the size is too big for a usual DFT approach. Probably the most acclaimed suggestion was one that claim to divide the problem in two parts; The internal part of a metal nanopaticle can be calculated considering a bulk system, so, easy solutions are possible, while the surface has to be properly done with DFT or GW.

It is important to point out that recently, there have been significant efforts to include quantum effects in classical plasmonics. Such approaches either modify the classical Maxwell equations of electrodynamics by introducing, for example, nonlocal, nonlinear and quantized fields or “borrow” quantization techniques used in empty cavities in quantum optics. However, such ad hoc approaches are fundamentally unsatisfactory and novel, microscopically accurate description of plasmonic systems that includes quantum effects is sorely needed.

On the other hand, the scope of first-principles theoretical approaches that aim at a parameter-free quantum-mechanical description of materials has increased drastically in recent years. Algorithmic and technological advances allow for the modelling of relatively large systems comprising thousands of atoms using density-functional theory. Moreover, several techniques for the description of electronic excitations are available, such as time-dependent density-functional theory and many-body perturbation theory (GW/Bethe-Salpeter approach). With these advances, we expect that first-principles approaches can contribute to the understanding of plasmonic systems and become valuable additions to the toolkit of

researchers in the field.

It is important to point out, however, while such first principle approaches describe the properties of electrons with high accuracy, the description of light is typically simplified. Moreover, the modelling of large clusters containing millions of atoms is currently still out of reach for these methods.

3 Community needs

The key requirements for progress are related to coordination and dissemination of the research in different communities.

This above discussion clearly highlights the need for the development of new approaches for the theoretical description of plasmonic systems. We have identified a strategic and significant opportunity to overcome this challenge by converging classical electrodynamics approaches, quantum-mechanical electronic structure theory and quantum optics methods from opposite length scales at the nanometer regime.

In sum, different disciplines are studying physical phenomena in plasmonic systems, but from different, often complementary points of view. The description of light-matter interactions in small nanoparticles, where quantum effect becomes important, poses a significant challenge to all approaches. This workshop has initiated an exchange of ideas to identify routes towards a complete and microscopically accurate description of plasmonic phenomena.

In fact, we strongly believe that all what we need is to make the plasmonic and electronic structure to interact!

4 Funding

In addition to the funding from CECAM we obtained €3000 from Psi-k, £500 from IOP and the rest was sponsored with an internal (Imperial College) program grant (EPSRC).

Further funding sources for this type of workshop are Royal Society, IOP and EPSRC.

5 Will these developments bring societal benefits?

Plasmonics aims at revolutionizing the actual electronic technology replacing circuits that works with electrons with something that will work actually with light! The main idea is to have faster and more efficient transistor and in general circuits. This will bring strong benefits to the economy if realized.

On the other hand, plasmonics has already showed its importance in sensing applications and the recent aim is to improve the plasmonic sensor up to detect single molecules. This will be extremely relevant for national security applications.

Also, a really recent goal is to build new materials with the desired optical and electronic properties using small metal nanoparticles, this is the goal of what is also called quantum metamaterials. In the same line but with a slightly different approach, recently we started to conceive nanoparticles that can be used to activate reactions or bring chemical in particular zones inside a cell. These new aspects could redraw the medicine giving a drug cellular

targeted release.

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Multiscale Simulation: from Materials through to Industrial Usage

Location: O´Brien Centre for Science University College Dublin Room, Dublin, Ireland
Webpage: https://www.cecam.org/workshop-0-1255.html
Dates: September 5, 2016 to September 7, 2016

1 State of the art

In modern physics, the evolution of computational capacity allows materials to be investigated over a wide range of length and time scales, often referred to as multi-scale materials modelling (MMM). This allows for the modelling of complex materials under realistic constraints in a wide range of situations. Almost all MMM discussions take a bottom-up approach, starting from ab-initio density functional theory and linking upwards via higher level models to predict key material properties at the micro- or nano-scale. From the other side, Integrated Computational Material Engineering (ICME) starts from the application requirements, and aims to understand how processes form material structures, how these structures give rise to material properties and how to select proper materials for applications based on this information. ICME uses computational engineering as a major component aiming to remove the need for a lot of experimentation. The aim is to design products alongside the materials that comprise them, and the end result is sought from investigations and simulations at multiple length scales during the product and process development.

2 Major outcomes

Outcomes of the meeting:

- Progress in addressing challenges in multiscale simulation
- Coupling and linking between “bottom-up” and “top-down” communities
- Building critical mass/consensus towards development of best practice and standardisation
- European leadership in this important area of multiscale simulations from first principles through to industrial applications

There is indeed much European activity thru the EUMMC, and this workshop is an important step in spreading information. However one aspect that succeeded even beyond expectations was the interaction with our US invited speakers. Several of these are leaders of projects with experience in standards development (e.g. OpenKIM and LAMMPS) which they generously shared with us.

Specific topics we addressed included:

- Supporting best practices: we shared what works among those involved in this type of activity.
- Reducing redundancy: what tools and frameworks are available and how reuse can be done most effectively.
- Developing standards: discussion of where standardization is needed will greatly increase

efficiency of the platform tools being developed, and their interoperability.

- Integration databases: avoid redoing calculations, increase standardization and data compatibility, providing opportunities for data mining.

- Roadmap key needs: seeking community agreement about what tools are most critical to develop, routes to interoperability and to platform sharing, and how to move forward most efficiently - may require a cooperative effort across different communities and continents to be realized.

- Building expertise: we held a plugfest and poster session devoted to hands-on overview, training and comparison of different platforms and linkage approaches.

The 3 days were arranged so that:

- Day 1 set the scene regarding the current status and vision for multiscale simulation, including the perspective of the multiscale materials modelling and the Integrated Computational Material Engineering communities, with keynote talks from recognised research leaders, and a panel discussion on interoperability. Discussion kicked off with comments on the classification of models, why this is needed and how this could be achieved. Overall the panel and the audience appreciated very much the multiscale approach, however, it was also highlighted that providing and agreeing the classifications is an extremely difficult. Discussion was followed by a discussion on keywords and metadata. The discussion focused on the requirements of industry partners and how they will use such a framework for their simulation and design purposes.

- Day 2 shared current practice, with a morning of presentations and discussions from a cluster of EU-funded multiscale simulation projects regarding current developments and challenges for interoperability and the afternoon poster and plugfest.

- Day 3 addressed next steps and challenges, with a series of overview presentations on Roadmaps, future plans and directions for integration being used to set the scene for chaired open discussions to identify and agree critical next steps for the widespread uptake of Multiscale Simulation going from Materials Modelling through to Industrial Usage. The discussion was mainly centred around the MODA and how a MODA is defined and used. It was argued that it is not a flowchart but it gives indication of the parts involved in the modelling process of a given project. A focus of the discussion centred around interoperability and integration, model development and validation. Given the participation from organizations in Europe and USA, there was a healthy discussion on how European and US initiatives can work together. A strong commitment from both sides of the Atlantic was expressed with the idea to start with a relatively small and focused collaborations, which will help define how to best work together.

3 Community needs

The main challenge, both in MMM and ICME, is the coupling and linking of models describing phenomena at different scales, from the nano-scale up to the device or macroscopic scale. These two communities need to be brought together to discuss in detail the challenges to be met in the structuring and realisation of integrated frameworks that facilitate linkage of various multi-physics models to achieve the predictive design of novel materials optimised for specified applications.

Current computational tools typically have their own non-standard schemas for input and output files, including also varying definitions of the model. At the same time, different

communities often rely on distinct nomenclature to describe the same model components or physical parameters, which makes it even harder to link and couple disparate tools.

Many multiscale problems require the linking of several levels of code, that span several research and application communities, and including open-source and commercial packages. Some existing tools use their own metadata schemas. Though these schemas are themselves distinct, translating from one to the other is often time consuming and inefficient. In addition, large quantities of data are being generated across different platforms, much of which is potentially useful and re-usable by the wider community, but often in ways that are not immediately obvious in the original context.

Further CECAM workshops in this area would continue the momentum we achieved in Dublin.

4 Funding

A number of funding channels already support work presented at the workshop. In addition to the Cluster of 5+1 EU projects that organised the workshop, several attendees at the Workshop have European funding relevant to the workshop, including the Nomad Centre of Excellence (www. nomad-coe.eu), and a Coordination and Support Action suporting the EMMC (http://emmc.info) which seeks to build a network to capitalise on the strong European position in materials modelling and to allow industry to reap the benefits of modelling. NMBP 07-2017: Systems of materials characterisation for model, product and process optimisation and NMBP 25-2017: Next generation system integrating tangible and intangible materials model components to support innovation in industry are relevant current calls, which involve further open innovation and interoperability developments. Joint research proposals were discussed on a one-to-one basis at the meeting, but were not a topic formally on the meeting agenda.

5 Will these developments bring societal benefits?

Materials are important for every aspect of modern life. Improved materials are essential for economic development of heavy industry and communications, for sustainability, efficient energy production and progress in drug design. There are many funding opportunities for research into better materials for energy production. We described some of these in the funding section above.

There were excellent exchanges between the Europeans and our US counterparts concerning the US experience with standards for potentials and formats relating to interoperability. The carefully selected US participants made major contributions to all discussions and helpful suggestions for working with larger collaborations from their experience.

One benefit that has already been achieved following discussions with Aidan Thompson, a co-developer of LAMMPS , is the preparation and release of a LAMMPS patch for the REBO potential. This may seem small, but it brings the efficiency of the standardized LAMMPS code to simulations involving carbon allotropes such as nanotubes which are central to many clean energy applications, such as hydrogen storage in nanotubes.

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Nonequilibrium Statistical Mechanics and Turbulence

Location: CECAM-IT-SIMUL
Webpage: https://www.cecam.org/workshop-0-1321.html
Dates: September 8, 2016 to September 10, 2016

1 State of the art

In recent years there has been a renewed interest for the problems of nonequilibrium statistical mechanics. The main reason behind this fervid activity has been the availability of improved computers, which have made possible experiments «in silico» hardly thinkable only a few years ago. In particular, numerical simulations have allowed detailed simulations of the stationary states of fluids, revealing the statistical features of observables elusive to real experiments, as for instance entropy production, dissipation and the contraction of phase space.

These efforts have led to numerous new discoveries for the dynamics of irreversible phenomena and fluctuating systems. Particularly relevant, the development of a sound framework for the behaviour of fluctuations of systems out of equilibrium. It is worth emphasising that, from a mathematical point of view, these developments find their general framework in the theory of Large deviations, a branch of probability theory that has matured in the last decades.

2 Major outcomes

In our CECAM workshop a group of renown expert of this field has presented their recent works. The interdisciplinary character has been largely emphasised and speakers with different background have met to look for possible interesting exchanges and new projects.

The main subjects considered have been: turbulence, particle dynamics, nonlinear waves, probabilistic approaches and statistical mechanics.

While the dynamics of small inertial particles has been captured much attention and can be said well understood, the workshop has allowed to identify new important issues, notably the dynamics of more complex particles, like finite-size ones ore non-spherical. This remains an open question and huge computationa effort will be needed to understand them.

Furthermore, some interesting results concerning modelling have been presented. The importance of the development of mathematical tools and in particular the application of stochastic processes has been stressed. From an applicative point of view, the need of sound turbulence models remains key. While some promising results concerning the stochastic modelling of gradients have been discussed, this issue seems yet to be addressed.

From a general point of view, some recent developments in statistical mechanics and probability, have been presented which appear particularly promising for the understanding of some general characteristics of turbulence flows. In particular, the macroscopic fluctuations theory has been discussed and it has been shown that the application to some problems of geophyscial interest has been successfull. While it is difficult to say if this kind of general theory can be applied to all systems, it appears appealing at least for some systems

which can be modelled simply.

The discussions have revealed that, thanks to computations, significant results have been recently obtained in the analysis of nonlinear wave systems. In particular, discussions have been carried out concerning elastic dynamics, intermittency, and solitons. This seems to be an active and challenging research field.

Last, some discussions have focused on two themes which has raised much interest very recently: the time-reversibility in turbulent trajectories and the presence of singularity. While some important results have been obtained, in particular finding the relation between numerical evidence and theoretical counterpart, these subjects need certainly to be better investigated.

3 Community needs

The numerical computations are essential for turbulence and more in general for statistical mechanics.

While many databases start to be available as well as some codes, the politics of open source performant codes should be strengthened. In this era, it appears illogical to not share existing codes.

The need of more computational hours appears vital for the community. The HPC resources are an example but more credits should be available. Many novel ideas seem to be constraint by the possibility to find computational hours.

The most important point is however the need of networking. Given the increased interdisciplinarity of the tasks, and the number of important contributions at european level, it is of the outmost importance to guarantee a timely and easy diffusion of knowledge. This has become particularly relevant since the national investment in research has shrinked in hte last years, making difficult the regular organization of such events.

In this sense, we think that it would be extremely useful for the community the organization of series of CECAM workshops with the same structure on the same topic. The large success of this first workshop underline this need.

4 Funding

Unfortunately, in this period of generalised economical austerity it is particularly difficult to receive adequate funding for research. However, discussions have been attempted among the different participants to figure out possible scheme of funding in the next future. At the national level, French and Italian gouvernments give some funding through national agency (ANR and MUIR). The rate of success is nevertheless extremely low (5% or less for ANR). A big deal has been made for Horizon 2020. While preliminary steps have been already made, the emphaisis on concrete industrial deliverable and the related needed presence of industrial partners appear particularly unfit for high-quality research.

5 Will these developments bring societal benefits?

Turbulence is ubiquitous in nature, yet it has to be admitted the lack of a sound model for realistic configurations. Possible applications are numerous; among the most remarkable, atmospheric and ocean dynamics even linked to climate changing issues, aerodynamics, combustion. More recently, enormous attention has been devoted also to Plasma, in relation to fusion and astrophysical problems.

In the last decades, we can say that most of the advances have been obtained thanks to computer simulations. In particular, not only numerics avoid very expensive experiments and hence allow more comprehensive studies, but it has given the possibility to analyse many observables almost inaccessible to real experiments, like fluctuations or instantaneous local measurements. Furthermore, as discussed in the CECAM workshop, numerical experiments permit to run thought experiments which are physically impossible, that which can be used to highligth particular mechanisms underlying important phenomena.

However, we are far from being able to run experiments in silico of realistic flows so that huge effort is needed.

A better understanding of turbulence and a more robust modelling based upon most advanced techniques, would be of great benefit from many point of view. In our opinion, the most intriguing possibilities appear the control in aerodynamics, also concerning the noise production and the simulation of droplets dynamics, notably bubbles and cavitation, which cause many damages to industrial products;

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Structure formation in soft colloids

Location: CECAM-AT
Webpage: https://www.cecam.org/workshop-0-1272.html
Dates: September 19, 2016 to September 22, 2016

1 State of the art

The insight into structure formation in soft matter from liquid crystals to polymers and colloids relies in many ways on our understanding of how the respective building blocks pack (the best-known examples being hard spheres, rods, and platelets). The packing of soft particles is much less understood, yet during the past decade the body of experimental and theoretical work on systems based on deformable and compressible colloidal particles (such as star polymers, hydrogel spheres, dendrimer micelles, and block copolymer micelles) reached a level where certain patterns began to appear. For example, the salient features of model dendrimers are cluster crystals as well as the otherwise exotic A15 and sigma phase.

In view of the rich phenomenology reported, the field is in urgent need of rules, mechanisms, and models relating the phase behavior, rheology, and other aspects of physics involved to the interparticle interaction. At the workshop, we aimed at make a step ahead towards universal models of soft colloids, ideally identifying a few working hypotheses to be explored in the future. This was a speculative endeavor, and the CECAM workshop provided a very suitable stage for out-of-the-box discussions of the possible form and scope of these models. The aim of the workshop was i) to compare the experimental and theoretical insight into the structure formation in soft nanocolloidal particles, attempting to outline the generic features of their phase diagram to including orientational, bond-orientational, and other partly ordered mesophases, and ii) to discuss experimental, numerical, and theoretical methods as well as models applicable to these problems so as to identify the most efficient approach leading to as unified an understanding as possible.

2 Major outcomes

The 4-day workshop was a focused and interconnected event, with all the participants without restrictions addressing the questions identified in the proposal. This was a strong signal that the theme is timely and that a meeting of this kind was long awaited in the community. With a total of 47 participants, of whom 19 were invited speakers, the program was fairly busy yet very productive, offering ample time for discussions. The main topics covered were:

1. Nucleation / This question remains among the outstanding challenges in both hard and soft condensed matter, and the insight provided by the latter can be quite helpful in general. A key question discussed is the choice of order parameters used to characterize the degree of order in crystal nuclei so as to monitor their growth: It seems that in many cases bond-orientational order is a precursor of translational order. Equally interesting is the effect of particle deformability on crystallization, which can be studied in the so-called deformable hard-sphere model.

2. Fluids / Soft-particle fluids are often modeled at a coarse-grained level based on effective pair potentials, and the many-body effects are left out. Although it is known that they may be quite important, especially in overlapping particles, the many-body effects are still poorly understood mainly because the theoretical framework for their quantification is complicated. At the same time, they may lead to fairly complex phenomenologies including chirality in fluids of non-chiral particles. Also of considerable interest is the structure formation and gelation in suspensions of magnetic particles, where particle shape may play an important role and particle self-assembly may additionally be steered

by capillary interactions.

3. Two-dimensional systems / Like in classical condensed matter, 2D soft colloidal systems are of particular interest too. The most paradigmatic problem in the field – the nature of the hexatic phase – remains difficult, requiring special simulation techniques that allow one to simulate a large enough ensemble. A popular experimental 2D system is a monolayer of magnetic particles trapped at an interface, which can be used to study the glass transition. Other physical realizations of 2D systems include colloids trapped between parallel walls. Recent results suggest that charged particles in such a confining geometry may form a rich variety of ordered structures hardly expected in advance.

4. New ordered structures in soft colloids / We discussed several types of crystalline, liquid-crystalline, and quasicystalline structures predicted by theory and simulations in systems characterized by either anisotropic pair interactions or by spherically symmetric multiple-well interactions. Some of the novel structures are marked by an enormous complexity; thus, their proper identification cannot be done just by inspection and requires a sophisticated algorithm. So far, the “artificial” crystal structures typically obtained in simulations were all identical to one or more natural crystals but some of the novel ones have passed beyond this point. Also discussed were new experimental results in the field of polymeric soft quasicrystals; especially interesting are the columnar 2D quasicrystals where several new types of order were observed.

5. Gels and glasses / These types of structures are very common in many soft particles such as microgel particles. The internal structure of such particles can be tuned by the radial profile of cross-linkers, which then controls their mechanical properties relevant for elastic and rheological behavior of the suspension. Additionally, these behaviors may also depend on ions embedded in the microgel, and we may expect that in the future these means of control will be further elaborated. Another related topic are glasses formed by rod-like anisometric particles, which turn out to be quite different from glasses of spherical colloids because of the nematic order.

3 Community needs

The workshop has clearly shown that the main objective of identifying one or more paradigms describing the behavior of classical deformable particles analogous to hard spheres is a distant yet very relevant goal of considerable interest to both experimentalists and theorists. There does exist a critical mass of researchers interested in the topic, each of them pursuing his or her own research agenda, and a more profound understanding of the generic features of soft colloids will invariably emerge from the many pieces of information provided by the specific projects with more focused objectives rather than from a single large scientific enterprise. The main needs of the community are thus not related to the individual projects themselves but instead to opportunities to exchange ideas in an unconstrained environment such as the present workshop. In our opinion, the funding agencies and institutes such as CECAM could contribute most appropriately to the development of the field by fostering these opportunities, ideally at a rate once per year or once in two years. A standalone meeting such as the CECAM workshop would be a perfect opportunity although longer retreats with duration of up to a few weeks would also be an appropriate format, allowing the participants to engage in joint projects. Compared to infrastructural costs, supporting such meetings is a modest investment yet one that could conceivably create circumstances where a qualitative step ahead can be envisaged.

4 Funding

With an emphasis on discussions rather than on direct joint research work, the objective of the workshop would ideally fit within a COST- or RTN-type framework of EC and ESF, respectively, or within a series of CECAM workshops. Although the expected outcome is somewhat speculative and potentially more interesting to senior researchers than to early-stage researchers, the topic could form a part of a future Horizon2020 Marie-Sklodowska-Curie ETN action – in fact, it is being addressed by an existing ETN COLLDENSE. At any rate, a more concentrated effort supported by a formal network may well produce far-reaching and potentially high-impact conceptual results, and the possibilities of establishing such a network reaching beyond EU alone should be explored in the future.

5 Will these developments bring societal benefits?

The question of a deeper understanding of structure formation in soft particles is of fundamental theoretical nature, and thus only indirectly related to immediate benefits of the society. At the same time, should one indeed be able to put the different results within a single conceptual framework, such a framework may well provide guidelines for future experimental and applied studies in the field, facilitating the design of tailor-made soft particles such as microgels. This impact will be even more prominent if relevant for the processing, synthesis, and performance of microgel-based materials used, e.g., in biomaterials, drug delivery, and oil recovery applications. In this context, it will be of paramount importance to include glasses as disordered arrested soft-particle structures simply because this is the dominant form observed in experiments. Equally important for the experiments and applications is rheology. While present at the 2016 workshop, these two subfields should perhaps be emphasized more at any follow-up meetings where ideally researchers from industrial laboratories (e.g., Solvay and Unilever) would participate too. Given the general consensus of the high relevance of the problem at hand, we have no doubt that a concrete benefit will eventually ensue.

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Non-equilibrium dynamics of thin films - solids, liquids and bioactive materials

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1261.html
Dates: September 20, 2016 to September 23, 2016

1 State of the art

A large range of high-resolution experiments are available today and allow for investigations at scales where no principal separation exists between inanimate and biotic physic-chemical systems, or between fluids and nanostructures. Examples are films, which extend a few single units across in one dimension, atoms or molecules (solids/fluids), or cells (biofilms). Novel multidisciplinary approaches are thus needed to address dynamical phenomena in thin films composed of such diverse types of materials.

Thin fluid films have been described quite successfully by continuum models derived in lubrication approximation. However, such descriptions are challenged at submicron scales, where fluctuations are expected to be relevant. Nonetheless they can still be useful, especially if effective potentials/parameters are employed that are extracted from microscopic modeling as e.g. Molecular Dynamics (MD), or with suitable noise terms.

Remarkably, similar thin film equations describe some solid systems. An example is the nanostructuring of solid surfaces by ion irradiation, where an amorphized layer acts as a viscous thin film with challenging multiscale properties. However, thin film equations fail to describe solid systems if e.g. facets are favored energetically. Validity conditions need to be established for the continuum modeling of thin solid films, using input from kinetic Monte Carlo simulations and MD data.

Thin films also occur in living systems, as in biofilm formation, the growth of colonies of sessile bacteria on solid-fluid interfaces. The spatial structure of the population is key to biofilms, which are composed of a large number of bacteria, making continuum descriptions viable. As for fluid and solid films, one needs to understand how large-scale properties and system performance correlate. Agent-based simulations, coupling the dynamics of a single cell to that of its environment, can be key to assess suitable continuum models.

2 Major outcomes

The presentations were both invited and contributed. Ample time was reserved for discussions, invited talks being 30 min.+15 min. for discussion and contributed talks being 25+10 min., respectively. In total, 12 oral (2-3 talks each) plus one poster session were celebrated. Two speakers (out of 27) cancelled their participation on short notice; one of these presentations was finally made in poster format. Overall, workshop attendees did actively engage in lively discussions which were perceived as productive by all.

At the end of each day, a critical review session was organised in which, moderated by meeting organizers, participants identified critical issues that impact their own research on fluids, solids, or biological systems. A main aim was to seek for synergies among participants and to identify future avenues of research with a potential to improve understanding and bring novel perspectives, and which could underscore similarities and differences in the thin film approach to the various types of systems considered.

Grossly speaking, the oral presentation+discussion sessions were devoted to

- Thin fluid films: Dynamic wetting/dewetting and challenges at the nanoscale (S. 1, 4, 6, 7); role of external fields on thin fluid films and droplets (S. 4, 7, 8); instabilities and patterns (S. 8); the role of the slip length (S. 6, 11).

- -Thin solid films: Solid-state dewetting (S. 5, 6); effects of growth kinetics and fluctuations (S. 5, 12); molecular systems (S. 9); coarsening effects (S. 9, 11).

- Films of biological or active matter: Mechanical instabilities and continuum models of bacterial biofilms (S. 2); growth and collective effects in epithelia, bacterial biofilms, and active nematics (S. 3, 10).

As can be seen, often we addressed systems of different nature (e.g. fluids and solids) within the same session in order to identify similarities and differences in their dynamical behavior and modeling aspects. In addition, sessions on different fields were mixed in each half-day.

During the critical review sessions, many relevant questions were raised. Among those, the participants finally selected 3 as the most pressing/challenging issues which are transversal to the 3 main themes of the workshop. Based on group discussions within each one of these 3 topics, several detailed issues were identified as pressing questions to be answered as soon as possible within the activity of researchers in these and related areas. They are as follows:

Wetting potentials, w(h):

- How does the wetting potential couple to curvature?

- Derivation of w(h) for non-flat films.

- Wetting potential for rough/heterogeneous substrates.

- Does w(h) act just on the surface or also as a bulk force? Typical form and length scales?

- What kind of w(h) are realistic and what kinds of materials lead to them?

- How to design a substrate with a certain w(h)?

- Fluid-fluid-fluid wetting (liquid/liquid/gas).

- Universal/typical relation between w(h) and mobility?

- Equivalence of wetting potential (exponential, power law)?

- Van der Waals / DFT: from single particles to w(h).

- Control of w(h); experiments.

Qualitatively novel features of anisotropy:

- Where does it make a difference?

- Induced by external fields; orientational transitions.
- Identifying order parameters; complexity (unavoidable).
- Dynamic faceting on the edge: limitations of continuum approaches? continuous degree of anisotropy:
- Emergence of new patterns in solids & active systems.
- Influence on dynamics, coarsening, morphology, fluctuations.
- Competing interactions: anisotropic diffusion.
- Role of pre-structuring/initial conditions.
- Close-to vs. far-from-equilibrium behavior.

Form of thin film equations:

- Gradient dynamics: automatic model generation.
- Where does it not work (jets without inertia, strong slip).
- Thermodynamical consistency vs good models.
- Higher order formulations.
- Improve mobility/energy; both? What is best, why?
- Qualitative vs quantitative assessment.

3 Community needs

The workshop put into practice an explicit multidisciplinary approach bringing together specialists from diverse communities (fluid dynamics, solid nanosystems, and biological systems; an alternative characterization can be solid and soft condensed matter practicioners) who share an interest in thin film systems, as suitably defined within the corresponding contexts. Actually, also the expertise of the attendees was quite diverse as we brought together experimentalists and a range of theoreticians (computationally and analytically working, including applied mathematicians). For some of the younger members of the individual communities the workshop was the first direct interaction with scientists from the other communities. As a result, we expect that new synergies will successfully develop from the intensive interaction of such diverse agents. In some cases, scientific collaborations between participants with heterogeneous backgrounds are already ongoing and the meeting can help them to intensify the interaction and incorporate further expertise. From the experience of the workshop we can conclude, that further actions that foster a sense of community would be highly beneficial. For instance, a series of workshops would be highly desirable, as it would allow participants to assess progress and foster development along the specific lines of interdisciplinary research areas which have been identified. A periodicity of two years seems adequate to allow for solid progress in between contiguous editions, while

the CECAM node structure across Europe would be ideal to underscore the multinational nature of these concerted efforts.

4 Funding

Typical funding channels range from local to international. The home institutions of the workshop organizers can offer small help to organize further workshops, as in this occasion. One can also envision larger workshops co-financed by two players, e.g., CECAM and a local centre as CeNoS in Münster. Further direct/indirect support can come from national sources, like CNRS or Univ. Claude Bernard Lyon 1 (France), Volkswagen or Hereaus Foundation (Germany), or MINECO (scientific grant system, Spain). The workshop scope also fits within the lines promoted by the Horizon 2020 EU Programme, promoting advance in key enabling technologies, from Nano to Biotechnology.

The field should also be strengthened by coordinated research efforts via dedicated grants. Such a possibility was informally discussed during the meeting among various single parties, not yet from the point of view of the workshop community at large. It might become a more consistent option as multilateral interactions unfold.

5 Will these developments bring societal benefits?

In a wider international context, the theme of our workshop is also fully in line with the "prospects for Condensed Matter and Materials Physics in the early part of the 21st century", as identified in the reports of the National Research Council of the National Academies USA (2010) "Condensed-Matter and Materials Physics: The Science of the World around Us" [by explicitly addressing aspects from 4, out of the 6 scientific challenges therein contained, namely, "how do complex phenomena emerge from simple ingredients", "what is the physics of life", "what happens far from equilibrium and why", and "what new discoveries await us in the nanoworld"] and "Research at the Intersection of the Physical and Life Sciences" [by explicitly addressing "common themes at the intersection of biological and physical sciences", such as self-organization, dynamics, and stochasticity]. As identified in these reports, a number of important benefits for society can be foreseen from scientific progress along these lines. For instance, improved understanding of wettability conditions (fluid thin films) can impact production of improved lubricants reducing mechanical wear and energy consumption. Full harnessing of solid surface patterning techniques at the nanoscale can increase the performance of optoelectronic, magnetic, and catalytic devices, while understanding biofilm formation can impact control of hospital infections, energy (biomass) production or waste disposal systems. Finally, a global understanding of thin film processes at scales and systems which can be highly diverse will contribute knowledge and eventually impact public awareness and education issues.

6 Participant List

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7th Workshop on Time-Dependent Density-Functional Theory: Prospects and Applications

Location: CECAM-ES
Webpage: https://www.cecam.org/workshop-0-1278.html
Dates: September 20, 2016 to September 23, 2016

1 State of the art

Time-dependent density-functional theory (TDDFT) is but one of the numerous methods used to model the electronic structure in atoms, molecules, and extended systems. Its use is growing fast, as its reliability for many purposes has been sanctioned by many successful applications over the years. The calculation of excitation energies of many varieties of molecules, and the optical absorption spectrum of many solids can be cited as examples. However, in other circumstances TDDFT has to be substituted by more accurate, yet more expensive techniques: advanced correlated post-Hartree Fock techniques, or many-body perturbation theory techniques such as any of the approximations to the solution of Hedin's equations. Yet TDDFT, as ground-state DFT, could in principle be exact, providing inexpensive solutions to all electronic structure problemas. How can one approach this goal was the starting question for this workshop – and, in fact, it has been the motivation behind the full series of the Benasque Workshop (and School) on TDDFT, since 2004.

2 Major outcomes

As stated by Hardy Gross in the concluding remarks of the workshop, perhaps the main conclusion is that TDDFT is still a young discipline. For example, pretty much as it happened with ground state DFT, it has taken a few decades since the "official" birth of the theory until we are witnessing fully rigorous mathematical studies of its foundations (we had one such example in the talk of R. van Leeuwen). Likewise, the youth of the discipline is demonstrated by the fact that it is only recently that somehow "obvious" applications of it, such as real-time simulations of high-intensity laser irradiation of solids, have appeared. Technical and theoretical difficulties slowed the progress of these studies for years; yet we witnessed in this workshop some excellent examples in the talks of K. Yabana, S. Sharma and H. Huebener, for example.

Although TDDFT is all about electrons (at least in its most widely used "standard" formulation), in reality these live in contact with the nuclei. The electron-ion coupling problem must be solved, and in this workshop we had the occasion to discuss the issue thanks to the presentations of, for example, F. Agostini, Ali Abedi, and E. Khosravi.

An exciting topic of discussion was the new developments in the merger of TDDFT and quantum optics. I. Tokatly presented his theoretical work on the formal foundation of a theory that treats quantum mechanically the set of electrons and photons on the same footing. H. Appel also contributed with a presentation full of practical applications, followed by one by C. Pellegrini about a proposal for a functional created for this type of developments. We have no doubt that this topic will grow steadily in the future.

However, the answer to the question stated in the previous section ("how can one make TDDFT approach exact results?") can only be answered by insisting on the research into better exchange and correlation functionals. This was of course the subject of some talks (such as the one by P. Gori-Giorgi on the adiabatic strictly correlated electrons functional, or

the work of S. Refaely-Abramson on hybrid functionals), and as usual in any workshop on density-functional theory, of much discussion at all times.

Highly non-linear light-matter interaction is clearly a topic on the rise. Starting with the inaugural talk of K. Yabana, we had plenty of time to discuss it: K. Varga reviewed his research on nanostructures irradiated with strong laser pulses; and D. Bauer presented his work on correlated two-electron quantum dynamics in intense laser fields, to give just some examples. In this area, TDDFT is a practical alternative, although it was clear from these presentations that serious work needs to be done to achieve predictive power for all materials and processes.

We wish to emphasize that a younger generation of scientist was present during the workshop, since this takes place after a corresponding school, and the forty students that participated in it stay for the workshop. They had the occasion of showing their research during a poster session, and in fact two of them, selected by a vote of the school teachers, could present it in the form of a talk at the end of the workshop. The topics: high harmonic generation in solids (I. Floss), and TDDFT coupled to quantum electrodynamics (N. Hoffmann).

3 Community needs

Fortunately, numerous codes have embraced TDDFT, and are active research tools both for applications and theory developments. This was obvious from the presentations of the workshop, in which we could see results obtained with many alternatives. It should be stressed, moreover, that various of those codes are accessible to all researchers through open licenses, and their implementation and details open and visible for inspection. This is felt as an important issue by a large part of the community.

These codes can nowadays be executed in large supercomputers, thanks to advances in their scalability for parallel architectures. This was also obvious in some of the talks, that presented results for extremely large systems. Despite being praised as a “computationally cheap” alternative, TDDFT requires large HPC resources because many researchers in the field are studying very large nanostructures or biomolecules (proteins, etc).

Finally, regarding event organization, TDDFT has been reviewed every two years by this series of workshops, since 2004. Also, we used to have a Gordon Research Conference in the alternate years, which unfortunately was discontinued, and which served to fill that middle year, on the one hand, and which was held in the US, on the other hand, in contrast to this European event. This was therefore an important meeting that is now missing. During the workshop, fortunately, N. Maitra and A. Schleife informed of an initiative to hold a TDDFT workshop next Summer in Telluride, Colorado. The goal would be to initiate a US-based series of schools and workshops, such as the Benasque series, in the alternate years. We are therefore convinced that a regular series such as the present one is highly appreciated by the community.

4 Funding

Many researchers in this field are concerned by the difficulty of accessing funding through many of the usual channels, due to the basic-research nature of the discipline, and to the orientation of many of those channels to more applied science. Oftentimes, basic research in DFT or TDDFT is performed under the umbrella of large projects with a more technologically oriented topic, in which the basic science aspect is regarded as a necessary but marginal sub-project. On the other hand, fortunately TDDFT is approaching the status of DFT, which is now regarded as a standard tool useful for technology and applied science.

No particular funding proposal was discussed during the workshop.

5 Will these developments bring societal benefits?

There are numerous technological processes and areas in which the excited-state electronic-structure of atoms, molecules, and materials (the object of study of TDDFT) is relevant, and therefore the possibility of using a first principles yet affordable technique to model these processes has potential economic benefits. During this workshop, for example, we could see the modelling of proton radiation damage in materials (A. Schleife), or the irradiation of intense laser on materials (K. Yabana, S. Sharma), or studies of conductivity in molecular electronics (S. Kurth). These are areas in which modelling based on TDDFT and related techniques may help industry, by easing the interpretation of the observations made in their research & development processes.

Excited electrons, and excited electronic potential energy surfaces, also play a fundamental role in bio-chemistry. We could learn about the relevance of TDDFT for bio-molecular studies not only during the workshop, but also during the previous school. This is of course an area in which bio-medical laboratories have an obvious interest, and it is to be expected that the more and more convincing TDDFT results will persuade the industry to incorporate this type of modelling into their processes.

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Numerical methods for optimal control of open quantum systems

Location: Free University Berlin, Institute of Mathematics,Berlin, Germany
Webpage: https://www.cecam.org/workshop-0-1309.html
Dates: September 26, 2016 to September 28, 2016

1 State of the art

Optimal control of open quantum systems has recently evolved as an important interdisciplinary research topic joining the fields of physics, chemistry, information sciences and engineering, with the goal of further developing scientific knowledge in quantum dynamics into the emerging field of quantum technologies. Despite of impressive progress in this field, there still is a lack of robust numerical methods and algorithms that impedes the applicability of the models when going to larger scales. However, numerical methods for bilinear control systems have recently been analyzed and developed by applied mathematicians—largely unnoticed by the physical-chemical community. Both fields have reached a certain degree of maturity, and this workshop mainly serves the purpose of joining forces.

A central theme of the workshop, therefore, will be both the physical concepts as well as the numerical methods for open quantum systems, intertwined with various approaches to manipulate them, stemming from the field of optimal control theory. This conference aims at fostering the fields of quantum dynamics and technologies, especially through its emphasis on algorithms and software. As reflected by the expertise of the members of this workshop, optimal control of quantum systems, typically exerted by electromagnetic fields, is of key importance in fields as different as molecular dynamics and (photo-) chemical reaction dynamics, manipulation of single spins in magnetic resonance (ranging from spectroscopy to medical imaging) or photons in optical devices, quantum information processing and quantum network technologies.

2 Major outcomes

The major scientific points discussed in the meeting can be grouped into four (partly overlapping) categories:

- Concepts of open systems, beyond the Markov approximation:

  Beyond the standard approach of modeling open quantum systems (dissipative dynamics) by Lindblad equations, one of the major topics of the present workshop has been on the extension of open quantum systems beyond the Markov approximation. For related control problems, the questions of controllability and/or reachability still represent open challenges. Also various other techniques of adding noise to the equations of motion have been considered in several contributions to this workshop, partly also involving the use of stochastic modeling.

- Model reduction for open quantum systems:

  Despite the advances in computing technology, the integration of the equations of motion of an open quantum systems represents one of the main computational bottlenecks nowadays. This considerably limits the practicability of various real-time applications, which is why reduced-order models are sought that approximate the

system response to a large class of possible input signals.
During the workshop, several approaches to obtain reduced-order models for open quantum dynamics have been discussed, ranging from singular perturbation to reduced-basis methods. It has been unanimously agreed that there is much room for improving available techniques and for further method development in the field.

- Quantum optimal control, from molecules to quantum networks:

  Pioneering work in the early 1990s demonstrated applications of quantum optimal control to simple systems from atomic or molecular physics. Since then, the field has emerged substantially, branching in different directions. Neglecting applications in chemistry and biology, one of the central aspects of the meeting was on quantum technologies based on superposition, entanglement and many-body quantum states. There, the control design often involves closed-loop strategies where feedback can be utilized to cope with unpredictable perturbations. The numerically efficient design of robust closed-loop network modules (e.g. using model order reduction) has been a matter of lively discussions in the course of the workshop and underpins the need for flexible and reliable algorithms for model reduction of open quantum systems.

- Algorithms and software for optimal control of open quantum systems:

  The objective of mathematical quantum optimal control is to optimize the temporal shaping of external fields, (typically pulses or sequences thereof), to reach certain (stationary or time-dependent) targets (observables) in a quantum system, and under which conditions such optimal solutions exist. Moreover, often the optimizations are subject to constraints such as energy and/or duration of the control. Quantum control builds on a variety of powerful tools from the fields of mathematical control theory, which is based on Pontryagin's Maximum Principle. However, most of the established theory is based on linear systems. Extensions to the bilinear case, which is prevalent for quantum systems, are still in an early phase, but are expected to be further cultivated in the coming years.

One focus of the present workshop was on numerical techniques to solve the control equations: among them are Krotov-type algorithms (and extensions thereof), where the disadvantage of the repeated forward-backward propagations is contrasted by the advantage of monotonic convergence properties. In order to speed up such simulations, the chopped random basis (CRAB) method can be used to generate a parametrization of the control sequence. Alternatively, gradient ascent algorithms (with possible extensions to second-order (quasi-)Newton methods) can be used which offer the advantage of updating the control for all times simultaneously.

3 Community needs

There are a number of individual software packages for quantum optimal control, such as QuTIP, QLib, QDyn, QNET, WavePacket, DYNAMO. However, they are still written in different languages such as Fortran, Matlab, Python, and further developed by different participants of the workshop; a common platform implementing all of the frequently used algorithms is still lacking. Further systematic work on the development of numerical approaches, along with the development of a common software platform would be desirable, where the challenge is to improve the computational speed and accuracy.

4 Funding

A funding channel relevant for many of the participants of the present workshop is QUAINT, a pan-European Coordination Action on Optimal Control of Quantum Systems, funded by the European Commission Framework Programme 7, Future Emerging Technologies FET-OPEN programme.

On a local level, there is also the Munich Quantum Center formed by groups from the two universities and the Max Planck-Institute for Quantum Optics, covering topics ranging from mathematical foundations, quantum information, computational methods, quantum nano-systems, quantum optics, and quantum many-body physics to superconducting devices.

At the current stage, the meeting was mainly aimed at bringing together the different sub-communities active in the field (mathematics, physics and chemistry), rather than assessing the possibility of joint research proposals. Nonetheless, plans to apply for a semester programme at the EPFL Bernoulli Center have matured, as discussed during the workshops social programme.

5 Will these developments bring societal benefits?

With most of the theory essentially established, the field of optimal control of quantum systems can be expected to reach maturity within the next few years, potentially leading to many technological advances. Most probably, on a mid-term time scale those will be in the fields of quantum information, quantum sensors, quantum metrology, and quantum encryption. In the long-term prospects the field will go towards the goal of quantum-computing. A roadmap to the research and development is sketched in the “Quantum Manifesto”, released in 2016 by leading scientists from all over Europe.

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Interface processes in photochemical water splitting: Theory meets experiment

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1303.html
Dates: September 27, 2016 to September 30, 2016

1 State of the art

The direct conversion of solar energy into chemical energy is among the most important scientific and technological grand challenges. Despite the recent success achieved in thin film photovoltaics, solar fuel production via photocatalytic water splitting remains a difficult task, with the record efficiency of ~12%, obtained by integrating two perovskite solar cells in series with an electrolyzed.

Efficient photocatalytic water splitting requires the simultaneous optimization of i) the band-gap of the light absorber so as to maximize visible light harvesting, ii) the efficiency/cost ratio of specific electrocatalysts, and iii) the interface processes both between photoelectrodes and catalysts and between photo-electrocatalyst and environment. While in the past years, materials' band-gap and catalysis have been the subject of extensive numbers of studies (and of several past CECAM workshops), interfaces in photoelectrochemical processes received much less attention.

This CECAM workshop on interface processes in water oxidation (WOX) aims at filling this gap. This field is growing and evolving very rapidly, and it is the subject of an ever-increasing number of studies. The challenge stems from the complexity of the interfaces (structure, composition, defects), of their electronic processes (charge transfer (CT), electron-level alignment, dynamics of excited states), of their chemical processes/conditions (stability of intermediates, effect of pH), and, most notably, from the coupling between all these factors with both the photon absorption and the reaction mechanism.

2 Major outcomes

The workshop was a meeting opportunity for chemical and physical communities that address similar challenges from different perspectives, ranging from experimental synthesis/characterisation, to theory and simulation. These communities agreed that an important breakthrough in photochemical efficiencies requires strategies to optimally connect research on fundamental processes (light absorption, charge separation, electron transport, …) to research on new working materials, up to the engineering device. A key issue is identifying well-characterised MODEL SYSTEMS, where theory and experiment can be efficiently combined.

This tight theory/experiment interaction fostered during the last 5-10 years an exponential increase in the performance of transition metal based catalysts for water oxidation, triggered by new complexes that abandoned the traditional mu-oxo architecture. Single-site catalysts are at the moment the most efficient. The spectacular progress in efficiency was not accompanied by substantial progress in stability, which is currently the major limitation for these systems. Theoretical simulations had a significant impact in elucidating the mechanism at play also in the natural catalyst for water oxidation. A new approach based on

spectroscopic fingerprinting of catalyst “states” during the catalytic cycle was presented. We remark again that these achievements stem from tight interaction between theory and experiments on well characterized systems.

Concerning solid-state heterogeneous catalytic interfaces, the request for well-defined model systems where theory and experiment can be efficiently combined is more critical. The emerging strategies for designing the next generation of devices may involve exploiting both the nanoscale and mesoscale. For example, growing functional oxide overlayers on hematite (Fe2O3) has a significant effect on the onset potential (~200 meV cathodic shift). These overlayers do not necessarily act as catalyst: Possible roles include facilitating electron hole separation, saturation of surface states that might act as recombination centers, electrostatic effects leading to higher concentration of holes in regions not coated with the overlayers. Another strategy involves electron-energy engineering at interfaces, for example by exploiting local electric fields, external bias or tandem systems, In the latter, photocatalysts for the anodic reaction like hematite are coupled with photoabsorbers like perovskites (whose function is to increase the chemical potential of the electrons), mitigating the known problem of a conduction band with insufficient redox potential to reduce protons to molecular hydrogen. From the mechanistic point of view, recent experiments show that under illumination the surface concentration of holes is very high, and a third-order reaction rate w.r.t. hole concentration was reported. This suggests a rate-limiting step that requires the accumulation of multiple holes at the reaction site.

The ability of ab-initio theory approaches to accurately predict electron-level alignment at photocatalytic interfaces is still debated. Significant progress involved simulations combining first-principles molecular dynamics of electrode/electrolyte interfaces and new approaches to compute redox potentials of reference electrodes. The higher performances of hybrid functionals were highlighted by several speakers. Departing from electron energy levels towards charge-transfer rates and to currents at interfaces is a key future challenge. Main limitations include the lack of model systems where to benchmark and validate theory approximations, and new theories for excited state dynamics.

3 Community needs

Close interaction between theory and experiments was advocated by all participants. Several speakers presented clear evidence that collaborative projects can lead to substantial new insights. One outcome of our discussions is that to improve the effectiveness of this collaborative approach we need benchmarking on model systems.

Theory cannot yet tackle the full complexity of realistic photoelectrochemical systems. To test the validity of current and emerging theoretical approaches and to improve the predictive power of theory, simulations need to be benchmarked against well characterized systems. While there is clearly a strong incentive for experimentalists towards designing and characterizing new systems with improved performance, this field suffers from lack of fundamental studies devoted to improve our understanding of the basic principles governing the functioning of photoelectrochemical devices. Here theory can have a remarkable role, but validation against experiments on model systems is critical. Many participants advocated for more funding and more collaborative (theory/experiments) projects aimed at filling this gap.

In this workshop, we decided to mix theoretical and experimental talks. All participants gave us positive feedback on this. They stressed the need to make sure the whole community understands what theory can/cannot simulate, and what is the predictive power of current approaches. At the same time, grasping the complexity of realistic systems, the different interpretations of well-established experiments, can stimulate a productive interaction between theory and experiments.

Two issues where significant progress is needed is obtaining a realistic model of the atomic structure electric double layer and of the effect of pH. Large scale simulations are needed in this case, calling for improved algorithms to tackle both size and time scale limitations of current approaches. Access to large scale HPC infrastructure is critical in this field.

4 Funding

The field of photocatalysis is the object of consistent national funding in US and in many EU countries. There are already networking actions that address either the chemical community active on molecular photo catalysts or the physical/chemical community focusing on surfaces and heterogeneous (photo)catalysis. The positive feedback received during this workshop suggest that there could be space for proposing a COST action on photocatalytic interfaces, that could bring together the EU communities of chemists, physicists and materials scientists working on molecular and solid-state systems.

5 Will these developments bring societal benefits?

Energy and environment are without doubt scientific grand challenges with enormous potential for social benefits. The production and distribution of energy from renewable energy sources are key components of sustainable development. Finding efficient strategies for mimicking natural photosynthesis can open the way to employ solar energy to directly convert abundant compounds (CO2, H2O, …) into useful products, such as fuels or chemicals. Finding cheap and efficient photocatalytic materials capable to promote this solar-to-fuel conversion, which is the main general goal of this research field, will prompt industrial investments. During the workshop, it emerged that photocatalytic systems for artificial photosynthesis is already attracting the interest of chemical and petrochemical industries, even if the cost of the device is still high and its efficiency relatively low. In perspective, the potential benefits resulting from the large-scale application of these technologies may reach health (since it can bring about a carbon neutral energy cycle) and may promote a sustainable economic growth accessible to both rich and developing countries.

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Multiscale Simulation Methods in Soft Matter Systems II

Location: CECAM-DE-SMSM, University of Darmstadt, Germany
Webpage: https://www.cecam.org/workshop-0-1286.html
Dates: October 4, 2016 to October 6, 2016

1 State of the art

Multiscale modeling is a central topic in theoretical condensed matter physics, materials science, as well as in applied mathematics and engineering. One prominent class of materials, whose properties can rarely be understood on one length scale and one-time scale alone, is soft matter. The properties of soft materials are determined by an intricate interplay of energy and entropy, and minute changes of molecular interactions may lead to massive changes of the system's macroscopic properties.

Many of the methods implemented today have been developed independently in the applied mathematics community and the soft matter community. The workshop brought together these communities in order to exchange ideas and develop a joint roadmap.

Methods for developing coarse-grained models, which are hierarchically linked to their fine-grained counterparts, have significantly advanced in the past decade. Important methodological challenges however remain. These include the understanding and modeling of dynamics of coarse-grained models, improvement and extension of mixed resolution models with dynamic exchange, and improvement and extension of methods that bridge the particle-continuum gap.

The workshop focused on the following issues:

- Fundamental issues related to coarse-graining:
  - Selected examples of successful coarse-grained models
  - (Why and in which sense are they successful?)
  - Generic strategies for coarse-graining
  - The role of multibody potentials
  - Coarse-graining strategies in the presence of uncertainties
  - The mathematical analysis of coarse-grained models

- Coarse-graining of dynamical properties
  - Mapping of dynamical properties
  - Sampling of rare events
  - Accelerated molecular dynamics
  - Markov State Models
  - Coarse-graining of nonequilibrium and active system

➢ Perspectives for multiresolution schemes

- Heterogeneous multiscale modeling
- Mixed Fine-Grained/Coarse-Grained Schemes
- Multiresolution in the time domain

2 Major outcomes

The workshop brought together 120 people from the applied mathematics and soft matter communities. Among established scientists in these fields, students from different disciplines in mathematics, physics, chemistry and biology participated in the meeting. The three-day program consisted of 18 invited talks of 45 minutes (35 +10) each, 5 contributed talks of 30 minutes (25 + 10) each, and 44 posters distributed over two, afternoon poster sessions. The invited talks were given by well-established scientists from different theoretical communities. This led to interesting cross-/interdisciplinary discussions throughout the meeting. The participating talks were selected from the abstract submitted to the organizers.

Several fundamental issues related to coarse graining were discussed during the meeting. These include mathematical aspects of inverse problems (inverse Monte Carlo and iterative Boltzmann inversion), integral equation methods, relative entropy methods, and the role of multibody potentials in coarse-grained modeling of water and hydrophobic polymer collapse transitions. The discussion of these topics clearly identified a need for extending these methods in order to alleviate limitations in state-point transferability of coarse-grained models. In this context, new developments in computing multibody coarse-grained interactions, regularizing inverse coarse-graining techniques, and application of integral equation methods were identified as promising.

Methods for hybrid simulations were discussed during the meeting. New developments in adaptive resolution methods (quantum/classical atomistic, classical atomistic/coarse-grained), hybrid particle/field methods, and particle-continuum coupling methods were discussed. The meeting identified that the interaction and discussion between researchers from the applied mathematics and soft matter communities is desired to address the open questions in this field.

In the field of dynamics, new developments in coarse-grained modeling using equilibrium and non-equilibrium Markov state models were discussed as well as methods to compute non-Markovian coarse-grained interactions using rigorous mathematical derivation based on the Mori-Zwanzig formalism. Applications discussed include dynamics of polymer melts, rare-event kinetics such as peptide binding and folding, as well as non-equilibrium dynamics such as polymers in shear flow. Further approaches discussed include field theoretical methods for dynamics of polymers/blockcopolymer systems and slip-link models for studying nonlinear rheology of highly entangled polymers.

3 Community needs

The field of soft matter simulations is highly interdisciplinary. Its progress relies on frequent interaction and exchange between mathematicians, chemists, physicists and materials

scientists. The feedback received from the participants of the meeting has been very positive, in particular in view of its interdisciplinary character.
In order to make progress in the most challenging problems in multiscale modeling of soft matter, intensification of scientific exchange of researchers of different communities is a major need. This exchange can be achieved by future interdisciplinary conferences and workshops. It is moreover desirable to enable exchange at the level of researchers and, in particular, PhD students.

The field of multiscale soft matter simulations relies on state-of-the-art codes. Methods for systematic coarse graining are typically implemented in in-house software. A need exists for implementing and further developing these methods within software packages that are freely available to the community. While activities in direction are ongoing, it is recommended that funding of these activities remains significant. This also holds for new methodological developments in hybrid simulation methods and methods for coupling particle- and continuum simulations.

4 Funding

The meeting contributed to identifying new questions and directions of research. The German Research Foundation (DFG) is currently funding a collaborative research center on multiscale simulation methods for soft-matter systems (DFG Transregio 146). Based on discussions at the meeting, we foresee that the renewal proposal for this center will strengthen aspects of quantum/classical hybrid simulations and development of multibody potentials. In this context, possibilities of joint research proposals were discussed at the meeting.

5 Will these developments bring societal benefits?

Multiscale modeling of soft matter has reached a level of maturity that allows providing answers for complex systems and questions relevant to the industry already now. There have been several successful examples of this already, e.g., in applications of modeling dynamics in polymer/monomer mixtures and investigating relations between chemical structure and interaction of polymer melts with solid surfaces in collaboration with several companies, including Merck, BASF, and Bayer. Linking chemistry and properties of materials by scale-bridging simulation approaches potentially offers solutions in materials science. The application of multiscale simulations methods to industrially-relevant problems ranges from flow problems (development of drag reduction additives in flow of complex fluids in tubes, fluid flow in nano- and micro-porous electrode environments in fuel cells) to computational materials discovery including drug design. Multiscale modelling is increasingly attracting large and medium-sized industrial research and development departments, a development which we foresee to continue in future.

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Computational insight into photo-induced processes at interfaces

Location: CECAM-DE-MM1P
Webpage: https://www.cecam.org/workshop-0-1307.html
Dates: October 10, 2016 to October 14, 2016

1 State of the art

There is enormous interest in understanding and controlling photo-induced charge transfer and chemical reactions for energy storage. These can be due either to water splitting and carbon dioxide reduction or by electro-hole pair separation at hybrid chromophore- or hybrid polymer-solid interfaces in photovoltaic devices, stimulating an increasing number of experimental and theoretical studies. Computational atomistic studies of experimental realistic setups require models that include an inorganic semiconductor nanostructure, acting as a catalyst and organic molecules in solvents. In photovoltaic applications, e.g. one has to consider multi-component systems, involving several chromophores tuned to absorb different wavelengths of light, an acceptor that removes an electron from the chromophores and creates separated electron-hole pairs, as well as electron and hole conducting media. Such models already may involve hundreds to thousands of atoms, extending far beyond the limits of any ab initio calculations. Furthermore, the non-equilibrium processes involved in the photo-induced charge separation and transport require explicit time domain modelling. Relevant processes occur on ultrafast time-scales and in most cases cannot be described by rate expressions. Charge separation, Auger-type energy exchange between electrons and holes, generation of additional charges by Auger mechanisms, energy losses to heat due to charge-phonon interactions, charge and energy transfer, and electron-hole recombination occur in parallel and competition requiring significant efforts in method development and clarification of multiple conceptual problems.

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.

As major scientific objectives of the proposed workshop we have achieved:

- Bringing together researchers from quantum chemistry and computational solid state physics working on photo-catalysis and photovoltaics. We were able to highlight recent progress and discuss challenges and opportunities in the materials aspect of tailor-made nanostructures and hybrid interfaces for highly efficient energy applications.

- We have fostered the exchange of methodological expertise and new developments between scientists working on different aspects of metal oxide photo-catalysis.

- We discussed possibilities for optimizing the materials properties and device design. The interdisciplinary character of the workshop helped finding solutions for overcoming current limitations.

- The workshop stimulated new worldwide interdisciplinary collaborations on computational photo-catalysis and photovoltaics for the mutual benefit of theoretical, experimental and applied researchers.

The program consisted of 30 invited talks of 40 minutes (35+5) each and one poster session presenting 39 posters. In addition, many social events (reception and conference dinner) to allow for informal exchange were held. The invited talks were given by well-established scientists from the different theoretical communities, which acted as platform for interesting cross-/interdisciplinary discussions. The invited talks were followed by a poster session where the younger participants could show their scientific work and exchange of ideas with a broad knowledge in computational chemistry, solid state physics and computational materials science. The organization was very compact with the scientists accommodated in the same hotel fostering exchange and discussion between the participants also outside the meeting room.

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 photocatalysis and photovoltaics necessitates a joint effort from experts in different fields. 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.

4 Funding

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.

5 Will these developments bring societal benefits?

Progress in the field of many body physics 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
- Photo-catalytic processes in energy storage and pollutant degradation
- Hybrid nano/bio-systems for medical applications
- Single-defect-based quantum optical and spintronic devices

Such directions can be strengthened by focused research projects for the development of new materials and devices in key enabling technologies. The field of nanodevices is currently opening to new materials, especially 2D. The EU flagship on graphene and 2D materials is indeed expected with the aid of computational predictions to produce several new outcomes. However, technological innovation is not limited to these novel materials.

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Mesoscopic Modeling in Physics of Molecular and Cell Biology

Location: Toulouse, France (CECAM-FR-GSO) - CEMES campus
Webpage: https://www.cecam.org/workshop-0-1269.html
Dates: October 10, 2016 to October 13, 2016

1 State of the art

With the involvement of an increasing number of physicists in the field of mesoscopic modeling of molecular and cellular biological processes, huge progress has been accomplished in the two past decades. However, many questions remain unsolved and the spectacular development of experimental techniques (e.g. as microscopy at super-resolution and single molecule experiments) promises that the number of open questions will keep growing in the future.

This workshop intended to gather theoretical physicists specialized in statistical physics and soft matter, and working on different subjects related to molecular and cell biology, but using very similar paradigms and tools. They belong to coarse-grained models (where a small group of atoms is modeled as one particle); effective mesoscopic models (where elementary particles are as large as molecules or subparts of macromolecules); analytical approaches using mesoscopic models from the statistical physics, eventually coupled to hydrodynamics, elasticity, or electrostatics.

One important goal of this workshop was to focus on the application of these various techniques to the physical mechanisms, depending on the time or the length scales under study and the biological issue.

The molecular or supra-moecular consituents of a cell, which were tackled in the workshop can be categorized as follows: cell membranes and their organization (micro-patterning, rafts collective signal transduction, translocation); the cell nucleus and the spatial organization of genes, genic regulation; nucleic acids, nucleosomes and chromatin in bacteria and eukaryotic cells; the cytoskeleton and its consitutants.

2 Major outcomes

The CECAM workshop « Mesoscopic Modeling in Physics of Molecular and Cell Biology » took place at the CEMES Marvig-CNRS campus in Toulouse, between October 10th and 13th, 2016. It gathered about 50 researchers, among which post-docs and Ph.D. students. Roughly, one half of the participants came from France and one half from Europe and the rest of the world (Japan, USA, India).

There have been 36 talks divided in 7 half-day sessions that covered the following topics:

GENOME PHYSICS; ACTIVE LIVING MATTER; NUCLEIC ACIDS; VIRUSES, CELLS AND BEYOND; BIO-MOLECULES & BIO-POLYMERS; DYNAMICS IN THE CELL; BIO-MEMBRANES.

Few posters were also presented.

The debates were rich and fruitful. When leaving many participants underlined the quality of the workshop and their happiness to have participated, and to have learnt a lot in research topics related to theirs. It was also acknowledged that the workshop focus was acurate

enough to enable the paticipants to feel concerned by most of the talks.

The issue of filling the gap between different scales of coarse-graining was tackled in several talks. When coarse-graining a system, one must take care of using the adequate effective parameters and to justify at best the choice of their values. This is not necessarily an easy task and issues remain open in this context.

The question of the relevance of mesoscopic models in spite of the apparent successes of the trendy all-atom models was discussed at the end of the workshop, after an introduction of the round-table by Nicolas Destainville (one of the workshop organizers). The participants rather were confident that mesoscopic models remain very important because, on the one hand, all-atom models are also based on approximations when building the force fields; and on the other hand, they are not always able to tackle the relevant time- and/or length-scales of interest. The gap can remain huge when milli-second (or even larger) lengthscales on micrometer-sized (or even larger) biological systems are at stake.

3 Community needs

The interest of mesoscopic modeling is that it is in part designed to avoid the need of huge numerical facilities, as required for instance by all-atom simulations. However, several talks presented highly demanding works in terms of computational needs.

As discussed in the "Major Outcomes" section, some members of our community feel a risk of being somewhat marginalized because they do not display consumption of huge computational power, and they are not always able to exhibit very spectacular pictures coming from their simulations. In the experimental biology community with which they daily collaborate, a regrettable fashion seems to emerge where all-atom simulations seem more trustworthy than mesoscopic modeling, either numerical or analytical, because of widespeard belief that they are "exact".

To this respect, it will be important to organize workshops with the same spirit, dedicated to mesoscopic modeling in physical biology, but even more importantly, we will have to find how to attract experimental biologists to these events.

4 Funding

The organizers did not identify the emergence of joint research proposals during the meeting, even though they cannot exclude that bilateral ones emerged.

5 Will these developments bring societal benefits?

Potential societal benefits of the research topics discussed in the workshop clearly come from their connection with experimental Biology. Health issues were not specifically addressed during the workshop, but most of the fundamental biology problems discussed have potential impact on health issues. The dramatic development of everyday more powerful experimental techniques (see, e.g. the recent Nobel prizes awarded for the discovery of GFP or the invention of the super-resolution microscopy) provides a large amount of experimental data that notably require the expertise of physicists to fully exploit and rationalize them.

Nucleic acids and genome physics (e.g. dynamic functioning and organization of genes in both human cells and pathogenic organisms); functioning of cell membranes as well as dynamics of parasite invasions; Viral self-assembly and modeling of viral capsids, are few obvious examples that were addressed in the workshop and where getting deeper insight will likely open the route to new therapeutic approaches. Topics more related to nano-technologies were also discussed, such as the modeling of the folding of DNA origami.

6 Participant List

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Molecular chirality from a physical and theoretical chemistry perspective

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1271.html
Dates: October 10, 2016 to October 12, 2016

1 State of the art

The understanding of molecular chirality, from a theoretical and computational chemistry viewpoint, is a main issue in molecular physics and chemistry. The origin of chiral specificity, a signature of life on our planet, ranks among the most interesting natural phenomena and is at the basis of the high enantiomeric selectivity of many processes involving biological molecules. Molecular recognition and asymmetric synthesis, asymmetric catalysis in organic, industrial and pharmaceutical chemistry are research fields, relevant for both basic research and technology and with perspective economic and social impact. Many hypotheses about the nature and role of the molecular chirality have been advanced, especially in speculating about the origin of biological homochirality. These hypotheses are controversial and lack of unanimous consensus: enantiomeric excess was argued to be generated by chance or by statistical fluctuations, followed by amplification mechanisms; from the viewpoint of fundamental physics, the hypothesis of a role of parity violation, due to weak nuclear forces, in determining an energy difference between the enantiomers is under scrutiny; external fields, specifically circularly polarized photons, can act as chiral environments. Interaction with macroscopic chiral environments also seems to induce selection (e. g. stirring of solutions during the formation of chiral aggregates). More recently, a stereodynamic mechanism for chiral selection in gas phase has been proposed examining the possibility that “oriented” molecular encounters may cause discrimination of chiral sign and emergence of chiral specificity.

2 Major outcomes

A number of topics came out from the presentations and the discussions held during the workshop sessions. Most of them were about advanced experiments and theoretical methods designed to study and understand the discrimination and detection of different enantiomers, chiral recognition, to measure enantiomeric excess in mixtures and to search for possible mechanisms of chiral selectivity in processes involving enantiomers.

Ideas about homochirality in nature and routes leading to enantiomeric excess have been also discussed. A brief account of the main topics follows.

The use of NMR to detect chirality (NMR is a technique in principle blind to chirality) has been discussed, based on the application of strong magnetic fields, which induce in precessing nuclear spins a rotating electric polarisation than is opposite for different enantiomers.

Synchrotron radiation as a source of VUV Circularly Polarised Light (CPL) has been recognised to be suited for simulations of physical environments promoting the occurrence enantio-specific processes, such as enantioselective photolysis and asymmetric production of amino acids upon CPL irradiation, with possible implications towards an astrochemical origin of homochirality.

Photoelectron Circular Dichroism (PECD) has emerged as a best suited method for the investigation of chirality in terms of asymmetries in the backward-forward scattering of the angular distribution of photoelectrons. It has been shown that the asymmetry effects characterising chiral ionisation, significantly stronger than in other chiroptical phenomena, can be exploited to investigate electron-nuclear interactions (e.g. vibronic interactions, vibrational resolved PECD calculations). In general, ab initio calculations, although effective in reproducing PECD spectra, need to be improved and validated to include the effects of different conformers. Molecules are flexible structures and conformational changes and solvation effects can greatly influence their chiral properties. The idea of introducing a continuous chirality measure as a distance from a reference achiral structure has been proposed and discussed.

Complementary to this point, the possible use of high resolution microwave spectroscopy to investigate chiral tagging and transient chirality (low interconversion barrier between enantiomers) has been also presented.

From a stereodynamic point of view, the effects of chirality in photodissociation reactions have been shown to be measurable in the universal angular momentum distributions of photoproducts. It has been also pointed out that no effect can be detected with unpolarised molecules, a constraint characterising also the chiral effects in collision involving atoms and molecules.

This latter topic has been also largely discussed, remarking the lack of experimental and theoretical works on it. In such a case, chiral effects could be observed under conditions of a significant degree of molecular alignment and orientation, a thesis sustained by analogy with electron-chiral molecule scattering, vector correlation studies and molecular dynamics simulations of atoms with H2S2 molecules.

Molecular orientation control techniques making use of electrostatic fields produced by hexapoles and their perspective use to set up molecular beam experiments about chiral discrimination in molecular collisions have been illustrated and discussed.

The estensive use of sophisticated quantum methods to study the dynamical effects due to chiral molecules has been illustrated for reactions and alignment and orientation by collisions with surfaces.

3 Community needs

Theoretical and experimental studies of chirality need strong computational support.

The need of the community in terms of the computational infrastructures is related to the computational costs of the quantum mechanical calculations of the electronic structure and intermolecular interactions involving chiral molecules, necessary to build up accurate potential energy surfaces and to model dichroism profiles. Ab initio calculations can in principle benefit from a number of existing commercial and also freely available codes, which are are supposed to be properly working. In this case what one hopes for is the prompt availability of high performance computing (HPC) resources. Collision simulations, especially when moderately large organic molecules are under consideration, are hardly performed by quantum mechanics, whose extensive applications is still limited today to three and four-atom systems, unless severe approximations are adopted, compromising accuracy and physical realism. Apart from the requirement of large HPC facilities, a certain lack of availability of quantum collision dynamics programs for more than three-atom systems, is still a limit in the field, since huge efforts are required to build up home-brew quantum dynamics codes.

Mixed methods (QM/Classical) can be used, which are based on quantization of the relevant degrees of freedom only, with some gain from a computational point of view.

4 Funding

An overall approach to molecular chirality and its manifestations as a consequence of light matter interaction, molecular collisions, influence of macroscopic rotating environments, should involve many fields of physical and theoretical chemistry (mw, UV, X-ray and NMR spectroscopy, circular dichroism studies, molecular beams) and the wealth of theories and methods at the foundation of them. Optimal funding schemes should be oriented to cooperation, to favour multidisciplinary efforts. COST Actions are well suited for that.

The applied-research character of most H2020 calls, except for ERC grants, makes them in general less appropriate for supporting a global approach to chirality, which even being in perspective promising in terms of technological applications, has not an high technology readiness level (TRL) and would probably fail to compete with other topics.

5 Will these developments bring societal benefits?

The research topic of the workshop implies the perspective improvement of theoretical approaches and experimental techniques for the accurate characterisation of recognition of chirality, enantiomeric excess production in gas and condensed phases and the contemporary development of new ones. The techniques range from molecular beam and spectroscopy based methods (e.g. circular dichroism, microwave spectroscopy etc..) to ab initio calculations and quantum, classical and semiclassical mechanics for molecular dynamics studies. Many of the theoretical tools and experimental methods are those used in research activities dedicated to asymmetric synthesis, asymmetric catalysis, drug discovery, in organic, industrial and pharmaceutical chemistry. The improvements will benefit these fields, with impact in terms of societal benefits. Particularly, advancement in the experimental characterisation of chiral recognition (think of absolute configuration determination) with the crucial assistance of theoretical methods and molecular dynamics simulations, could greatly improve the search for effective drugs, when chiral molecules are involved and also the development of synthetic techniques necessary to produce enantiomerically pure drugs. Materials science is another important field, which the outcomes of the research on this topic could favourably impact.

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Computational methods towards engineering novel correlated materials

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1240.html
Dates: October 24, 2016 to October 26, 2016

1 State of the art

The intention of the workshop ”Computational methods towards engineering novel correlated materials” was to gather a group of influential but comparatively young theoretical and computational physicists in the field of correlated materials to discuss the main challenges of today’s state-of-the-art ab-initio calculations.
The program consisted of i) 23 workshop presentations including four keynote talks focussed on the main topics of our meeting: Novel materials (two keynote talks), Collective phenomena, and Theoretical Methods; ii) a poster session for which we had 11 contributed posters; iii) a round table discussion chaired by the organizers.
It was taken care that there was substantial time for questions and discussions after each presentation.
It turned out that the mix of participants, which covered a wide spectrum of experts ranging from density functional theory to quantum many-body theory, was an essential part for vivid discussions throughout the three days of the workshop. In particular the round-table discussion was very inspiring and included critical exchange about strengths and weaknesses of different methodologies as well as common challenges and goals of different research units in the field.
Below, we first report on the status quo of our community regarding computational methods and their applications, and then outline future goals and challenges that we identified during our workshop.

2 Major outcomes

In terms of computational methods, the merger of density functional theory with dynamical mean-field theory is still the dominating choice for ab-initio materials simulation for correlated materials. However, an increasing number of extensions of the DFT+DMFT methodology have been developed to an extent that their application to realistic modeling of strongly-correlated materials has started. These extensions can be categorized mainly into two classes.

The first type of extensions are focused on the link between first principle calculation and dynamical mean-field theory. A lot of work is put, e.g., into the development of GW-based approaches, which improves conceptually over standard DFT-based methods. This is due to the fact that the GW formalism is formulated in the same language as DMFT and the long-standing double-counting problem is, different from DFT+DMFT approaches, well defined. Such approaches are already used to study physics of, e.g., iron based superconductors or correlation physics in more exotic systems like e.g. semiconductor surfaces or even Graphene.

The second type of extensions is focused more on the many-body problem itself. To overcome the intrinsic local limit of single site DMFT, field theoretical methods which might be coined as ’diagrammatic’ approaches are developed. These range from renormalized Fermion-Boson vertices in the ’Dual Boson’ approach, or the novel TRILEX scheme, to computationally expensive approaches attacking the fermionic" "two-particle vertex like the

dynamical vertex approximation or the dual fermion approach.
All of these beyond-DMFT approaches have in common that they include (more or less) non-local fluctuations and correlations into the calculation by systematically pushing the approximation from the single particle self-energy to vertices of higher order.

Given that the mentioned extensions are all comparatively recent it is expected that their usage for realistic materials calculations will increase and, depending on the usability and reliability, that the approaches will be more accessible throughout the community."

3 Community needs

Given the recent improvements of algorithms, the range of materials where DFT+DMFT like approaches are applied has grown significantly over the last decades. New impurity solvers allow to reach very low temperatures and to deal with complex crystal-field and spin-orbit-coupling situations.
In terms of materials, this means that for instance the ab-initio description of heterostructures, including low-symmetry crystal structures, is now possible. Another emerging field is the investigation of oxide materials based on heavy transiton metals, such as iridium oxides. They are promising for application as topological insulators, with an amount of chemical flexibility that cannot be reached by semiconductor materials. And last but not least we can now study the precise evolution of physical properties at very low temperatures. This allows us to investigate coherence phenomena in bad metallic regimes, which is important for, e.g., pnictide supercondutors or ruthenates.

In terms of materials, we expect that the number of compounds, where the above described ab-initio methods are applied, will increase. While there is a number of materials where the 'simplest' DFT+DMFT works well, it became apparent - also during this workshop - that extensions of DMFT beyond the local limit can be motivated also very pragmatically from a materials science point of view. One example that sticks out are non-local correlations that arise from magnetic fluctuations in unconventional superconductors like cuprates or the new iron-based compounds. One might hope that methods which are currently developed will be able to resolve some of the long standing puzzles. One criterion will for sure be the feasibility of treating also orbital degrees of freedom; while in cuprate high-Tc compounds an effective single band description might be justified, iron-based superconductors are a good example for non-trivial physics that emerges from a generic multi-orbital setup.

While high-Tc compounds are surely amongst the more spectacular examples they are only a fraction of compounds which pose similar challenges. Therefore, we conclude that in particular extensions of the single-site DMFT methods will be far more than an academic excercise and rather decisive for the development of the entire field. At the moment, the main obstacle is that most of these methods, such as DGammaA or Dual Fermions, are computationally still much too expensive in order to use them in a truly realistic setting. Therefore, in our opinion, the community needs to also work on methods that are a bit lighter (like, e.g., the TRILEX approach), but still include the main non-local properties. A problem that will remain is that the application of these new methods will be limited to experts only due to their complexity.
Time will tell if the implementations can actually be improved to a standard where also non-experts can use them. At the moment, however, this is rather doubtful.
Another recent development that we deem absolutely essential to continue is the effort to share and benchmark new codes. There are already a number of public DMFT and impurity-solver implementations, which can be used as a basis to set some standards that new implementations have to fulfil. We see that in particular the younger members of our community appreciate code sharing and benchmarking. However, there are dangers connected to code development for young researchers that should not be taken lightly.

Spending time on implementations and code maintenance is not recognised enough as a valuable duty in our community. Especially due to the structure of a standard academic career (which means a severe lack of long term perspectives for most researchers for a long period after their Ph.D.), coding heavy projects can easily lead to a dead-end track.
Finally, in addition to 'black-box' methods that aim at full ab-initio predictions, we also highlighted at the workshop the need for model calculations. The latter ones are sometimes better suited to disentangle relevant microscopic origins than full-fledged ab-initio calculations. We should not forget about the big advantage of computer simulations over experiments, that is that we can play with the material much more than nature allows in real life. This playing is crucial for gaining physical insight.
We think that the workshop was a great success. In particular, we collected participants of different schools, but all working in simulations of correlated matter. This diversity was decisive for this event to work and the feedback we got from the participants was extremely positive. We did encourage especially younger members of our community to consider organizing workshops with the help of CECAM and/or PsiK.

4 Will these developments bring societal benefits?

The topic of the workshop is still not at the appropriate stage to discuss societal benefits. However, the long term goal of accurate modeling and engineering of materials will have a clear societal impact.

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Water at interfaces: from proteins to devices

Location: CECAM-AT
Webpage: https://www.cecam.org/workshop-0-1304.html
Dates: November 29, 2016 to December 2, 2016

1 State of the art

The properties of water at biological/inorganic interfaces or in confinement have received large attention in recent years by the scientific community due to their fundamental role in biochemical processes and for their technological applications.

On larger scales, water-membrane interplay is relevant for technological and medical applications. According to recent data, one person in six lacks the access to clean water, making the purification of wastewaters a serious technological and political challenge for the coming years.

At the molecular scale structure of water at the interface of hydrophobic surfaces has important implications for the protein properties. Moreover, the formation of a hydrogen bond network around a protein could be related to changes in the protein tertiary structure and, consequently, of its biological function.

Water also governs the rate at which proteins, nucleic acids and membranes recognize ligands and molecules. Accurate models are of fundamental importance for drug design.

At low temperatures, the dynamics of water near protein surfaces instead are highly relevant for the safe preservation of organic material. In fact, water-protein interactions may influence the phases of the water itself, a feature that is exploited by several proteins to promote or impede the formation of ice. For example, experimental and numerical results show that long-range protein-water interactions play an important role in explaining the hyperactive antifreeze protein activity of insects. Some fungal spores, among the most abundant organic spores observed in the atmosphere, are known to use ice nucleation proteins to facilitate water nucleation.

Rationalizing the behavior of water in biological environment may provide the key to understand many of the complex self-organizing mechanisms of biological matter.

2 Major outcomes

The key points discussed during the workshop were the following:

1. The importance of water behavior close to inorganic interfaces was a central theme at the workshop. On the one side the discussion focused on the dynamical properties of recent filtration membranes applied in water desalination, sanitation and transport phenomenon in fuel cells. On the other side, we discussed about the general properties of hydrophobic surfaces, introducing a strongly interdisciplinary session with contributions ranging from biology all the way to atmospheric science.

   The studies presented showed the remarkable experimental and theoretical advances in the understanding and exploitation of the properties of ions dissolved in water. Overall, the speakers presented interesting new concepts to control the transport of ions and exploit such control to either remove the ions (desalination) or to store energy (fuel cells).

2. The accurate description of the solvation of bio-molecules was another central theme of the workshop. In particular, during the workshop we discussed current problems and future perspectives of water models regarding both equilibrium and dynamical properties of proteins. Moreover, current computational and conceptual challenges related to ice nucleation and ice inhibition materials, important in fields like cryo-preservation of tissues and frozen food storage, among which proteins play an important role, were discussed. An important conclusion of the discussions was that in order to further advance the field it is necessary to improve our current representation of water polarization properties and to reduce the computational cost of the simulations.

3. A special session was dedicated to a general discussion on the impact of water studies both in the scientific community and, more in general, to society.

   This workshop demonstrated the growing importance of interfacial water in many fields of science among which there are physics, biology, medicine, water treatment, atmospheric science, engineering. This field of study has been emphasized in recent publications but, contrary to bulk water, it was subject only lately of few meetings. The central goal of this workshop was to gather leading scientists, from a wide spectrum of disciplines ranging from biophysics to material sciences, working on modeling and experimental aspects of water at interfaces and at different length scales. We believe that the workshop fully achieved this aim.

   The long-term goal of this workshop is to catalyze interdisciplinary collaborations that integrate our knowledge on different length scales and coarse-grained modeling to address the study of large bio-molecular/polymeric systems and of the design of new functionalized materials. Based on the discussion stimulated and the feedback obtained from the participants, we believe that also this objective was reached.

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 water 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, working on modeling and experimental aspects of water at interfaces and at different length scales. We believe that the state of the art in water modeling is now sufficiently mature to address important applications in the fields aforementioned, hence the timeliness of this meeting was optimal and the location ideal with many local groups working on related problems. 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 organization:

   The success of the meeting and the feedback of many participants that appreciated the novel wide interdisciplinary program suggests that it would be important to transform such an isolated event into a recurrent meeting opportunity either yearly or every two years.

4 Funding

During the meeting, several discussion occurred about funding options to support research collaboration on water related projects in particular Horizon2020 and ETN network grants.

Other possibilities were presented by Max Paoli who introduced the TWAS grant programs. From the website (http://twas.org/opportunity/twas-research-grants-programme-basic-sciences-groups) of this program: "The TWAS Research Grants Programme in Basic Sciences aims to: Reinforce and promote scientific research in basic sciences in developing countries; Strengthen developing countries' endogenous capacity in science; Reduce the exodus of scientific talents from the South; Build and sustain units of scientific excellence in science and technology lagging countries over a longer period to help them achieve a critical mass of highly qualified and innovative scientists capable of addressing real-life problems facing their countries."

The participants responded with interests to this option.

5 Will these developments bring societal benefits?

Water covers 2/3 of the Earth and affects life in countless aspects and length scales. It is the main component of living beings, confined in cells or flowing below tissues. A great effort has been done to model water behavior in order to account for its many properties and anomalies (e.g., near the freezing point, water is not much susceptible to temperature changes, a property essential for life in cold climates), yet many aspects remain still controversial.

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.

Water sanitation is one of the goals set by the United Nations and in order to reach such goal we need a better understanding of the properties of water at the interface of novel materials used as filters (e.g. graphene).

For medical applications, the field of drug design is in desperate need of a better understanding of the effect of water on the description of protein-protein and protein-drug 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.

Finally, the ice nucleation properties of water have enormous repercussion to our planet from food and organ preservation to the understanding of large scale climate models.

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.

6 Participant List

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Biomimetic and living materials: active matter at high densities

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1322.html
Dates: December 7, 2016 to December 9, 2016

1 State of the art

Active matter is still at its infancy and the increasing number of experiments, conducted to either verify or falsify active matter theory results, reflects the importance that this area of research has acquired in recent years. Its importance lies ultimately in its applicability to understand biological physical problems such as tissue formation and cancer growth as well as to design and fabricate biomimetic materials. The understanding of the physical properties of active materials, such as biological tissues, requires acquiring a solid knowledge about the large-scale properties of active particle systems at high densities. At low densities, we can assume that the system is diluted enough as to attempt the use Boltzmann approaches, which fundamentally depend on the validity of the molecular chaos assumption. At high-densities, on the other hand, such assumption is likely to be violated. Moreover, recent studies indicate that the dynamics at high densities are dominated by the presence of active stresses. The observation of anomalously large density fluctuations and stresses in such systems suggests that the use of mean-field approaches cannot be blindly trusted. Large-scale computer simulations become then a necessary first step towards a reliable characterization of the statistical properties of active matter at high densities. From an experimental point of view, the tracking at high densities, as well as the measurement of active stresses, is a technical challenge, independently of whether the active particle are bacteria, eukaryotic cells, or artificial self-propelled particles. Finally, it has been shown that emerging collective effects in active systems are highly dependent on boundary conditions, the presence or absence of spatial heterogeneities, and/or the properties of the surrounding medium. In summary, a dialog between theorists and experimentalists in this field is highly needed.

2 Major outcomes

The workshop brought together experimentalists and theorists that during 3 days discussed several timely relevant topics on active matter, some of which are listed below:

- Liquid crystal physics and its connection to active matter. This included the study of bacteria swimming through a liquid crystal as well as the study of active entities exhibiting nematic interactions.

- The modeling of tissue growth was an important topic discussed during the workshop. Living tissue consistent of many interacting cells is a prominent example of the active matter at high densities. Different tissue models were proposed and discussed during the workshop.

- Self-propelled particles with (exclusively) repulsive interactions have been presented as a useful, simple, non-equilibrium system that allows addressing several relevant questions. For example, the non-linear rheology of such system was discussed, including the transition between “active fluid” and “active solid”.

- Active elastic networks together with active gels have received renewed interest and appear as a powerful theoretical framework to describe various biological systems.

- Experiments with bacteria have been always occupied a central role in active matter research. During the workshop, it became evident that the current focus is on the observed decreased of viscosity due to the presence of active swimmers. Studies of swimming in the presence of flows as well as the impact of the physical properties of the surrounding liquid on the observed swimming patterns are also in the spotlight.

- The emerging collective properties in models of aligning active particles were discussed. The main focus was put onto different modifications and variations of the famous Vicsek model, including actively moving rods. Recent developments in the construction of kinetic theory were shown. Some experimental systems such as Quincke rollers emerge as well-controlled realizations of active particles with aligning interactions.

- Several exciting new questions were identified during the workshop. Active particles that interact with the trails left by them, as in gliding myxobacteria, represent a challenging theoretical problem. The emergence of vortex patterns for chiral microswimmers, as well as the design of navigation strategies for robots, including a sensorial delay, appear as new promising research directions.

In summary, the discussed topics included various questions related to the physics of active matter at the level of theory and experiments. Special focus was put on active systems at high densities as well as on biological and biomimetic materials

3 Community needs

Computer simulations play a very important role in the study of active matter. Moreover, many of the existing models were first formulated as computational algorithms, and only later on formulated in term of continuum-time Langevin equations. Furthermore, due to the presence of anomalous fluctuations and anomalous transport in active systems, theoretical advances require the use of large-scale individual-based simulations. In addition, the numerical integration of hydrodynamic equations for several active systems is also computationally demanding. In short, the field of active matter is in a constant need of computational power. The access to computer cluster of high performance computing represents a serious limitation for several of us; and it provides a clear advantage for those groups having unlimited access to them.

The active matter community is growing fast, with several new groups joining this collective effort. And while the level of interconnection among the groups is high, the community is strongly influenced by a small social clique having access to a large number of resources, which leads to a natural overrepresentation of this social clique in workshops and conferences. It would be crucial for the community to provide to small players the necessary funding to organize workshops and conference with the hope this will open the door to new research groups, potentially coming from different field, bringing new fresh ideas in the active matter domain.

4 Funding

Typical funding comes from national research funds as well as from few European ones. One can mention the projects by DFG (Germany), ANR (France), and NSF (USA). Recently, a number of projects has benefited from ERC grants. Junior researchers could get finance from Marie-Curie Program, which is implemented in the framework of Horizon 2020. The possibility for researchers from different countries to apply with common research proposals to the European funding grants in the framework of Horizon 2020 was discussed. However, a serious problem for the success of active matter proposals is given by its interdisciplinary character, often providing a physical perspective to a biological system, and with the proposal floating in a grey area between physics and biology.

5 Will these developments bring societal benefits?

The developments in the field of active matter can bring important progress in different areas. The understanding of collective cell behavior is crucial to tissue formation, wound healing, and cancer growth. Bacterial motility and biofilm formation is fundamental to an understanding of bacterial infections. For instance, during the workshop the dynamics of cell infection and cancer growth, in the framework of tissue modeling, were discussed. These studies will lead to the design of better drugs and treatment techniques. The ability to control active particles may help to conceive precise drug delivery techniques, for instance by using micro-swimmers to deliver the drugs.

On the other hand, the use drones following simple rules derived from the active matter algorithms, was proposed during the workshop, with the emphasis on the potential application in search and rescue units during natural disasters.

Finally, the theoretical works on the dynamics of dense active matter are also important to understand the behavior of huge crowds of people in panic. This may help to design a complex landscape to avoid the often observed deadly human stampedes, hopefully providing protection from injuries in big crowds.

6 Participant List

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E-CAM
The European Centre of Excellence for
Software, Training and Consultancy
in Simulation and Modelling

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State-of-the-Art Workshop: Reaction Coordinates from Molecular Trajectories

Location: CECAM-NL (Lorentz Centre LC)
Webpage: https://www.cecam.org/workshop-0-1349.html
Dates: August 29, 2016 to September 2, 2016

1 Overview

Many processes in nature and technology are dominated by rare transitions between long-lived stable states separated by high free energy barriers. Examples include phase transitions in materials, chemical reactions and conformational changes of biological macromolecules. The state-of-the-art workshop recently held at the Lorentz Center in Leiden discussed current methods and future perspectives on statistical mechanical approaches to perform computer simulation of such rare event processes in complex many- particle systems and extract information from these to gain mechanistic insight. In particular, the workshop focused on the identification of reaction coordinates and the construction of reliable and meaningful models from atomistic simulation data. The computational methodologies discussed by the participants are of relevance in a wide range of fields ranging from physics and chemistry to materials science and molecular biology.

Advanced molecular simulation techniques running on today's high performance computers can sample transitions between long-lived states effectively, resulting in large sets of simulation trajectories, from which one has to extract useful models that capture the essential features of the process under study. These models should have a minimal number of degrees of freedom and should be expressed in terms of physically meaningful variables to render them understandable to humans. Moreover, such models serve as the basis for the construction of reaction coordinates that enable in-depth studies of the process at hand, e.g. by computing thermodynamic and kinetic properties. Many approaches have been developed to find good low-dimensional reaction coordinates, for instance, by seeking functions of physical variables that best approximate the committor, by identifying projections that separate transition paths and the transition state ensemble from equilibrium fluctuations, by extracting the dominant pathways in master equation and Markov-state models (MSM) or by using data-driven methods such as diffusion and sketch maps. However, these methods require the a priori definition of some collective variables that are capable of describing the process under study and thus rely on the physical and chemical intuition of the researcher apply these methods. Central goals of the workshop were to explore routes to improving algorithms, to minimize the required human intervention, and to develop practical analysis tools accessible to a wide scientific community.

2 Program of the workshop

Monday **Creating Collective Variables and Reaction coordinates**

09.00-09.30	Registration and coffee
09.30-09.45	Welcome and introduction by the LC staff and Chair of the day
09.45-10.20	Kresten Lindorff-Larsen (U. Copenhagen) *Reaction coordinates in molecular simulations – input or output?*
10.30-11.05	Carlo Camilloni (TU Munich) *Collective variables, Experimental data and PLUMED*
11.15-11.50	Pratyush Tiwary (Columbia U, New York) *Identifying and enhancing important fluctuations for sampling molecular systems with rare events*
12.00-14.00	lunch & discussion
14.00-14.45	*Discussion on mapping out of workshop goals* (Discussion leader Peter Bolhuis)
14.45-15.20	Bettina Keller (FU Berlin) *Harnessing chemical intuition to find the slow dynamic subspace*
15.30-16.00	coffee
16.00-16.35	Alessandro Laio (SISSA, Trieste) *Automatic topography of complex and multidimensional probability distributions*
16.45-17.30	*Plenary discussion* (Discussion leader: Gerhard Hummer)

Tuesday **Methods to extract reaction coordinates from molecular simulations**

09.00-09.35	Baron Peters (UCSB, Santa Barbara) *Rare Events Methods, Reaction Coordinates, and Useful Rate Theories*
09.45-10.20	Ron Elber (U Texas, Austin) *Global and local approaches for calculations of reaction pathways*.
10.30-11.15	coffee
11.15-11.40	Pietro Faccioli (Trento U, Trento) *Variational principles for reaction coordinates and biased reaction pathways*
12.00-13.00	lunch & discussion
13.00-14.45	discuss & work & collaborate on goals
14.45-15.20	Titus Van Erp (NTNU, Trondheim) *Analyzing complex reaction mechanisms using path sampling*
15.30-16.00	coffee
16.00-16.35	Michele Ceriotti (EPFL, Lausanne) *Finding patterns and mapping landscapes.*
16.45-17.30	*plenary discussion* (Discussion Leader Alessandro Laio)
17.30	end of the day

Wednesday **Fundamental issues in Reaction coordinates**

09.00-09.35 Cecilia Clementi (Rice U, Houston)
Low dimensional representation of protein conformational dynamics: tools and challenges
09.45-10.20 Robert Best (NIH, Bethesda)
Mapping protein folding dynamics onto 1D reaction coordinates — how far can we push this idea?
10.30-11.15 coffee
11.15-11.50 Sergei Krivov (U Leeds)
Nonparametric variational optimization of reaction coordinates.
12.00-13.00 Lunch & discussion
13.00-14.45 Discuss & work & collaborate on goals
14.45-15.20 Daan Crommelin (CWI, Amsterdam)
Importance functions for multilevel splitting
15.30-16.00 coffee
16.00-16.35 Peter Bolhuis (U Amsterdam)
Networks of reaction coordinates or reaction coordinates of networks
16.45-17.30 *plenary discussion* (Discussion Leader Baron Peters)
17.30 end of the day
19.00 Workshop dinner

Thursday **Machine Learning and Markov Modeling**

09.00-09.35 Max Welling (U Amsterdam)
Modern Machine Learning Tools Relevant for Molecular Dynamics
09.45-10.20 Frank Noe (FU Berlin)
Machine learning methods for dimension reduction, reaction coordinate identification and extracting kinetics from molecular dynamics
10.30-11.15 coffee
11.15-11.50 Edina Rosta (Kings College, London)
Identification and Analysis of Transition and Metastable Markov States
12.00-13.00 lunch & discussion
13.00-14.30 discuss & work & collaborate on goals
14.30-15.05 Xuhui Huang (HKUST, Hong Kong)
Using the Projection Operator Approach to Identify Optimal Kinetic Lumping and Recover Slowest Conformational Dynamics of Complex Systems
15.15-15.45 coffee
15.45-15.55 David Swenson (U Amsterdam) (contributed talk)
Generation and Analysis of Arbitrary Path Ensembles using OpenPathSampling
16.00-16.35 Jocelyne Vreede (U Amsterdam)
Path sampling simulations of the mechanisms and rates of transitions between Watson-Crick and Hoogsteen base pairing in DNA
16.45-17.30 *plenary discussion*
(Discussion Leader Christoph Dellago)
17.30 end of the day

Friday	**Applications and Experimental testing of reaction coordinates**
9.00-9.35	Michael Woodside (U. Alberta, Edmonton) *Measuring transition paths in the folding of single molecules*
9.45-10.20	Dmitrii Makarov (U Texas, Austin) *Reaction coordinates and pathways of mechanochemical transformations*
10.30-11.15	coffee
11.15-11.50	Christoph Dellago (U Vienna) *Reaction coordinate for freezing: do we understand crystallization?*
12.00-13.30	lunch & discussion & work
13.30-13.40	Ruben Demuynck (Genth U, Zwijnaarde) (contributed talk) *Advanced molecular dynamics simulations to construct free energy profiles of complex transformations in nanoporous materials.*
13.45-13.55	Rodrigo Casasnovas (Forschungszentrum Julich) (contributed talk) *Understanding protein-ligand unbinding kinetics from metadynamics simulations*
14.00-15.35	Gerhard Hummer (MPI Frankfurt) *Reaction coordinates in the analysis of single-molecule experiments*
14.45-15.00	coffee
15.00-16.00	*Overview of the workshop + discussion plans for the future* (Discussion leader Peter Bolhuis)
16.00	End of the workshop

3 List of participants

Organizers

Bolhuis, Peter
University of Amsterdam, The Netherlands
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University of Vienna, Austria
Hummer, Gerhard
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Last Name	First name	Affiliation
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Mackernan	Donal	University College Dublin, IR
Makarov	Dmitrii	University of Texas at Austin, US
Noe	Frank	FU Berlin, DE
Peters	Baron	UCSB, US
Rosta	Edina	King's College London, UK
Swenson	David	Universiteit van Amsterdam, NL
Tiwary	Pratyush	Columbia University, US
Van erp	Titus	NTNU, NO
Vreede	Jocelyne	University of Amsterdam, NL
Welling	Max	U. of Amsterdam, NL
Woodside	Michael	University of Alberta, CA

Major outcomes

The workshop discussed methods and techniques to sampling and analyzing rare events in complex systems, such as nucleation at phase transitions, drug binding, protein-protein interactions, protein folding, association, and self-assembly to name but a few. In talks and discussions, the workshop participants reviewed current state of the art methods to address such process including path sampling (including Milestoning), metadynamics, Markov state modeling, diffusion maps, dimension reduction, reaction coordinate optimization, machine learning, and unsupervised cluster methods, and explored ways to improve these methods. Particular attention was devoted to the integration of popular MD packages such as Gromacs, NAMD Charmm, Amber, ACEMD, MOIL, LAMMPS with enhanced analysis and advanced sampling tools including Plumed (a package for enhanced sampling and collective variable analysis), pyEmma, and MSMBuilder (packages for Markov sate model analysis).

Notwithstanding the great capabilities of existing methods and software, several unsolved issues were identified. In particular, during the workshop the following topics were discussed:

1. *Extracting order parameters from molecular simulations to construct low dimensional models.* This point is important because there is no straightforward recipe to reduce the dimensions to meaningful variables and progress in this area is urgently needed. Speakers contributing here were Lindorff-Larsen, Camilloni, Tiwary, Keller, Laio, Ceriotti, Rosta, and Huang.
2. *Methods for sampling rare pathways*. Here the goal is to create the molecular trajectory data using advanced sampling algorithms. Speakers contributing here were Peters, Elber, van Erp, Faccioli. Vreede, and Swenson.
3. *Methods to construct reaction coordinates*. This subject was discussed by Peters, Best, Clementi, Krivov, Crommelin and Bolhuis.

4. *Machine learning algorithms*. The prospect of automatic methods to construct RCs from molecular trajectories is very appealing. Various speakers discussed this approach, including Welling, Dellago, Ceriotti, Noé.
5. *Better ways to integrate simulations and experiments.* It is important to connect the proposed computational methods to experimental probes. This was discussed by Woodside, Makarov, Hummer, Vreede, Casasnovas, and Demuynck.

More specifically, during the discussion sessions the following questions were raised and partially answered:

1. What properties should a simulation method predict?
2. What is a reaction coordinate?
3. Is the committor really the perfect reaction coordinate?
4. How to obtain the best low dimension model for the committor?
5. How to connect high dimensional reaction coordinates to physically meaningful variables?
6. How can we use machine learning to find collective variables and reaction coordinates?
7. Is it always possible to devise an optimal reaction coordinate? If so, what is the meaning of this optimal coordinate?
8. When can reaction coordinates, which often constitute the slow variables of a process, be used to coarse-grain the dynamics? When not?
9. How do we get the order parameters for testing?
10. Can we make use of diffusion or sketch maps for reaction coordinate analysis?
11. What if multiple transitions are important? Do we resort to kinetic networks or use multiple reaction coordinates? Should one identify a single (possibly complicated) reaction coordinate, or try to construct a Markov state model (MSM) using many metastable states?
12. When is it possible to reduce a complex problem to diffusion on a one dimensional free energy landscape, and when do we need a network Markov model?
13. How can experiments test reaction coordinate predictions? How do we connect to experiments?
14. What are the predictions that one can make with an optimal reaction coordinate (as opposed to reasonable RC)?
15. To what degree does the computational efficiency of free energy calculations depend on the chosen coordinates, and how can these coordinates by optimized, possibly "on the fly"?
16. Experiments are almost always interpreted in terms of 1D models. What are the limits of this approach? When does it fail? How good is 'good enough'?

To review the current state of the field, identify stumbling blocks, and point out possible future research directions, the workshop participants discussed the possibility to collectively write a review paper co-authored by all of them.

5 Community needs

Several sessions were devoted to identifying what currently slows down progress in the field and to address the specific needs of the scientific community to overcome these problems. During the discussions, it became clear that here is a need for methods and software tools to carry out the following tasks:

1. Sample rare event processes, either by a) configuration or b) trajectory sampling.
2. Construct kinetic networks or Markov state models from trajectory data.
3. Construct and identify order parameters from arbitrary configurations.
4. Dimensionality reduction of large data sets and reaction coordinate analysis.

Several software packages already exist, e.g. MSMBuilder and PyEmma for item and Plumed for items 1a) and 3). Therefore, it makes sense to focus on items 1b) and 4). Indeed, that is the main goal of Work Package 1 of the ECAM Center of Excellence. Developments in this direction will be carried out mainly within The Open Path Sampling (OPS) framework, a Python library to facilitate path sampling simulations (http://openpathsampling.org).

Software modules to be developed in WP1 of ECAM partly based on OPS will address the follow specific issues:

1. Specific modules that perform transition path sampling, TIS, FFS
2. Modules to optimization interface for TIS and FFS
3. Modules for executing the reactive flux algorithm
4. Module for the calculation of the transition state ensemble
5. State definition assessor modules
6. Wrappers for popular MD engines (LAMMPS, Gromacs)
7. Interface to Plumed for use of collective variables
8. Reaction coordinate analysis modules for use with TPS/TIS/FFS
9. Analysis tools to work with path sampling

The development of these modules is the objective of the extended software development workshops organized within Work Package 1 of ECAM.

6 Funding

To make progress in the development of new methods and tools for the sampling and analysis of rare events, 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, an Innovative Training Network focused on rare event sampling and analysis could be used to create a collective research and training effort with strong ties to industry. Other opportunities for funding might be available in the Future and Emerging Technologies (FET) Program of H2020.

7 Developments for society and industry

The societal benefits are twofold. On the fundamental level, the tools will enable new discoveries and developments, for instance in material science and molecular medicine. This will be made possible by the scientific community using the sampling and analysis tools that re being developed.

On an economic level, industry would benefit from software containing efficient and easy to use simulation and analysis tools to extract observables for applications in

- Drug binding: binding affinities, kon/koff rates, effect of mutations on these quantities (this implies mechanistic insight).
- Food/dairy industry: protein aggregation, chocolate crystallization, grain size in ice cream, food preservation, all of which requires knowledge of the freezing mechanism
- Materials science: nucleation, crystallization of polymers, ageing of materials, soft matter, self-assembly of nanomaterais, colloids, defect formation in crystals.

Finally, society will benefit from methods and ultimately software that make drug development cheaper, improve food quality, and help in the development of high-tech materials.

State-of-the-Art Workshop: Electronic Structure

Location: CECAM-UK-HARTREE, Daresbury, United Kingdom
Webpage: https://www.cecam.org/workshop-0-1351.html
Dates: September 12, 2016 to September 14, 2016

1 Overview

The field of quantum mechanical calculations has grown enormously over the last 25 years and has become an indispensable tool in many diverse research areas. One illustration of this importance is that the publication rate of papers based on density functional theory (DFT) now exceeds 30 thousand papers per year and is still growing. This remarkable statistic can too easily mask the problems associated with DFT. The primary aim of this E-CAM State of the Art Workshop was to review the field of electronic structure calculations and identify emerging trends and potential new capabilities entering the field over the next five to ten years. An overview of the most relevant points presented by each speaker can be found on the following pages along with a brief summary of the discussion.

After years where large-scale applications were dominated by DFT, we are now seeing the broader adoption of post-DFT methodologies. These techniques offer higher accuracy than is possible with DFT and can address a wide range of problems where DFT has been shown to struggle. These advanced methods can, in some cases, reach absolute accuracy significantly higher than the apocryphal 'chemical accuracy' of 1 kcal/mol. Going beyond DFT, our description of electronic structure is no longer solely based on the electron density; instead it is increasingly expressed in terms of the electronic wave function, or Green's functions.

Typically, a choice of methods and implementations are available for tackling a new problem and this choice may present an additional hurdle to the use of electronic structure codes in new studies. One encouraging aspect of the meeting was the general consensus that accessibility to non-experts is a vital dimension in future method development; indeed, the success of DFT in addressing this issue is at the heart of its widespread use. Electronic structure theory is increasingly employed in a variety of situations beyond the academic research environment, which brings with it new requirements, including development of efficient means for treating extended time and length scales, an almost indispensable feature for industry.

One of the most important developments of the electronic structure field in the last few years has been the emergence of careful verification of solid-state codes within the so-called D-Codes project [1]. This is long overdue: chemists will correctly point out that verification and validation has been at the heart of their work for decades. The D-Codes project marks only the beginning. To date, the exercise has been limited to density functional theory codes, the majority of which being plane wave pseudopotential codes along with only a few all electron implementations. The success and usefulness of this first effort clearly highlights the importance of providing resources to follow the verification and validation roadmap that Cotennier, and the community he has created, have already mapped out.

[1] K. Lejaeghere et al., Reproducibility in density functional theory calculations of solids, Science **351**, 2016. DOI: 10.1126/science.aad3000

2 Programme of the workshop

Monday, 12 September

14:00—16:00	R*egistration*
16:00—16:45	Mike Payne, University of Cambridge 16:45—
17:30	George Booth, King's College London *Are wavefunction methods a future of computational materials science?*
17:30—18:15	Alessandro de Vita, King's College London *Inference-accelerated molecular dynamics: can we predict first-principles forces?*

Tuesday, 13 September

9:00—9:45	Mark van Shilfgaarde, King's College London *Green's function methods in electronic structure*
9:45—10:30	Leonardo Bernasconi, STFC *Electronic excitations and dynamics in the condensed phase*
10:30—11:00	break
11:00—11:45	Ivan Rungger, National Physical Laboratory *Beyond mean-field correlations for electron transport calculations*
11:45—12:30	Stefaan Cottenier, Ghent University *Verification and validation of DFT methods and codes: what's next?*
12:30—14:00	lunch
14:00—14:45	Julie Staunton, University of Warwick *Density functional theory and slowly varying fluctuations to describe magnetic and alloy phase diagrams*
14:45—15:30	Neil Drummond, Lancaster University *The CASINO quantum Monte Carlo program: current status and future directions*
15:30—16:00	break
16:00—16:45	David Rugg, Rolls-Royce *Electronic structure for improved predictive capability in structural materials - academic dream and/or industrial folly?*
16:45—17:30	Mark Casida, Université Grenoble-Alpes *Precision and accuracy in quantum (photo)chemistry*
17:30—18:15	*discussion of workshop report (1)*

Wednesday, 14 September

9:00—9:45	Nicola Marzari, EPFL *The ADES model for computational materials science: Automation, Data, Environment, and Sharing*
9:45—10:30	James Kermode, University of Warwick *Towards predictive multiscale materials modelling: uncertainty quantification for density functional theory*
10:30—11:00	break
11:00—11:45	Andrea Ferreti, CNR–Istituto Nanoscienze *Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functionals*
11:45—12:30	*discussion of workshop report (2)*

3 List of participants

Organizers

Payne, Mike
University of Cambridge, United Kingdom
Petit, Leon
Daresbury Laboratory, United Kingdom

Last name	First name	Affiliation
Bernasconi	Leonardo	STFC RAL, UK
Booth	George	King's College London, UK
Casida	Mark	Université Grenoble-Alpes, FR
Castagna	Jony	STFC Daresbury Laboratory, UK
Cottenier	Stefaan	Ghent University, BE
De Vita	Alessandro	King's College London, UK
Drummond	Neil	University of Lancaster, UK
Engel	Edgar	University of Cambridge, UK
Fabris	Stefano	SISSA, Trieste, IT
Ferretti	Andrea	CNR-Institute of Nanoscience IT
Hasnip	Phil	University of York, United Kingdom
Jackson	Jerome	STFC Daresbury Laboratory, UK
Kermode	James	University of Warwick, UK
Lueders	Martin	STFC Daresbury Laboratory, UK
Marzari	Nicola	EPFL, CH
Migliorato	Max	University of Manchester, UK
Rugg,	David	Rolls-Royce PLC, UK
Rungger	Ivan	National Physical Laboratory, UK
Searle	Barry	STFC Daresbury Laboratory, UK
Staunton	Julie	University of Warwick, UK
Tomic	Stanko	University of Salford, UK
van Schilfgaarde	Mark	King's College London, UK
Weber	Cedric	King’s College London, UK

4 Major outcomes

The organisers are particularly grateful for the speakers for carefully addressing their brief for the meeting by giving talks covering the broader issues related to their research areas and are equally grateful to all the participants for their contributions to the discussions.

Mike Payne introduced the meeting and provided an introduction to E-CAM, which is the recently launched Horizon 2020 Centre of Excellence (CoE) associated with the CECAM network. He then reiterated the aims of the meeting namely to review current status and emerging trends in the electronic structure field. In the following we note only the most important and relevant points made by each speaker.

George Booth provided a review of progress in wave function based methods, both the classic explicitly correlated wave function methods of theoretical chemistry, such as Configuration Interaction (CI), and the rapidly developing Full Configuration Interaction Quantum Monte Carlo (FCIQMC) method. The approach has to confront the exponential scaling of the CI wave function but succeeds because the majority of the weight of this wave function is in a relatively small number of determinants. This method has been shown to be accurate well beyond the classical "required level" of theoretical chemistry of 1 kcal/mol.

Alessandro de Vita talked about methods to intelligently extract interatomic force data from ab initio calculations. Machine learning techniques were presented in the context of molecular dynamics simulations of crack propagation, where force field parameters were obtained on-the-fly from DFT calculations, but only when geometries are encountered that had not previously been calculated, with a significant reduction in computational cost. Examples were provided where this method fails, but equally other examples were provided where forces were accurately predicted - reducing the number MD steps where ab initio calculations were required by an order of magnitude.

Mark van Schilfgaarde described Green's function based approaches to electronic structure, specifically the quasiparticle self-consistent GW method (QSGW). GW originates in many-body theory and gives an accurate description of optical properties, considerably superior to DFT. Traditionally the GW method has been applied perturbatively on top of DFT. QSGW is a self-consistent, non- perturbative scheme, which shows considerable improvements over earlier methods. Possibilities of combining QSGW with methods for treating strong correlation (DMFT), which is missing from the theory, were discussed.

Leonardo Bernasconi discussed calculations of excited states – for a long time a taboo subject for DFT which is strictly a ground state theory. However, with the introduction of time dependent DFT (TD-DFT) and time dependent Hartree Fock (TD-HF) there are now methods which can work very well for a range of excited state problems. In particular, TD-B3LYP, which mixes DFT and HF, gives good results both for Wannier-Mott excitons and Frenkel excitons but does not work well for charge transfer excitations. The next challenge is excited state dynamics where state crossings present a major challenge to theory, this is important for instance in describing fluorophores in dye-sensitised solar cells.

Ivan Rungger talked about realistic calculations of electron-transport beyond the standard Landauer-Buttiker model thus including beyond mean-field correlations. This was based on a multiscale approach: standard electronic structure methods, such as the Smeagol TD-DFT transport code, were combined with the Anderson impurity model, which describes correlation. There are significant technical challenges with this approach but it will be an important tool to model electrical spin manipulation in electroactive molecules.

Stefaan Cottenier provided an overview of the D-Codes project – covering both the scientific and sociological successes of the work. He correctly stated that the physicists had been left a long way behind the theoretical chemists in the area of verification and validation (V&V) and that we had only just started to put this right. The work to date has, in fact, only addressed the issue of verification of codes – proving that they yield consistent result. The question of validation -- is the answer correct? -- has yet to be addressed. A roadmap for future V&V, which now just requires a moderate investment of resources to pursue, was presented.

Julie Staunton presented a theory of magnetic materials based on a statistical mechanics treatment of spin fluctuations. Building upon the local moment picture of magnetism, a formal theory of the free energy, as a function of temperature and field, is provided by the disordered local moment (DLM) theory. The applications of this theory to metamagnetic FeRh and to spin- fluctuations in MnO were presented as well as discussion of rare-earth intermetallics and the a-g martensitic transformation in steel. Developments of the method, involving the non-local coherent potential approximation, were exposed.

Neil Drummond convinced us of the accessibility of Quantum Monte Carlo (QMC) calculations by setting up and running an entire QMC calculation during his talk! Various technical developments such as optimised Jastrow factors and backflow corrections have enhanced the method and can be packaged with relative ease. Even though a great deal of attention has been paid in ensuring the use of QMC codes is easy and intuitive, making it possible for non-experts to use multideterminant trial wavefunctions remains challenging.

David Rugg, as Senior Research Fellow in charge of materials research at Rolls Royce, provided an industrial perspective. The role and importance of university-based collaborations in their research programme was pointed out in a wide range of different materials science areas. The complexity and potential cost implications of the materials challenges facing a company like Rolls Royce are both daunting and humbling. It was pointed out that understanding and/or rationalising materials behaviour is what they really require – not only parameter free, atomic scale simulation of an event.

Mark Casida provided a historical perspective of the rise of theoretical chemistry from its breakthrough era in the 1970s and the development of Hartree-Fock and post Hartree-Fock methods. In this context, he talked generally about accuracy and precision in quantum chemistry and more specifically about TD- DFT for photochemical applications. He also discussed technical issues, such as scaling, and emerging methods such as “dressed TD-DFT”, where double excitations are included in the theory, and over what timescale adoption of such methods can be expected.

Nicola Mazari described technical work to address the issue of predictive accuracy in DFT and realistic complexity. He discussed the rapidly growing field of materials informatics by describing the development and application of the AiiDA tool, which aims to address the issues of automation, provenance (of calculations), reproducibility of calculations as well as providing the ability to generate workflows and protocols for complex derived properties and then use these in high-throughput applications. A case study was provided by the finding of new 2-dimensional materials out of the set of all known layered 3-dimensional systems.

James Kermode described the 'Python-isation' of Fortran codes, which can be semi-automated and thus applied to any electronic structure code. Controlling calculations using python brings many advantages of modularity and interoperability and allows a much more flexible use of DFT technology. He described his work on uncertainty propagation in electronic structure methods based on Baysian analysis. By examining the effect of errors in the exchange functional used in DFT, a measure of the absolute error in calculated properties could be obtained.

Andrea Ferreti discussed the use of Koopman's compliant functionals as a method of bridging between DFT and Many Body Perturbation Theory (MBPT). The Koopman's compliant approach re-introduces the derivative discontinuity present in the exact, but unknown, Kohn-Sham functional which is lacking in the usual approximations. This leads to the concept of orbital dependent density functionals, which do not have unitary invariance, but which allow accurate prediction of spectroscopic properties.

5 Community Needs

In the first discussion session, the organisers asked those not giving presentations, for their thoughts about the status and prospects for the field of electronic structure and then the discussion was open to all participants. The following summarizes the resulting debate:

Density functional theory is now a mature technology that is increasingly finding application in industrial settings. Industrial use demands accuracy and precision, which are now being addressed by validation and verification exercises such as the D-Codes project. A recurring theme of the meeting was the importance of having well specified error bars, and clear definitions of the applicability of the different methods. These specifications are prerequisites for use of electronic structure codes outside of the academic environment and by users who are not necessarily familiar with the underlying theoretical basis. Significant progress towards these goals is being made in the software engineering of different electronic structure packages and this has been shown to provide not only a robust framework for conducting DFT-level calculations but also makes advanced methods as as approachable as possible. While these developments suggest a "black-box" mentality, the importance of physical insight was expressed, particularly in an industrial setting where modelling is often used to support interpretation of experimental findings. While new methods for very high accuracy prediction of ground-state and optical properties were discussed, it is clear that dynamics, multiscale modelling and finite temperature remain challenging topics, each being addressed by different efforts. To expand the applicability of existing DFT and post-DFT theories, advanced techniques from computer science are already being applied and can be expected to play an ever increasing role, these include not only the use of massively parallel, hybrid CPU/GPU hardware but also efficient strategies based on machine learning.

6 Funding and resources

Members of our community are under increasing pressure from funding agencies to do industrially relevant research. This brings with it the requirement for industrial standards of quality control, namely error quantification. In this context, consistent investment is required in order to dedicate development resources to verification and validation. At present, there is widespread uncertainty as to how such work should be financed, because, unlike feature addition, this work is, with notable exceptions such as the UK's CCP projects, not normally funded through research g r a n t s .

7 Developments for society and industry?

Developments in electronic structure theory have wide reaching technological implications. The workshop featured mostly, but not exclusively, physicists and methods from solid state theory; developments in these particular areas lead to societal benefits by improving the understanding of materials, and their properties, and in the discovery of new materials for applications. Specific classes of materials directly addressed at the workshop include, but are not limited to, photovoltaic materials, catalysts, fracture resistant alloys for aerospace applications and magnetocalorics.

Enabling the use of current state-of-the-art techniques of electronic structure theory in industry promises to allow many more problems to be addressed than can be examined by academic research groups alone and means that research efforts are focused on problems of direct commercial relevance. This will allow cheaper and more effective product development in a wide range of industries. Detailed reviews of the economic impact of electronic structure and molecular modelling have recently been provided [2,3].

1. https://gerhardgoldbeck.files.wordpress.com/2014/01/the-economic-impact-of-modelling.pdf
2. https://gerhardgoldbeck.files.wordpress.com/2014/02/psik-industry-interactions-report1.pdf

State-of-the-Art Workshop: Different Routes to Quantum Molecular Dynamics

Location: CECAM-HQ-EPFL, Lausanne, Switzerland
Webpage: https://www.cecam.org/workshop-0-1319.html
Dates: June 6, 2016 to June 10, 2016

1 Overview

Quantum molecular dynamics is a rich and rapidly growing field, involving different communities in physics, chemistry, and applied mathematics. Applications range from controlling photochemistry, to predicting the effect of hydrogen diffusion in materials, to quantum computing. The key challenge is that simulating the exact quantum dynamics of multi-component systems of electrons and nuclei is a task currently out of reach, except for the simplest molecules with a few degrees of freedom. Approximations must then be developed to surpass the exponential scaling of computational (mainly memory) power needed to solve the time-dependent Schrödinger equation, describe more realistic molecular systems, and take simulations closer to experiments by improving the accuracy of available methods and developing new ones.

Current approaches can be roughly divided in the following sets: exact quantum calculations (applicable to low dimensional systems), wave-function based methods (where the wave-functions are expanded in convenient truncated basis, variationally optimized during the evolution), trajectory-based and trajectory– guided methods (in which the properties of the quantum system are mimicked via averages over ensembles of generalized, interfering, classical trajectories), semi-classical dynamics (based on second order approximations of the path integral representation of the quantum propagator), and path integral methods (employing exact methods to sample the quantum thermal density to tackle the time-domain). The main challenge for all these schemes is to maintain the balance between efficiency and accuracy, i.e. to keep the computational costs manageable while preserving the ability to predict and interpret experiments.

The available approaches span a wide range of formal frameworks and involve different communities. However, opportunities to establish common goals, unifying theoretical grounds, and solid and shared benchmarks are missing. Comparing shortcomings and advantages, understanding the restrictions of each approach, and defining benchmarks to assess merits and limitations of the different approaches to identify the different areas of applicability were then the main goals of this workshop. In addition, the issue of transferability of the methods to the industrial community was specifically addressed.

2 Programme of the workshop

Monday, 6 June

Quantum dynamics (Chaired by Ali bedi and Guillermo Albareda)

09:00-10:00 Tucker Carrington
Computing (ro-)vibrational spectra with the Lanczos algorithm

10:00-11:00 Uwe Manthe
Wavepacket dynamics and the multi-configurational time-dependent Hartree approach

11:00-11:30 Coffee Break

11:30-12:30 Discussion

12:30-14:00 Lunch

14:00-15:00 Review of critical issues & identification of work groups

15:00-15:25 Guillermo Albareda
Towards ab-initio Molecular Dynamics without Born-Oppenheimer Potential-Energy Surfaces

15:25-15:50 Neepa Maitra
Non-Adiabatic Dynamics in Strong Fields: Enhanced Ionization

15:50-16:15 Edit Matyus
Pre-Born--Oppenheimer Molecular Structure Theory

16:15-16:40 Aurelien Patoz
Geometric integrators of arbitrary order of accuracy for molecular quantum dynamics in electromagnetic fields

16:40-17:05 Martin Mosquera
Non-standard Approach to Linear-response TDDFT and the Calculation of Excited-state Spectra

17:05-17:20 Coffee Break

17:20-18:00 Round Table Discussion: Future Directions

Tuesday, 7 June

Trajectory-based and trajectory-guided methods (Chaired by Philipp Marquetand, Basile Curchod, and Ivano Tavernelli)

09:00-10:00 Joe Subotnik
Surface hopping in solution and at metal surfaces: Nonadiabatic processes all around us

10:00-11:00 Dmitry Shalashilin
Coherent States and their use for Multidimensional Quantum Dynamics

11:00-11:30 Coffee Break

11:30-12:30 Discussion

12:30-14:00 Lunch

14:00-15:00 Review of critical issues & identification of work groups

15:00-15:25 Antoine Carof
Electron Transfer in Organic and Biological Materials

15:25-15:50 Benoit Mignolet
In Silico Photochemistry of the Thioformaldehyde S-oxide Sulfine. Beyond the Initial Ultrafast Decay

15:50-16:15 Clemens Rauer
GAIMS-Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes
16:15-16:40 James Snyder
GPU-accelerated multireference electronic structure calculations enabling large-scale nonadiabatic dynamics simulations
16:40-17:05 Seung Kyu Min
Coupled-Trajectory Approach of Mixed Quantum-Classical Dynamics Based on Exact Factorization
17:05-17:20 Coffee Break
17:20-18:00 Round Table Discussion: Future Directions

Wednesday, 8 June

Semiclassical methods (Chaired by Michelle Ceotto and Jiri Vanicek)

09:00-10:00 Kenneth Kay
Semiclassical Initial Value Representation Methods: Some Future Directions
10:00-11:00 Eli Pollak
Ab-initio semiclassical dynamics
11:00-11:30 Coffee Break
11:30-12:30 Discussion
12:30-14:00 Lunch
14:00-15:00 Review of critical issues & identification of work groups
15:00-15:25 Riccardo Conte
Simulating Vibrational Spectra of Variously-sized Molecules via Multiple Coherent Time Averaging Semiclassical Initial Value Representation
15:25-15:50 Giovanni Di Liberto
Accurate and Efficient Pre-exponential Factor Approximations for the Semiclassical Initial Value Representation Ppropagator
15:50-16:15 Chiara Donatella Aieta
A quantum approximate method for the calculation of thermal reaction rate constants
16:15-16:40 Fabio Gabas
An Efficient Computational Approach for the Calculation of the Vibrational Density of States
16:40-17:00 Coffee Break
17:00-17:40 Round Table Discussion: Future Directions
19:30-22:00 Dinner

Thursday, 9 June

Path integral molecular dynamics (Chaired by Giovanni Ciccotti)

09:00-10:00 David Manolopoulos Ring polymer molecular dynamics
10:00-11:00 Stuart Althorpe
Quantum statistics + classical dynamics: what is it?
11:00-11:30 Coffee Break
11:30-12:30 Discussion
12:30-14:00 Lunch
14:00-15:00 Review of critical issues & identification of work groups
15:00-15:25 Timothy Hele

	Derivation of the exact non-adiabatic quantum propagator in the classical-like mapping variable representation
15:25-15:50	Michael Willatt *Approximate Quantum Time-correlation Functions from Matsubara Dynamics*
15:50-16:15	Romain Dupuis *Path Integral Methods for Isotopic Fractionation of Li and Proton Diffusion in Hydroxides*
16:15-16:40	Aaron Kelly *Accurate Nonadiabatic Dynamics on the Cheap: Harnessing Quantum-Classical Theory with Generalized Quantum Master Equations*
16:40-17:00	Coffee Break
17:00-17:40	Round Table Discussion: Future Directions

Friday, 10June

Discussions on standardized outputs, benchmarks and industrial engagement (Chaired by Dominic Tildesley)

09:00-11:00	Discussion
11:00-11:30	Coffee Break

3 List of participants

Organizers

Abedi , Ali
University of Basque Country, Spain
Albareda, Guillermo
Universitat de Barcelona, Spain
Ceotto, Michele
Università degli Studi di Milano, Italy
Curchod, Basile
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Last Name	First Name	Affiliation
Gomez Rodriguez	Sandra	University of Vienna, AT
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Manthe	Uwe	University of Bielefeld, DE
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Aieta	Chiara Donatella	University of Milan, IT
Ciccotti	Giovanni	University of Rome, La Sapienza, IT
Conte	Riccardo	University of Milan, IT
Di Liberto	Riccardo	University of Milan, IT
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Mosquera	Martin	Northwestern University, US
Parrish	Robert	Stanford University, US
Sanchez	David	Stanford University, US
Seress	Laszlo	Stanford University, US
Snyder	James	Stanford University, US
Subotnik	Joe	University of Pennsylvania, US
Varga	Kalman	Vanderbilt University, US

4 Major outcomes

Given the spirit of the workshop, focused on a survey of the state of the art, the main outcomes of the discussions aim at setting the stage for promoting further development and creating the best research environment for them. In fact, it was recognized that quantum dynamics is transitioning from the pioneering to a more established phase of development. The consensus was that the next five years will lead to a consolidation of the different methods developed over the years, eventually producing new physical and chemical insights in the reaction dynamics of polyatomic molecules and condensed phase systems.

The following points were singled out of the discussion:

1. Given the cost of approximate quantum dynamics, its application to realistic systems usually requires accurate potentials at lower cost than full first-principles electronic structure calculations. In this context, the workshop highlighted a clear recent development extending the range of exact quantum dynamics simulation: the availability of high-dimensional high-quality potential energy surfaces (mainly for ground state reactions). Key to this achievement is the development of new fitting and interpolating techniques, in particular those based on neural networks. With these potential energy surfaces, gas-phase quantum dynamics simulations of relatively complex reactions were carried out ($CH4 + H^+$, for example), highlighting new physics and chemistry for the reaction of polyatomic molecules. Furthermore, alternative approaches were discussed, where electronic structure calculations are avoided by defining a fully time-dependent framework for electrons and nuclei

2. The importance of communication with the electronic structure community was highlighted. In fact, while until recently the development of electronic structure techniques was focused on the simulation of large systems, it is expected that in the next years a lot of effort will be devoted to accelerate the existing algorithms, with speed-ups of several orders of magnitude. Ab initio quantum dynamics and its applications to molecular systems will benefit greatly from this tremendous acceleration.

3. The recent development of fast Ring Polymer Path Integral techniques allows for the inclusion of nuclear quantum effects (zero-point energy or tunneling effects) in the computation of molecular reactions and condensed phase simulations, and, in some cases, at the cost of standard ab initio molecular dynamics. Semi-classical molecular dynamics is also now available on-the-fly and it has been mainly employed for spectroscopic calculations of gas phase molecules, up to hundred degrees of freedom.

4. The recent inclusion of spin-orbit coupling in more approximate methods makes it now possible to simulate complete photochemical relaxation pathways with techniques such as surface hopping or ab initio multiple spawning.

5. New areas of application for quantum dynamics were identified. In particular, Ring-polymer molecular dynamics (RPMD) at the cost of classical molecular dynamics, presented in this workshop, paves the way for the inclusion of quantum effects in condensed phase reactions and in biological processes.

Other significant applications include: reaction mechanisms of polyatomic molecules, tunneling in proteins, electrochemical processes with surface hopping, photochemistry with both surface hopping and ab initio multiple spawning, hydrogen diffusion on surfaces and in the bulk in connection to battery technology and materials design via linearized approximations of the dynamics.

To fully exploit the recent progress in quantum dynamics, the discussion stressed the need to continue practical testing and theoretical analysis of the methods. This is particularly important since it was anticipated that in the near future the quantum molecular dynamics community will split into two groups: one interested in method development, and another more focusing on applications. This change is similar to the splitting that occurred in the electronic structure theory community. It will lead to the formation of a community of "computational chemistry for quantum dynamics" and it is crucial that methods are sufficiently reliable to be used as a "black box" by academic community oriented towards applications. This is also key when discussing transfer of methods and software in the field to industrial partners.

During the discussions, the community highlighted different challenges for the field. Four main questions were identified:

1. How can we reach statistical limits with the current quantum dynamics methods?
2. How can we treat electrochemical problems in the context of non-adiabatic quantum dynamics?
3. How can we deal with gas-surface reactions?

5 Community needs

The community did not express any particular need in terms of computational infrastructure. This is mostly due to the "exponential scaling" law of quantum dynamics, which requires more brainwork than brute-force computational power to be circumvented. In this relatively young area of research then, the development of new methods and refinement of existing ones is still the major driving force. It was hence a common impression among the participants of the workshop that the major need in the community is man power.

Procuring sufficient human resources is all the more important given that the part of the community focused on development of new techniques and algorithms is rather small, and tends to reduce over time due to the decreasing funding for fundamental research.

However, the discussion also 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, currently mostly in house codes, towards the creation of packages, again in analogy to the history in electronic structure. In this sense, the youth of the field and the existence of the new E- INFRA5 CoEs, and in particular of E-CAM, offers a unique opportunity to create a more organic environment for software development, documentation, and maintenance. Identifying the optimal hardware architecture (GPU vs CPU, for example) for quantum dynamics is also an interesting, and at the moment largely unexplored question that will benefit from interactions with E-CAM.

The community is eager to promote opportunities for interaction and exchange that bring together a wide spectrum of researchers active in quantum dynamics. These opportunities are at the moment extremely rare but 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, as the community is not yet large enough for considering the organization of a big conference, most likely scientifically sterile due to the lack of intensive discussions.

6 Funding and Resources

In terms of funding, discussions during the workshop indicated that the field of quantum dynamics would tend to be more and more application-oriented, as fundamental research tends to be harder to get funded. Horizon 2020 is clearly a potential funding channel, and recent developments, which pave the way to biological 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 quantum dynamics methods.

7 Developments for society and industry

As technology reaches smaller time and length scales, the quantum properties of matter gains relevance for society and industry. Furthermore, the ubiquitous presence of hydrogen in materials (e.g. impurities in steal) and devices for clean energy (proton based batteries) makes these simulations relevant also in macroscopic devices and at ambient conditions. Finally, the recent interest in the potential revolution of quantum computing – both in terms of simulating devices that could be used as q-bits, and developing quantum algorithms for application in areas ranging from chemistry to cryptography – has opened a whole new set of opportunities for interactions with hardware developers

Quantum dynamical simulations are then increasingly important in many industrial sectors, including hardware design (e.g. coherence and interference effects for quantum control or design of q-bits), pharmaceutics (tunneling in enzymatic reactions), energy production or storage (when light is used to induce quantum physical or chemical transformations).

Collaborations in these fields are already active. In the context of E-CAM, new simulation methods and algorithms for quantum computing are being developed in collaboration with IBM. Similar collaborations involve some of the participants to the workshop. Surface hopping and multiple spawning are methods of choice to simulate the excited-state dynamics of molecular systems. 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 (collaborative projects, for example with, Dyesol, Greatcell) or organic light emitting diodes (collaborative projects, for example with, BASF, Novaled). Excited state, and in particular non-adiabatic, dynamics is potentially interesting also for pharmaceutical companies, for example in connection to preventing photo-damage (leading to skin cancer).

Applications of quantum dynamics techniques are also central to reveal reaction mechanisms of atmospheric molecules. Models for these reactions currently employ experimental data, but usually require to complement insufficient data with very simplified models, often not accurate enough. Using quantum dynamics to circumvent the problem of missing experimental data would lead to more accurate atmospheric composition models, with a direct societal impact related to the study of chemical reactions involving small molecules on current climate changes.

It was stressed that, while it is extremely important to evaluate each potential collaboration individually to avoid creating expectations that cannot be met, the field of quantum dynamics is now approaching sufficient maturity to pursue more actively industrial engagement. To promote this, it will be important to create communication channels between academia and industry to disseminate the potential applications of the field. It was also pointed out, however, that the technical difficulties and the earlier stage of development of quantum molecular dynamics compared to classical molecular dynamics or electronic structure calculations, currently prevent “blind” knowledge transfer to industry and that the best strategy at the moment seems to encourage one-to-one collaborations with experts.

Extended software development workshop: trajectory sampling

Location: CECAM-AT, Traunkirchen, Austria
Webpage: https://www.cecam.org/workshop-0-1356.html
Dates: November 16, 2016 to November 25, 2016

Organizers

Dellago, Christoph
University of Vienna, Austria
Kahl, Gerhard
Vienna University of Technology, Austria

1 State of the art

During the past decades, classical molecular dynamics (MD) simulations have become an indispensable tool in many branches of science: in particular, in molecular biology, chemistry, physics, and materials science MD simulations are nowadays able to provide insights into molecular mechanisms with a spatial and temporal resolution that is not accessible to experimental probes and/or to *ab initio* computer simulations. Due to this capacity, classical MD simulations have also become a standard tool in industrial research, as for instance in the fields of materials design, biomolecular engineering, or drug design. The broad application of these simulation techniques is supported by the availability of related software packages, which rely on efficient and accurate implementations and which are regularly maintained, receiving on a regular basis methodological updates: LAMMPS, ESPRESSO, GROMACS and OPENMM are a few of these products that are available. Despite this progress, an even broader application of MD simulation is limited by the relatively short (real) times scales accessible to these techniques, a problem which becomes in particular apparent if the project at hand is characterized by substantially disparate time scales: thus rare, but important barrier crossing events, as they occur in protein folding, chemical reactions in solution or nucleation phenomena are still out of reach for standard MD simulations.
During the past two decades, considerable progress has been made in developing methods that allow detailed and reliable investigations of the above-mentioned processes. Only in recent time, groups of researchers have started to develop packages in the field of trajectory-based rare event simulations, however these products have not gained, so far, the broad distribution of standard MD program packages. The E-CAM state of the art workshop “Reaction Coordinates from Molecular Trajectories” (29 August – 2 September 2016, Leiden), helped to identify some specific software needs of the scientific community to overcome these problems. A scientific report from this workshop can be found here.

The central goal of Work Package 1 (WP1) of E-CAM is to develop robust and efficient code for path based simulations for the simulation of rare event processes. This development is carried out within the framework of the OpenPathSampling package, which provides easy-to-use tools for performing transition path sampling simulations and analyzing the results, for instance in terms of committor distributions or collective variables. The underlying dynamics are generated using external MD engines such that it can be used in conjunction with available MD codes. Currently, support for OpenMM is available and development to support other MD engines, such as LAMMPS and Gromacs is underway.

2 Training provided

The first extended software development workshop of WP1 took place in Traunkirchen (Austria), from November 16 to 25, 2016. Among the 18 participants there were ten experienced, senior researchers and eight junior participants, recruited from some of the research groups of the senior researchers and from other groups interested using path sampling approaches in their research. The program contained, in particular during the first days, talks given by the senior researchers, providing an (i) overall view of the problem and (ii) focusing on the particular problems to be dealt with during the implementation phase of the workshop: overview was given on theories that provide the basis of how to simulate rare events in complex molecular systems and an introduction was made to the OpenPathSampling package. Complementary information was given on quantum nuclear effects in rare events and an industrial partner (from Biki Technologies) reported about the relevance of these simulation techniques in technological applications. These scientific presentations were complemented by more technical talks, dedicated to the GIT system, the software development guidelines developed for E-CAM, and tools for performance analysis of the codes.

3 Software development projects

The following software modules were defined at the beginning of the workshop:

I. Basic shooting and shifting algorithm
II. Aimless shooting algorithm
III. Reactive flux algorithm
IV. Calculation of the transition state ensemble
V. Maximum likelihood optimization of the reaction coordinate
VI. Optimal placement of interfaces for transition interface sampling

The junior participants chose one of the problems based on their own research interests and then worked on them individually or in teams of two. Close to 60 % of the workshop was then dedicated to the software development. Guided by the program manager (Jony Castagna) and two senior researchers (David Swenson and Donal MacKernan), the young researchers worked very efficiently: according the feed-back that was collected during the workshop on a regular basis, a progress in the code development was achieved that was beyond expectations.

Currently, the modules are finalized, adapted to the software development rules of E-CAM and tested. A round-up workshop will be held in Vienna (April 4 and 5, 2017), where these packages will be finalized such that they can be uploaded into the E-CAM repository for Classical MD. These modules will also be part of Deliverable 1.3 of WP1.

Extended software development workshop: electronic structure library coding - solvers

Location: CECAM-ES
Webpage: https://www.cecam.org/workshop-0-1274.html
Dates: June 6, 2016 to June 17, 2016

Organizers

Artacho, Emilio
CIC NanoGUNE Consolider, Donostia-San Sebastián, Spain, Spain
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Corsetti, Fabiano
Imperial College London, United Kingdom
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University of Cantabria, Spain

1 State of the art

Electronic structure software and methods development still work predominantly within the historical paradigm of separate, complete and self-contained packages, typically depending only on a few compilers and basic libraries. This approach has undoubtedly been successful in producing the rich variety of electronic structure codes available today. However, it has led to a lot of replicated development, and makes it hard to introduce common data standards. It has also made it increasingly difficult for researchers to contribute new ideas without becoming deeply involved with the development of one of the pre-existing packages.

At the moment, it is widely recognized in the community that these are important, yet unsolved, problems. There are however a number of interesting new European initiatives aiming to help communication between codes, in conjunction with big data research (e.g., NOMAD, AiiDA, MARVEL) and close integration with HPC (e.g., E-CAM, MaX). It is also important to note that there are already a few examples of communal software libraries specific to electronic structure which have found some success in bridging between different codes, e.g., Wannier90 for maximally-localized Wannier functions, and Libxc for exchange and correlation functionals.

The aim of the Electronic Structure Library (ESL, esl.cecam.org) initiative is to develop the research infrastructure underpinning a huge amount of scientific research, spanning materials physics, physical chemistry and biology, nanotechnology and nanomedicine, Earth science, and more. Indeed, the importance of atomistic modelling from first principles electronic structure is widely recognized, and its applications outside of academia are many.

In particular, the opportunity to collaborate with researchers in industry involved in such modelling projects would allow us to develop software that could drive innovation and growth.

Our goal is to create a common repository of high-quality software and data standards in the field of electronic structure simulation, which will facilitate reuse of code, interoperability between different code bases, and development of new methodologies. This ESL initiative was born two years ago from a CECAM extended software development workshop; the current workshop is the third annual one, plus a January 2016 workshop organized in collaboration with the NOMAD project.

2 Training provided

The theme of this year's workshop was "solvers", as our objective was to develop three libraries focusing on eigensolvers, Poisson solvers, and atomic solvers.

The first day of the workshop was dedicated to talks and discussion. These revolved around three topics: the integration of ESL within the larger E-CAM project, technical issues relating to the quality and usability of software libraries produced with the ESL, and the details of the specific libraries which we planned to work on during the workshop. We had representatives present both from E-CAM and commercial atomistic simulation ventures (QuantumWise, SIMUNE).

The rest of the workshop was dedicated to coding and related work (software documentation, ESL wiki maintenance, code repositories) in small teams of 2-4 people.

3 Software development projects

The major outcomes are summarized below:

Integration of ESL and E-CAM: creation of the E-CAM GitLab code repository; migration of ESL projects to GitLab; creation of online collaboration tools for ESL projects on the E-CAM server; initial work on adopting the EasyBuild installation framework for ESL modules.

Eigensolver library: development work on the ELSI project (Electronic Structure Infrastructure), including the ELPA, libOMM and PEXSI eigensolvers; initial work on including also the CheSS solver from BigDFT; complete restructuring of the ELSI interface to increase flexibility and portability by making use of the MatrixSwitch and FUTILE libraries; creation of a new subproject for automatic generation of realistic test Hamiltonians.

Poisson library: creation of the PoKE project (Poisson Kernel for Electrons), based partly on a previous effort to create a Poisson solver library within BigDFT; discussions on the interface; implementation of periodic and free boundary conditions; initial testing.

Atomic library: creation of the SQARE project (Solvers for Quantum Atomic Radial Equations); setup of coding framework; discussions on the interface and code layout; implementation of ODE solvers.

ESL wiki: restructuring and clean up, addition of data standard documentation (UPF).

There has already been some noticeable improvement in the computational infrastructure for the ESL project, partly as a result of our activities during this workshop and our ongoing collaboration with E-CAM. Currently, CECAM is hosting the ESL wiki on one of its servers, while the software has been partly migrated to a new GitLab repository hosted by E-CAM. Some of thesesoftware modules are part of D2.1 of WP2.

Planned future developments, which we hope to be able to implement in coming years, include the regulated mirroring of externally-developed software (with the permission and collaboration of the original authors) and integration of the ESL libraries into package management systems for both personal workstations and HPC centres.

It would be important for the future strategy of the ESL to provide dedicated machines not just for storing code but also performing nightly builds and automatic testing. This would help the ESL maintainers to ensure consistent high quality amongst all contributions. Similarly, quick access to HPC facilities would allow for in-house development and testing of massively parallel code.

Finally, providing training in collaboration with the ESL could be useful for attracting new researchers and giving them the tools to contribute to the projects being developed. Training areas of interest would be software engineering, modern coding practices, data analysis tools, and development for HPC. On top of this, ESL maintainers could benefit from meeting HPC companies and learning about developments in hardware.

Extended software development workshop: Wannier90

Location: San Sebastian, Spain
Webpage: https://www.cecam.org/workshop-0-1357.html
Dates: September 12, 2016 to September 16, 2016

Organizers

Mostofi, Arash A.
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1 State of the art

Wannier90 is a code for generating maximally-localized Wannier functions and using them to compute with high efficiency and accuracy a host of advanced materials properties. Wannier90 is a paradigmatic example of an interoperable software tool, achieved by ensuring that the quantities that need to be input into it are entirely independent of the underlying electronic structure code from which they are obtained.

All of the major electronic structure codes in the world have an interface to Wannier90, including Quantum-Espresso, AbInit, VASP, Siesta, Wein2k and Fleur. In this way, the developments that are released in Wannier90 are immediately available to a very large fraction of the electronic structure research community and the impact of this has been evident in the large number of publications resulting from the use of Wannier90 (around 900), many of them in high profile journals such as Nature on topics ranging from the strongly correlated physics of topological insulators and iron-based pnictide superconductors, to the chemistry and bonding of ionic liquids.

The aim of this workshop is to share recent developments related to the generation and use of maximally-localised Wannier functions and to either implement these developments in, or interface them to, the Wannier90 code. It is also an opportunity to improve and update existing interfaces to other codes and write new ones. The format was deliberately open, with the majority of the time allocated for coding and discussion.

This workshop was an activity of the E-CAM European Centre of Excellence (https://www.e-cam2020.eu) that supports Software, Training and Discussion in Simulation and Modeling, and MARVEL, the Swiss National Centre on Computational Design and Discover of Novel Materials (http://nccr-marvel.ch).

2 Training provided

This workshop was instrumental in catalysing the transition of Wannier90 from a code developed by a small handful of developers to a community code with a much wider developer base. This has been achieved in two principal ways through the workshop: (i) situating the source code and associated development efforts on a public GitHub repository (wannier- developers/wannier90); and (ii) building a community of connected Wannier90 developers by facilitating new and hopefully lasting personal interactions between individuals at the workshop. There were 25 attendees at the workshop.

The response to this workshop from the community was highly positive. Aside from the Wannier90 Developers Group, there were 20 attendees at the Workshop, actively participating and contributing to discussions and the code. An anonymous feedback form that they were asked to complete at the end of the workshop demonstrated its success. Of the 14 respondents: 93% agreed or strongly agreed that the workshop was useful; 96% said that it should be repeated either once a year or every other year; and 100% agreed or strongly agreed that it was a good occasion to meet with other researchers and that it was a good opportunity to learn something new. Further to the feedback of the participants of the workshop, our intention is to hold a community Wannier90 software development workshop once every two years, with the next one in the second half of 2018.

3 Software development projects

The major technical outcomes were as follows:

Migration of the Wannier90 repository to GitHub: the Wannier90 revision control repository was previously hosted on a server hosted by the Theory of Condensed Matter group in Cambridge. This was migrated to GitHub in order to make it much easier for the community to contribute developments. The GitHub repository can be found at https://github.com/wannier-developers/wannier90.

A Guide for Contributors: now that the code has a much wider developer base, a formal coding style guide and guide for developers is needed.

An interface to the Yambo code: Wwrite an interface between Yambo and Wannier90, taking into account the possibility that eigenvalues need to be resorted if GW corrections swap them.

Update to the interface to Quantum-Espresso (non-collinear spin + USPPs): add non-collinear support with ultrasoft pseudopotentials to the QE interface (pw2wannier90).

AiiDA plugin for Wannier90: development of a plugin for AiiDA to be able to automate Wannier90 runs.

SIESTA interface: Wannier90 Interface for the SIESTA code.

CP2K interface: Wannier90 Interface for the CP2K code.

Matrix elements of the position operator: output the matrix elements of the position operator between Wannier functions in a format similar to the one for the Hamiltonian (seedname_hr.dat file).

Gollum interface: Wannier90 Interface for the Gollum code.

Improve the current library mode to support new features: improve the current library mode to support new features such as spinors and symmetry-adapted Wannier functions.

Design a new library interface: major re-design a new library interface for enhanced usability.

Add support for automatic output of bibTeX files: add functionality in the Wannier90 code so that at the end of each run it produces a bibTeX .bib file with all the citations to be used according to the functionality used in the run.

Symmetry-adapted Wannier functions: implement the code to compute the symmetry-adapted Wannier functions.

Improvements to the interpolation routines: improve the interpolation routines (bands and operator interpolation) to shift WFs into the Wigner-Seitz cell centred on the other WF when computing matrix elements.

Test suite for Wannier90 and integration with Travis-CI: implement the infrastructure for having tests in Wannier90, integrate it both with the test farms used for the EPW code (nightly builds) and with Travis-CI.

Z2PACK interface: implement the necessary changes in Wannier90 to allow Z2PACK to be able to use the Wannier90 routines.

FORD infrastructure implementation for automatic code documentation : implement the core infrastructure to have FORD automatically document the Wannier90 Fortran codes and routines.

Some of the software modules developed during this workshop will also be available in the E- CAM repository for electronic structure. These modules will be part of deliverable 2.2 of WP2.

Extended software development workshop: quantum mechanics and electronic structure

Location: CECAM-FR-MOSER, Maison de la Simulation, France
Webpage: https://www.cecam.org/workshop-0-1357.html
Dates: June 27, 2016 to July 8, 2016

Organizers

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1 State of the art

Simulating the exact quantum dynamics of multi-component systems of electrons and nuclei is a task currently out of reach, except for the simplest molecules with a few degrees of freedom due to the exponential scaling of exact methods. Available approximate algorithms can be broadly classified as follows: exact quantum calculations (applicable to low dimensional systems), wave-function based methods (where the wave-functions are expanded in convenient truncated basis, variationally optimized during the evolution), trajectory-based and trajectory– guided methods (in which the properties of the quantum system are mimicked via averages over ensembles of generalized, interfering, classical trajectories), semi-classical dynamics (based on second order approximations of the path integral representation of the quantum propagator), and path integral methods (employing exact methods to sample the quantum thermal density to tackle the time-domain). The main challenge for all these schemes is to maintain the balance between efficiency and accuracy, i.e. to keep the computational costs manageable while preserving the ability to predict and interpret experiments. Due to this variety of methods, none of which has clearly outperformed the others, software development in quantum dynamics has so far been less systematic than in other fields of modelling, such as classical molecular dynamics or electronic structure. Thus, one of E-CAM WP3's goals is to provide an environment to stimulate the transition from in-house codes, often developed and used by single groups, to the development of modular, community-based, packages capable of multiple functionalities and adopting common benchmarks.

The approach pursued in the ESDW is in direct connection with the outcomes of the E-CAM state-of-the-art workshop (SAW) "Different routes to molecular quantum dynamics", CECAM- HQ Lausanne June 6-10 2016. In that workshop, the importance of defining well-established benchmarks and potential libraries to provide a fair comparison ground for alternative methods was stressed. This task was initiated in the

ESDW (see below). The need to encourage discussion among the developers of existing packages and promote modular programming was also stressed in the SAW. A scientific report from this workshop can be found in the E-CAM website here.

In this ESDW, three codes dedicated to quantum dynamics (QUANTICS, PAPIM, AND TNUM) were compared and common future work to homogenize their development and avoid overlap of capability was planned. Two more codes (CPMD and CP2K) were also discussed in the framework of combining approximate quantum methods with first principle evaluation of the forces. The need to systematically promote these discussions and explore alternative means of generating potentials was also indicated as urgent in the SAW outcomes.

2 Training provided

10 students and 6 tutors, including Dr. Ivano Tavernelli representing the industrial partner of the WP, IBM, participated to the ESDW. The key scientific topics discussed were:

1. Quantum Computing (of interest to the IBM industrial partner);
2. Exact quantum propagation methods for low dimensional systems to be used to provide benchmarks for approximate schemes (of interest to the IBM industrial partner);
3. Single and multi-surface potentials for benchmark systems (of interest to the IBM industrial partner);
4. Calculation of approximate quantum time correlation functions (Linearized methods and the Quantum Thermal Bath approach);
5. Coupling of approximate methods with first principle force calculations.

Training on software development included the following items: The on-line E-CAM tools for software development, the E-CAM Git repository, tools for the documentation (Doxygen) and performance analysis. Instruction occurred via tutorials and hands-on practice.

Interactions with experts on software and hardware development working at La Maison de la Simulation were also integral part of the training activities. These experts gave talks on hardware architectures and programming paradigms and the use of advanced visualization tools such as the Image wall hosted by the Maison de la Simulation

3 List of the software development projects

The modules developed or initiated in the ESDW (see also E-CAM deliverable 3.1) are:

1. **SodLib:** exact wavefunction propagation using the second-order differencing integrator scheme to solve the time-dependent Schoedinger equation. This routine has been implemented and tested as an added functionality within the Quantics quantum dynamics package.
2. **ChebLib:** Chebyshev integration scheme for exact wave function propagation on the grid. This routine has been implemented and tested as an added functionality within the Quantics quantum dynamics package.
3. **SpoLib**: solver for the time dependent Schroedinger equation using the Split Operator Fourier Transform method.
4. **InpTnum**: two main subroutines to read input data and set up information into two fortran derived types: zmatrix (coordinates definition) and Tnum (information to compute the numerical kinetic energy operator).
5. **PhysConst**: enables the use of physical constants and the correct isotopic masses.
6. **PotMod**: a library in which users can store new potentials. Potentials currently available in the module are: harmonic and Morse potentials; empirical potential, based on high level electronic structure calculations, of the ground state of $CH5^+$.
7. **AuxMod**: a set of subroutines which enables any user to construct easily a Fortran input parser. It also contains a library of adapted MPI subroutines for easier programming of Fortran MPI parallel codes.
8. **ClassMC**: Metropolis Monte Carlo sampling of the classical Boltzmann distribution function and calculation of classical time correlation functions from the sampled initial conditions.
9. **PIM**: exact sampling of the Wigner density. It provides quantum initial conditions for the approximate calculation of the time correlation functions.
10. **ClassMd**: a solver for the Hamilton evolution of the and computing autocorrelation functions. This subroutine outputs the Kubo autocorrelation of the dipole moment.
11. **CoorTrans**: set of subroutines enabling transformations between coordinates and a subroutine which transform the gradient and the hessian from Cartesian to curvilinear components for exact wave function propagation.

Modules 1,2,4,5,7,8 have been uploaded in the E-CAM repository for WP3 and are documented in deliverable D3.1. Work on the other modules is on-going. Although not directly originating them, IBM is interested, in particular, in the development of the modules for exact quantum dynamics (1,2,3) and for approximate time-correlation functions (8,9) in view of future applications to modelling of open quantum system for quantum computing.