SUMMARY (maximum 1 page)

The workshop "Common trends between Kinetic theory, Dynamical Density Functional methods and mesoscopic methods based on effective free energy models" was held in Lausanne, in the dependencies of CECAM (Centre Européen de Calcul Atomique et Moléculaire), from 2nd until the 4th October 2008.

In recent years there has been an upsurge of interest towards the study of non equilibrium phenomena, relaxational problems and transport processes.Different theoretical approaches have been developed in order to understand such issues and many new and promising results have been obtained. The objective of the workshop has been to bring together experts working on different, complementary fields related to the study of the dynamics of fluids in confined geometries at the meso and nanoscale.

Specifically, in this workshop we have gathered experts in the fields of density functional theory and its extensions to fluid dynamics, lattice Boltzmann techniques, kinetic theory as well as experts in the development and foundations of mesoscopic and hybrid techniques.

The workshop has focused in the foundations and use of these different approaches. It has paid attention to the interconnections and complementarities of these different approaches. The format of the workshop has promoted discussions and scientific exchange of ideas among the participants. To this end, enough time for lunch and at coffee breaks has been ensured. Also the format of the talks favor the discussions along the presentations to make them more lively. We have taken advantage of the facilities at CECAM to promote informal meetings among the participants. These meetings have emerged as a natural follow up of the discussions carried out along the workshop and have been very fruitful for the participants.

The workshop has become an excellent venue to contrast the challenges posed by these different approaches. It has encouraged in depth discussions in the foundations of kinetic methods and how the underlying thermodynamic behavior is ensured. There were also interesting discussions related to how length scales are bridged and how molecular simulations can be used to provide quantitative tests on dynamical properties extracted from mesoscopic approaches.

DESCRIPTION OF THE SCIENTIFIC CONTENT OF AND DISCUSSIONS AT THE EVENT (maximum 4 pages)

The workshop lasted for three days. It was organized in five sessions that collected the different open topics which we wanted to be covered. The first day we arranged two initial lectures of more general scope with the aim to set the stage of the questions to be addressed. Two outstanding lecturers presented two lectures on density functional theory and on kinetic modeling, "Density Functional Theory:Statics and Dynamics,Origins and Challenges" and "Entropic lattice Boltzmann models". They put forward the challenges which lay ahead. Afterwards, we organized a first session on the foundations and capabilities of dynamical density functional theory.

This starting session was followed by a first session centered on dynamical density functional theory. The talks "Dynamical Density Functional methods", "Dynamical density functional theory for confined colloids:" and "Dynamical density functional theory: connections to hydrodynamics and applications to dynamical pair correlation functions in inhomogeneous liquids" show the possibilities of this framework to tackle new challenges in the physics of colloidal systems. The second session extended to the foundations of kinetic models from a general perspective, and also how to use them to simulate complex fluids. The talks "Statistical mechanical perspectives of lattice Boltzmann complex fluids models", "Nucleation pathways from density functional theory", "Dynamic Boltzmann Density Functional theory", and "Mesh free models of orientationally ordered liquids" addressed several issues covering the foundations of a number of kinetically based approaches to the dynamics of soft materials extending the capabilities of current methods and pointing in new directions along which progress in modeling complex fluids with variable degree of microscopic details can be achieved.

The second day started with a session centered on microscopic approaches to dynamic phenomena. The talks "Testing effective free energy models by molecular dynamics simulation", "Microscopic flow around a tagged diffusing particle: effects of fluctuations on the hydrodynamics

description", "Polymer and Biopolymer Dynamics in Crowded Environments", "Concurrent multiple scale simulation of molecular liquids: combining adaptive coarse-graining and hybrid particle-continuum hydrodynamics schemes", and "Mixed quantum-classical theory of solute-solvent dynamics: an extended hydrodynamics approach" covered molecular studies of dynamic phenomena of interest for complex fluids and colloidal suspensions, the analysis of kinetic phenomena from kinetic theory, the foundations of multiscaling modeling and also the development of hybrid methods which couple molecular details of the system with effective solvents. There was also a discussion on hybrid approaches which take care of quantum aspects of the system dynamics, whenever they become relevant issues to be taken into account. Specific examples where introduced and the corresponding discussions served to clarify the limitations and capabilities of the complementary approaches.

The fourth session was devoted to the foundations of kinetic modeling and their extensions to deal with complex fluids. It was based on diverse talks, "Dynamics and lattice-based simulation of inhomogeneous fluids", "Multi-component multi-phase lattice Boltzmann methods", "Thermal Effects in Phase Separation of Binary Mixtures" and "Hybrid lattice Boltzmann model for binary fluid mixtures" which considered different types of complex fluids and mixtures. In this context, the speakers were careful to expose clearly what are current challenges to such an approach and delivered presentations on the connection with molecular aspects of the fluid and also on extensions based on effective free energies and their consistent thermodynamic formulation. In the opposite direction, the session also covered hybrid methods which couple a kinetic description of the fluid with a macroscopic description of specific degrees of freedom. The final session of the workshop focused on the applications of kinetic models to dynamic phenomena on the micro and nanoscale. The presentations " Lattice Boltzmann Simulations of Capillary Filling", "Lattice Boltzmann Methods for multi-phase flows and contact line dynamics", "Forced thin films on heterogeneous substrates" and "Lattice kinetic methods for the study of electrokinetic phenomena in charged porous media" discussed dynamic capillary phenomena, fluid instabilities and electrohydrodynamics and how the versatility of kinetic methods to address such a variety of phenomena.

During the duration of the workshop we have put emphasis to promote discussions as much as possible. To that end, we have encouraged questions along the presentations and left time for continuing questions at the end of the talks. The gatherig of people with different background and the size of the event favoured such a goal. All along the sessions participants have benefited from an exchange of points of view and open questions relating how different approaches can tackle the issues raised by the speakers. The atmosphere has remained informal enough to promote lively discussions. As a result, participants have not been afraid to pose not only specific questions, but also raise more general issues. This has given rise to interesting discussions on the basic problems associated to the fundamentals of some of the techniques describes, and also on what type of tests can be used to challenge them. In the context of these wider discussions relevant challenges and physical situations which must be understood have also been debated.

As a result, the workshop has managed to address both issues related to the foundations and conceptual problems and challenges of the different approaches to the dynamics of fluids and complex materials, together with their application to open challenges and relevant problems for the scientific community.

ASSESMENT OF THE RESULTS AND IMPACT OF THE EVENT ON FUTURE DIRECTIONS OF THE FIELD (maximum 2 pages)

The event has served to clarify which are the relevant open issues and challenges when trying to analyze systems where a clear separation of time and length scales is lacking. This is the case when dealing with systems in the nanoscale, when treating dynamics in situations where a variety of relaxing time scales are present, or when confinement plays a relevant role.

The event has discussed the challenges related to the foundations of complementary, different approaches. It has also served to analyze how various theoretical frameworks can be related with each other and how such interrelationships can serve to clarify their use in novel situations. The discussions carried out have been benefitial to elucidate the relationship between the need to capture molecular specificity and the coupling with effective, collective modes of the system at different scales in nonequilibrium conditions.

The discussions carried out during the workshop have helped to address open and relevant problems which will promote future research in different directions. Regarding the foundations of kinetic models, the connection with the underlying thermodynamic treatment on inhomogeneous situations remain as an open question for generic non-ideal fluids, the advantages of entropic formulations of these models also remain to be fully explored. The use of dynamical density functional theory is promising; the understanding of when hydrodynamics becomes relevant remains always as an issue to keep in mind. The new results on detailed microscopic dynamics provides quantitative predictions against which mesoscopic models can confront their results to validate the assumptions on the coarse grained usually assumed by researchers in the field.

The new results reported and the discussions carried out have opened new directions of research and have helped to focus relevant issues. The use of the complementary approaches in biologically motivated problems appears as a natural direction where a number of the problems raised merge naturally. The understanding on how to formulate hybrid schemes and how to develop methods to use them together also appears as a promising direction in situations where different time scales coexist. Dynamical density functional theory also appears as a promising framework to

account for molecular structure in colloidal systems. The studies reported on glassy dynamics, or kinetics of non-spherical particles offer promising possibilities which will be exploited in the coming years. Also the prospectives of blending density functional density ideas together with coarse grained kinetic models on a variety of complex fluids will be further explored and exploited. Specially, combining the idea of excluded volume in a consistent kinetic framework, introduced in one of the talks, offers the possibility of a well posed kinetic model for complex fluids with high potential in confined geometries. Hybrid kinetic models have been discussed as a flexible scheme to tackle a variety of complex fluids. New challenges in this area include the extension to new type of complex systems, such as electrolytes or the proper handling of thermal transport. This is in fact an open issue common to a number of the approaches presented in the workshop and remains a common challenge. The ability to treat appropriately into account fluid/solid interactions when capillarity cannot be neglected have also shown to be a fruitful ground of application for a number of coarse grained approaches. The relevance of molecular details in the dynamics of a contact line and its implications in the motion of liquids in heterogeneous environments also will promote research projects in the near future.

The workshop has served to identify and pose a number of general questions which are meaningful to the scientific community and which must be tackled in order to make progress. Among these,

Which are the relevant microscopic details that must be captured in a problem, and which degrees of freedom can be eliminated in a coarse grained description?
How can a thermodynamic approach be generalized to include dynamical aspects of he evolution of the system?
How should we benefit from kinetic theory to address kinetic phenomena of activated processes, where fast processes become crucial ingredients?
How can we build hybrid schemes with enough thermodynamic consistency to address new complex fluids?

The discussions and unresolved questions which have come out during the workshop will promote research to answer these questions and challenges in the near future.

FINAL PROGRAM OF THE MEETING

First Day

* 09:10 to 09:50 - Robert Evans
  Density Functional Theory:Statics and Dynamics,Origins and Challenges
* 09:50 to 10:30 - Ilya Karlin
  Entropic lattice Boltzmann models
* 10:30 to 11:00 - Coffee Break

* 11:00 to 11:40 - Pedro Tarazona
  Dynamical Density Functional methods
* 11:40 to 12:20 - Hartmut Löwen
  Dynamical density functional theory for confined colloids:
* 12:20 to 13:00 - Andrew Archer
  Dynamical density functional theory: connections to hydrodynamics and applications to dynamical pair correlation functions in inhomogeneous liquids
* 13:00 to 14:30 - Lunch Break

session 2

* 14:30 to 15:10 - Xiawen Shan
  Statistical mechanical perspectives of lattice Boltzmann complex fluids models
* 15:10 to 15:50 - james lutsko
  Nucleation pathways from density functional theory
* 15:50 to 16:20 - Coffee Break
* 16:20 to 17:00 - Burkhard Duenweg
  Statistical Mechanics of the Fluctuating Lattice Boltzmann Equation
* 17:00 to 17:40 - Pep Español
  Dynamic Boltzmann Density Functional theory
* 17:40 to 18:20 - Chris M. Care
  Mesh free models of orientationally ordered liquids

Second Day

session3

* 09:00 to 09:40 - Juergen Horbach
  Testing effective free energy models by molecular dynamics simulation
* 09:40 to 10:20 - Rodolphe Vuilleumier

Microscopic flow around a tagged diffusing particle: effects of fluctuations on the hydrodynamics description

* 10:20 to 10:50 - Coffee Break

* 10:50 to 11:30 - Raymond Kapral
  Polymer and Biopolymer Dynamics in Crowded Environments
* 11:30 to 12:10 - Rafael Delgado Buscalioni
  Concurrent multiple scale simulation of molecular liquids: combining adaptive coarse-graining and hybrid particle-continuum hydrodynamics schemes
* 12:10 to 12:50 - Irene Burghardt
  Mixed quantum-classical theory of solute-solvent dynamics: an extended hydrodynamics approach
* 12:50 to 14:30 - Lunch Break

session4

* 14:30 to 15:10 - Simone Melchionna
  Dynamics and lattice-based simulation of inhomogeneous fluids
* 15:10 to 15:50 - Alexander Wagner
  Multi-component multi-phase lattice Boltzmann methods
* 15:50 to 16:20 - Coffee Break

* 16:20 to 17:00 - Giuseppe Gonnella
  Thermal Effects in Phase Separation of Binary Mixtures
* 17:00 to 17:40 - Antonio Lamura
  Hybrid lattice Boltzmann model for binary fluid mixtures

Third Day

session 8

* 09:00 to 09:40 - Julia Yeomans
  Lattice Boltzmann Simulations of Capillary Filling
* 09:40 to 10:20 - Luca Biferale
  Lattice Boltzmann Methods for multi-phase flows and contact line dynamics
* 10:20 to 10:50 - Coffee Break
* 10:50 to 11:30 - Ignacio Pagonabarraga
  Forced thin films on heterogeneous substrates
* 11:30 to 12:10 - Benjamin Rotenberg

Lattice kinetic methods for the study of electrokinetic phenomena in charged porous media