NEW TRENDS IN SIMULATING COLLOIDS:

FROM MODELS TO APPLICATIONS

Scientific report

Giuseppe Foffi

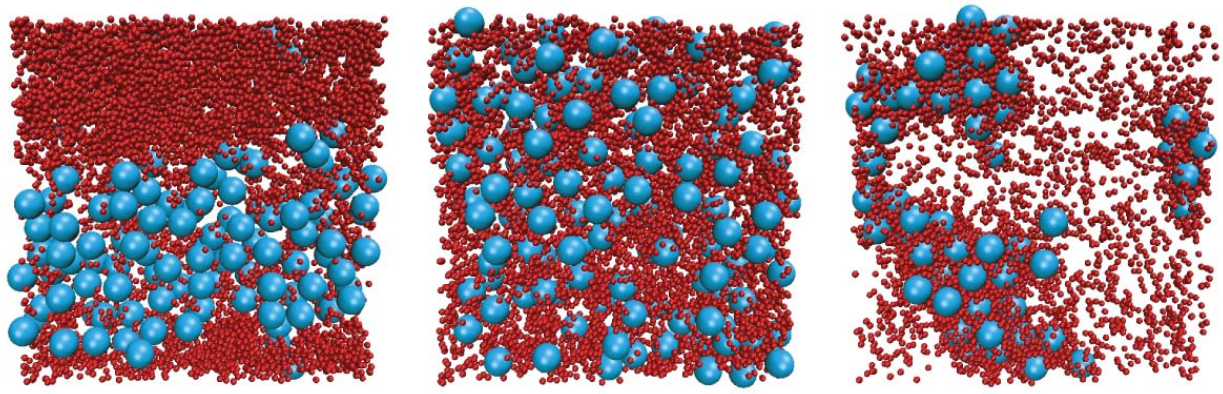
Institut of Theoretical Physics
Ecole Polytechnique Fédérale de Lausanne (EPFL)
Lausanne

Gerhard Kahl

Institut für Theoretische Physik &
Center for Computational Materials Science (CMS)
Technische Universität Wien
Wien

Richard Vink

Institute of Theoretical Physics
Georg-August-Universität
Göttingen



1 TOPIC OF THE WORKSHOP

The CECAM workshop "New Trends in Simulating Colloids: from Models to Applications" took place in Lausanne from the July 15th to the July 18th.

Over the past decades, attention in colloidal physics has grown at an incredible pace. To a great extend this remarkable development is due to the fact that colloidal systems are of high relevance both in everyday applications as well as in basic research. On one hand, colloids are ubiquitous in our daily lives and a deeper understanding of their physical properties is therefore highly relevant in applied areas ranging from biomedicine over food sciences to technology. On the other hand, a seemingly unlimited freedom in designing colloidal particles with desired properties in combination with new, low-cost experimental techniques make them -- compared to hard matter systems -- considerably more attractive for a wide range of basic investigations.

The aim of the present workshop was two-fold. On one side, we wanted to bring together people from in simulations and theory to discuss the new trends in the field, with the emphasis on novel problems and emerging technique following the path of CECAM tradition. The second important driving force was the idea to bring together few key experimentalists to put in the right perspective the whole workshop. This is, perhaps, an uncommon feature for a CECAM workshop. In this field, however, the continuous interaction with the experimentalists is vital. Indeed all the time a coarse grained description of a real system is undertaken, the investigator has to be sure that he is addressing a problem of real interest. We believe that Physics of colloids, using mainly coarse graining modeling, has to obey to this principle.

2 SCIENTIFIC CONTENTS AND PROGRAM

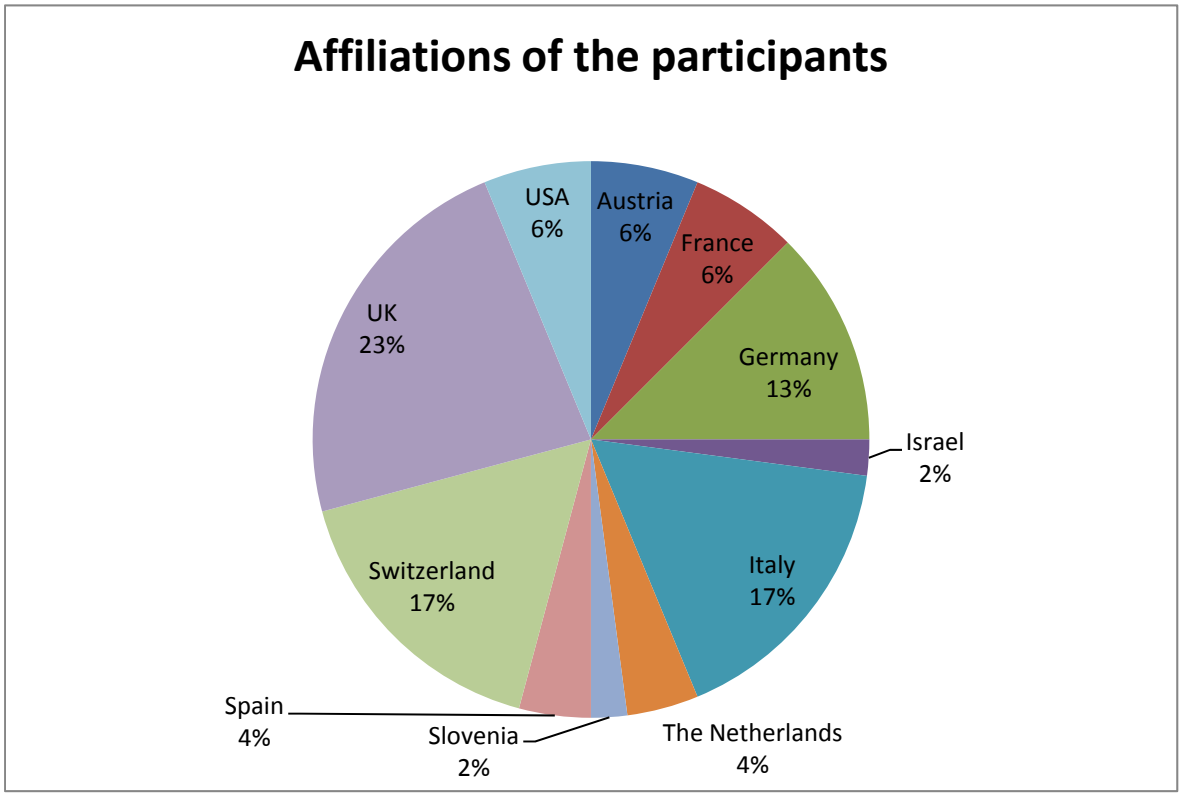
The workshop was organized with two sessions per-day. Each session was opened with a key note presentation from an experimentalist. During the three days of the workshop 31 oral presentations were delivered. Moreover, during the poster section (15 posters presented) PhD students and young post-docs presented their work. In order to boost the discussion, we

explicitly asked these speakers to present and discuss their point view on simulations. In particular, we gave them the possibility to be as critic as they wanted. Several scientific issues were discussed. The emerging trend in studying, theoretical and numerically, patchy interactions was stressed in the opening day. This was a common day with the work shop "Computer Simulation Approaches to Study Self-Assembly: From Patchy Nano-Colloids to Virus Capsids" organized by Ard A. Louis, Athanassios Panagiotopoulos and Jonathan Doye. What emerged is that, in these systems, several properties can be tuned by properly chosen patchy interaction potentials. This is a very promising path to explore the possibility of smart self-assembly. Another important issue, a traditional problem in colloidal systems, was the dynamical and glassy properties of colloidal systems. In this framework, there were discussions on glasses as well as on self assembly and biological properties. A special role in the discussion was played also by proteins systems, both as model colloidal systems and for their applications. In the CECAM tradition, several technical tools have been discussed during the workshop. The focus was on density functional theory, hydrodynamics interactions, event driven Brownian and molecular simulations and genetic algorithms, only to mention few of them.

Since we foresaw a number of relevant points would have been raised during the workshop, we asked an experimentalist and a theoretician (Dr. Erika Eiser and Prof. Christos Likos) to summarize and animate the finale discussion. This choice was indeed successful. This 'round table' discussion meeting was highly useful to provide an overview of yet unsolved problems and to point out directions for future work. From the phenomenological point of view, among those are the questions on the relevance of hydrodynamic interactions, the problem whether to treat solvents in an explicit or an implicit way, or the relevance of multibody interactions. With respect to the methods it was agreed that future developments on dynamic Monte Carlo simulations or on rare events and multiscale techniques are urgently required. We are particularly pleased with the experimentalists who provided an excellent overview of the current state-of-the art in experimental colloidal physics.

3 PARTICIPANTS

The venue was attended by more than 50 participants and most of the colloidal physics community was represented. In particular we managed to get a good representation of the international communities. More than 4/5 of the participants came from outside Switzerland (see pie chart). In this way new connections were established while old ones were renewed. We were also extremely satisfied by the fact the participants belonged to very different stages of their career. There was indeed a good mixture of young investigators as well as more established leading figures. For a lot of PhD students this was their debut in the scientific community and the informal CECAM atmosphere helped them participate to the round tables at the end of each session and to discuss with more experienced researchers.



4 FEEDBACK FROM THE PARTICIPANTS

We have asked all the participants to send us a sentence about the workshop. The feedback has been very positive. Here we report some representative sentences from this feedback.

"The program was particularly well constructed with a combination of experiment, theory and simulation." (Denise Rapaport)

"Due to the careful thought of the organizers, the workshop provided an ideal environment in which to meet leaders in the field. Existing contacts could be renewed and deepened. For example, it was possible to put together plans for future international/Europe-wide collaborations." (Paddy Royall)

"The workshop allowed me to gain a first-hand experience in cutting-edge, state-of-the-art research in self-assembly of modern colloidal/soft matter science. I have been exposed to a wealth of new information pertaining to systems, problems methods and techniques, as well as open questions. Of particular relevance and value was the presence of a number of leading experimentalists in the workshop, who presented their view, confronted existing theories and approaches with hard experimental data and gave impetus for thought and exchanges. I have already established one new contact as a result of the meeting." (Christos Likos)

"It was very useful to gather this focused section of the international soft matter community to share new ideas on simulation of colloids and self-assembly. Input from leading experimentalists helped anchor the discussion in reality. By the end we agreed that a similar meeting in two or three years' time should be a target, and we can expect many exciting advances in that time. This was the first conference for my PhD student (Vera Batista), and was invaluable for introducing her to the leading researchers, both young and more established, in the field." (Mark Miller)

"For me this workshop was very useful since it allowed me to meet some people that I already knew and thus to discuss with them. In addition I had a very good opportunity to meet people that I didn't know before and thus to get familiar with their work. Last not least I want to mention that the accompanying infrastructure of the workshop was very good (lecture hall, hotel, transport to the city,...)." (Walter Kob)

5 SPIN OFF AND CONCLUSION

In the final discussion, most of the speakers and of the participants expressed the appreciation both for the contents of the workshop and for the CECAM organization. The general consent was that within a few years' time events with similar aims should be organized to discuss the progress that has been achieved meanwhile. Finally the Liquids, Soft Matter and Biological Physics Board of the Journal of Physics: Condensed Matter has decided to dedicate a special issue to this workshop (together with the workshop "Computer Simulation Approaches to Study Self-Assembly: From Patchy Nano-Colloids to Virus Capsids"). This special issue will contained original peer-reviewed articles written by the invited speakers of the workshop. It is expected to be published between the end of 2009 and the beginning of 2010.