MOLECULAR SIMULATIONS IN BIOSYSTEMS AND MATERIAL SCIENCE

(SimBioMa)

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ABSTRACT
The aim of the proposed programme is to initiate a concerted European effort to develop those computational tools that can be used to obtain a better molecular understanding of the emergence of mesoscopic structure and dynamics in biological systems ("molecular systems biology") and in man-made nano-structured materials.

In order to establish the link between molecular properties on the one hand and mesoscopic materials properties on the other, one must use an integrated approach that seamlessly integrates quantum calculations, molecular simulations and mesoscopic modelling techniques. To achieve this, we must translate the recent advances in computational methodology into practical tools that allow us to construct detailed models of biological systems and nano-structured materials. For these systems, numerical simulations are expected to be of crucial importance because they will allow us to gain "microscopic" insights that cannot be obtained experimentally. A concerted research effort will be required because conventional molecular modelling techniques, whilst adequate to model simple molecular systems or very small numbers of biomolecules, cannot access the length and time scales relevant for mesoscopic structure and dynamics. To focus our research effort, we aim to concentrate on a small number of relevant and representative problems. For these problems we will:

- Identify the limitations of the current techniques
- Identify the focus of novel simulation techniques
- Identify those static and dynamics properties that allow for experimental validation of the computational approach
- Improve the power of computational techniques

The success of this proposal crucially depends not only on collaborations of those simulation groups in which these novel techniques have been developed with those working in these areas, but also on collaborations between those developing techniques in different domains.

The trend of applying such advanced simulation techniques to these type of systems is clearly visible in leading groups in the US and Japan. Since Europe has a leading role in the development of molecular simulation techniques, the proposed ESF-program could translate this strong position in technique development into a strategic advantage in the areas of molecular systems biology and nano-materials science.

KEYWORDS
molecular simulations, molecular systems biology, material science, mesoscopic modelling

Status of the relevant research, scientific context, objectives and envisaged achievements

Status of the relevant research

Molecular simulation has evolved to become the tool of choice to model the physical properties of complex systems. Interestingly, the increase in power of simulations is only partly due to the large increase in computing power during the past 50 years. Ten years ago state of the art simulations could barely access the nanosecond time scale and the increase in cpu power has pushed this limit two orders of magnitude. Even if the cpu-power continues to increase at this speed, we cover only a very tiny fraction of the experimental length and time scales. This gap can only be bridged by the development of novel computational techniques.

The technique-oriented ESF-programme SIMU has helped the molecular simulation community to focus on developing novel algorithms that extend molecular simulations towards longer time and length scales. As part of SIMU important progress has been made in the development of a number of computational techniques (many of which have been reported at the final SIMU meeting that was held in Genoa in 2004):

- *Hybrid quantum/classical techniques*: biological systems are far too large to be treated fully quantum chemically. The idea here is to apply full quantum computations on a small part of the system and treat the rest of the system classically. The computational issues that have been solved deal with the details of the boundary between the quantum and classical part.
- *Solvent effects in chemical reactions:* Ab-initio molecular dynamics allows us to study the effect of the environment (solvent, ligands etc.) on a chemical reaction. These computations are very time consuming and are in most cases far too short to observe a chemical reaction. It has been shown that such simulation can be used to compute the free energy of a given reaction coordinate. This free energy is a first step in understanding the reaction kinetics.
- *Identifying complex reaction coordinates/rare event simulations*: Very long simulation times are often the results of (free) energy barriers a system has to take. Identifying such barriers in complex systems is far from trivial as this barrier is an ensemble of transition states in a very high dimensional state. Computational techniques have been developed to locate this transition state ensemble.
- *Mesoscopic modelling:* to access longer length scales in a simulation one has to coarse grain, i.e., lump groups of atoms or molecules together in an effective particle. The computational challenge is to develop methods to derive the effective interactions between these mesoscopic particles.

From a scientific point of view the above list is impressive: each technique has pushed the time and length scales by 5 to 10 orders of magnitude more than can be expected from the increase of CPU power. These techniques have been applied to relatively simple model systems that were chosen for their computational convenience, rather than their intrinsic relevant for current experimental research. The next scientific challenge is to use these techniques to solve important scientific questions in emerging fields of research.

In contrast to the *technique-driven* SIMU programme, the proposed programme will be *application* driven. The techniques developed by the SIMU programme have to be integrated and will be applied in two carefully selected scientific domains where we expect that molecular simulations can make key contributions. As stated above, the research fields that we have identified are *molecular systems biology* and *nano-structured materials science.* Whilst the scientific objectives in these two domains are rather different, the computational techniques needed to address them are surprisingly similar. For this reason, the proposed programme aims to stimulate interdisciplinary transfer of knowledge.

Scientific context
To illustrate how techniques have to be integrated consider as an example the Photoactive Yellow Protein. This protein plays an essential role in some bacteria as it is responsible for a response when it is in contact with UV light. The present computational approaches are limited to the structure of a protein. Our ambition goes beyond this. We aim to develop computation methods that contribute to our understanding of the *functioning* of a protein in its biological environment. In this case one would like to have a molecular understating of the chain of folding events that are induced by a chemical reaction which is triggered by light hitting the photoactive centre. A *hybrid quantum/classical* approach is required to understand the role of the protein in the chemical reaction. As the folding events occur on a time scale much longer than the time scale accessible with conventional molecular dynamics, *rare events simulations* are required to study the chain of folding events. Clearly "brute force" simulations cannot cover the full range of length and time scales that are needed to understand the functioning of such a protein. The way of achieving this is an intelligent way of combing molecular computational techniques that work at different length and time scales. While several techniques have been thoroughly tested in small systems, the complexity of the biological context will require novel approaches. As the expertise is available in different European groups, the ESF-programme provides the essential means to simulate this development.

Yet, the above example is simple compared to the true holy grail of molecular system biology. The ultimate aim is to have a particle-based model of a system that contains a large number of interacting (and reacting) bio-molecules. Such a model should be able to predict the response of a biochemical network to a change in the external conditions. The scientific questions require a molecular description, and molecular simulation is the technique by excellence to complement the novel experimental techniques that operate on the single molecule level. Yet, the time and length scales posed by biological questions do limit the conventional techniques and the potential of the novel techniques is exciting.

A second domain is related to the recent developments in material science, an area in which examples of similar importance can be described. The miniaturization of electronic devices in the near future will reach the nanometer length scale, where quantum effects become important. Experimentally it is now possible to construct materials at the nano meter length scale. At this length scale materials often do not behave as bulk material but are dominated by their interfacial properties. Understanding materials at this length scale requires the molecular approach that is developed in the context of the present proposal. Other examples of modern materials are soft matter systems, in particular colloidal dispersions. The effect of external potentials on the static and dynamic properties of such systems is at present a scientific question of high priority in order to be able to design such materials with well defined elastic and structural properties at a later stage. The computational approach to such systems spans several orders of magnitudes in length and time scales and thus is a significant application area for the "bridging" methods developed in the ESF programme "SIMU".

Domain: Molecular Systems Biology

Domain coordinators: Prof. Berend Smit (CECAM)
Within this domain, the programme aims to identify those techniques that are missing to obtain a better understanding of biological systems and stimulate the development of these methods. Below we list some case studies that illustrate our ambitions.

Proteins in action

Case study coordinators Dr. Peter Bolhuis (UvA, Amsterdam) and Prof. Ursula Röthlisberger (Lausanne)

Often an external stimulus such as light, pressure, or chemicals induces a chemical reaction in a protein causing a chain of events. The PYP protein or rhodopsin are reference systems in which there is a large body of experimental data to validate a computational approach. Key issues are whether a quantum chemical description on the femto-second time scale can be linked to the description of a conformational change of a protein at the micro second time scale.

Interactions between peptides embedded in membranes

Case study coordinators: Prof. Reinhard Lipowsky (Potsdam) and Prof. Helmut Grubmüller (Gottingen)

Understanding the details of the interactions between molecules (proteins, peptides, cholesterol) in membranes is complicated by the response of the membrane. All-atom simulations give insights in parts of the interactions, but mesoscopic models are requires to access the length and time scales involved in the understanding the collective behaviour of these imbedded molecules. Key issues are whether coarse graining techniques can be developed that relates changes in the molecular structures to changes in the effective interactions between these embedded molecules.

Protein crystallization and amyloid aggregation

Case study coordinators: Prof. Daan Frenkel (AMOLF, Amsterdam) and Dr. Michele Vendruscolo (Cambridge)

Crystallization of (membrane) proteins is a problem of significant practical importance. How can we modify the conditions such that crystallization can be tuned requires a detailed understanding of the physical chemical properties of proteins. For colloids simulations have contributed to this understanding, extending these to proteins is the key issue here. This problem illustrates a key aspect of the present programme: at present simulations of proteins are usually limited to one, or a few such molecules. However, to study a cooperative effect, such as crystallization, it is essential to simulate thousands of proteins. This can only done by using a coarse-grained model. Yet the model has to be constructed in such a way that it adequately represents the microscopic interactions between real proteins. The aberrant behaviour of proteins may result in amyloid aggregates, which have been associated to misfolding diseases, such as type II diabetes, Parkinson's and Alzheimer's diseases. Under-standing the molecular mechanisms of this type of ordered aggregation will provide new insights for the development of rational treatments to combat these medical conditions.

Active transport in and between cells

Case study coordinators: Prof. Roland Netz (München) and Prof. Jean Pierre Hansen (Cambridge)

Molecular motors and ion channels are mechanisms of the cell to transport material. To fully understand the mechanism of molecular motors models have to be extended from motors operating in vacuum to include the details of the hydrodynamics in the cell. How to combine the atomic description with the hydrodynamic length scale will be the key issue in this case study. Ion channels and aquaporins are physiologically important examples of the wider topic of highly confined fluids (fluids in nanopores), which are also relevant in Molecular Material Science. Major issues are the understanding of molecular mechanisms for selectivity and gating.

Domain: Molecular Material Science

Domain coordinators: Prof. Peter Nielaba (Konstanz)

Within the domain Molecular Material Science the aim is to develop those computational techniques that can be used to understand and guide experimental material science at the nanoscale.

Quantum effects in nano-sized materials

Case study coordinators: Prof. Karsten Jacobsen (Denmark), Prof. Matthias Scheffler (Berlin), and Dr Ali Alavi (UK)

Many of the interesting effects recently studied in systems on nanometer length scales take place at low temperatures so that the consideration of quantum mechanics is important. Examples are Au- atoms in single-atom wires, molecules in cylindrical pores or clusters of a few atoms or large atomic islands deposited on surfaces. Experimentally, many structural-, elastic-, electronic-, and phase- properties of systems in the size of a few nanometers have been obtained. As these systems contain about 10-10.000 particles, which is nearly ideal for computer simulations, since these systems are too large for analytical methods and to big for bulk techniques to hold. Progress is expected by using ``bridging'' techniques which have been developed for classical/quantum systems, e.g. classical and path integral Monte Carlo and Car-Parrinello- and classical- molecular dynamics simulations.

Microfluidics:
Case study coordinators: Prof. Pep Espanol (Madrid, Spain), Prof. Michael Cates (Edinburgh, UK), Prof. Jean-Louis Barrat (Lyon, France)
Many emerging applications in material science, micro and nano-engineering and biology, critically depend on the dynamical behaviour of fluids at the meso and microscale. While such scales are still beyond reach of genuinely atomistic methods, such as molecular dynamics, they are not directly addressable by sheer fluid dynamics either. The reason is that microfluidic behaviour shows specific features with little or no counterpart in the macroscopic world. Europe has played a trailblazing role in developing a new class of mesoscopic techniques, most notably the Lattice Boltzmann method (LBM) and Dissipative Particle Dynamics (DPD) which now can be applied to a variety of micro-rheological applications, such as dynamic phase-transitions in porous media, multiphase flows in capillary channels, blood flows, liquid crystal simulations and many others. From a computational point of view, a new class of hybrid schemes, combining LB upwards with continuum methods and downwards with atomistic methods, possibly DPD itself, will also be pursued. The potential impact of such multiscale approach for microfluidics applications is hard to overestimate.

Colloidal systems, glasses and liquid crystals:
Case study coordinators: Prof. Kurt Binder (Mainz) and Prof. Michael Allen (Warwick),
Colloidal dispersions have been much investigated recently, by experimental and simulation methods and are of great interest for companies like Schlumberger, Henkel, Bayer or BASF. They can be both prepared and characterised in a controlled way, and the effective interaction between the colloidal particles can be tailored. Exciting questions on the many-body effects induced by co-operation and self-organisation of many particles can by studied by experiments as well as by computer simulations. This has been demonstrated for the bulk freezing transition, the kinetic glass transition and for the crystal nucleation rates. At present many interesting questions concern the behaviour of colloids in external shear-, electric-, laser-optical-, and magnetic fields as well as in a confined geometry. In the ESF programme we intend to contribute to the classification of the different self-organisation processes of these important soft matter systems as a function of particle complexity and the kind of external manipulation.

Objectives and envisaged achievements
The key target of the programme is to facilitate the development of a European collaborative computational research effort that can support and guide experimental efforts in two carefully selected domains: biomolecular and material science. The success of such an approach is crucially dependent on networking activities that each has their own targets and milestones:

- *Educational:* to ensure an excellent good European infrastructure that allow students and junior researchers from various group to acquire state of the art molecular simulation techniques from the top researchers in the field
- *Dissemination of knowledge:*
    - *Conferences:* to ensure an excellent visibility of the European strength in the area of molecular simulations

  - *Workshops:* to ensure an optimal exchange of ideas on a well defined focused case study.
- *Planning of research programmes:* to initiate two coherent and collaborative European research programmes in the domains of the application.

Expected benefit from European collaboration in this area

European research teams have played an important role in the technical advances in Molecular Simulations. In many areas of Molecular Simulation, European groups occupy a leading position. The SIMU initiative has been instrumental in fostering this success and, generally speaking, we can say that the SIMU community has been internationally at the forefront. Of the many research groups that are organized under the "SIMU" umbrella, the present proposal will invite those that are expected to make major contributions to the molecular modelling in the context of molecular systems biology or nano-structured materials science. In addition we will stimulate those computational groups that are currently involved in microscopic simulations of biological system or material science to become part of the present programme. Such collaborations lead to an increase of quality of the various teams. Equally important, the programme activities that we propose will make it possible to ensure uniform high scientific standards for computer simulation throughout Europe.

We believe that, in order to maintain the leading position of Europe in molecular simulation, it is essential to train a next generation of brilliant young scientists in this field. Our proposal is designed to do that. By focusing on emerging applications, we aim to maximize the impact of these young scientists on society at large. The proposed members of the steering committee partly reflect this view.

In this proposal we have outlined in some detail the activities that are, in our view, most promising because they are the focus of our strongest groups. The programme itself will gather the best teams in the molecular simulation community, both in Europe and in North America. The participation of US scientists will be supported through applications by our American associates to the international NSF programme which has opened recently to ESF-NSF joined activities. Thus the activity of our community has given to Europe a very strong position and our community is committed to maintain and strengthen this position. We should make sure that we exploit our strategic advantage by defining new, timely and daring challenges. The present initiative aims to achieve this by widening the scope of molecular simulations to new fields.

European context:

The proposed ESF-programme will clearly benefit from the expertise in the area of multi-scale simulation that came together in the ESF "SIMU" programme. In fact, at the end of the SIMU programme the participating groups decided spontaneously that it was of crucial importance to keep in touch. They have therefore organized in the ESF-COST action MOLSIMU (P13). MOLSIMU is not a research programme – it is a means to keep a strong community together and allow them to formulate promising research programmes in areas of great scientific importance. In 2004, the objectives described in the present proposal were identified by the MOLSIMU representatives as an important research focus. However, it should be stressed that the present proposal concentrates on a small subset of all the research topics that are studied by MOLSIMU groups. We believe that such a focus is essential, in order to make progress on the specific applications described in the present proposal.

The educational part of the programme will benefit from the Marie Curie Training Courses that are coordinated by CECAM. The proposed ESF program will benefit from the CECAM infrastructure to organize workshops and tutorials. The study of nanofluidics and its extension via mesoscale methods to the nano-regime is the subject of one of the UK Collaborative Computational Projects (CCP5).

Proposed activities and budget

Management structure

To ensure a maximum of the support for research related activities we will use a light management structure. For each domain there will be a programme committee and their members form the steering committee of the programme. The steering committee will meet once a year and is responsible for the actions taken. Within a domain the programme committee is responsible for initiating and coordination of the various actions and will be supported by the Case Study coordinators. To save funds, parts of the decisions should be done, if possible, by e-mail discussions and decisions.

Workshops:

The workshop activities should contain groups from the simulation community as well as from the experimental community. During the programme the focus of the workshops will shift from identifying the key challenges for each of the case studies to providing solutions to solve them. The Case Study coordinators will play an important role in initiating a workshop related to their case study. The input from leading experimental groups will be essential to ensure that the case studies focus on important experimental issues. Some of the workshops will be focussed on the preparation of a coherent European research program (EUROCORE). We count on 7 workshops a year each about 9 kEUR for on average 15-20 participants.

Schools and tutorials:

Training of young students and scientists of community is very important in order to spread the state-of-the-art knowledge. In the first part of the programme schools will focus on bridging knowledge gaps between the old SIMU community and the computational biocommunity and material science. To provide such a training we plan to arrange two schools (25kEUR each) and two tutorials (10 kEUR each) per year.

Microworkshops and short term visits:

The exchange of ideas in small groups discussing a well defined issue or by direct short term visits between the SimBioMa- laboratories shall be supported as well. Experimentalists will be included in these activities on a regular basis. Five to ten short term visits should be supported per year with an average amount of 2.5 to 5kEUR.

Conferences

Two major international events are scheduled. The Europhysics conference on Computational Physics in 2007, in which a special section on computational biomolecular and material science will be organized, and a conference to conclude the program. Both events will be open to all programme participants. This justifies higher expenses for these scheduled activities of 60 kEUR for each of these conferences.

***Duration*:** 5 years (2006-2010)

BUDGET ESTIMATE (numbers in EURO per year)

1) Workshops:	60,000
2) Conferences (sequential savings):	34,000
3) Short time visits:	25,000
4) Schools:	50,000
5) Tutorials:	20,000
6) External administrative costs:	15,000
7) Committee meetings:	9,000
Sum:	213,000
ESF Administrative Costs (7.5%)	16,000

In addition to the scientific activities the above budget includes web site maintenance and local administrative expenses (15 kEUR per year), steering committee meetings (9 kEUR per year) on the average. The number of research groups interested (>300) and number of countries involved (21) justifies this budget.

Appendix A: CURRICULUM VITAE principle applicants

Professor Dr. Berend Smit

08.11.1962:	Born in Deventer (the Netherlands)
1981-1987:	MSc study Chemical Engineering (Technical University of Delft, NL)
1982-1988:	MSc study Physics (Technical University of Delft, NL)
1990	Ph.D (Utrecht University NL)
1988-1997	Researcher at Shell Research Amsterdam (NL)
1990-1992	Visiting scientist University of California at Berkeley (Prof D. Chandler)
1997-present	Professor of Computational Chemistry University of Amsterdam
2004-present	Director of CECAM, Lyon

Recipient of the 1997 Gold medal of the Royal Dutch Chemical Society

Area of research: computational methods in biophysics (cell membranes), chemical engineering (porous materials, phase equilibria), physical chemistry (surfactants, clays)

Professor Dr. Peter Nielaba

25.5.1959:	Born in Marl (NRW, Germany)
1977-1982:	Study of Physics in Goettingen (Diplom thesis in Theoret. Physics)
1983-1986:	Ph.D.-study at the FU Berlin (Theoretical Physics)
1987/1988:	Postdoc in USA (Mathematical Phys., Prof. Lebowitz, Rutgers U.)
1988-1992:	Scientific Assistant at the U. Mainz (Prof. Binder)
17.6.1991:	Habilitation in Theoretical Physics (U. Mainz)
1992-1997:	DFG-Heisenberg-Fellow
1997/1998:	Interim-Professor for Theoretical Physics (C3) at the U. of Saarland
1998-present	Professor for Theoretical Physics (Chair) (C4), U. Konstanz
2002-2004:	Chairman of the ESF-programme SIMU
2004-present:	Chairman of the COST-action MOLSIMU

Area of research: Statistical Physics, Computational Physics, Theoretical Solid State- and Surface Physics

FIVE RECENT RELEVANT PUBLICATIONS OF THE APPLICANTS:

1. *Understanding Molecular Simulation.* From Algorithms to Applications. D. Frenkel and B. Smit, Academic Press, Boston (1996) and (2002 2nd edition)
2. *Bridging time-scales: Molecular simulations for the next decade*, P. Nielaba, M. Mareschal, G. Ciccotti (eds.), Springer, Heidelberg (2002).
3. *Simulating the effect of alcohol on the structure of a membrane*, M. Kranenburg and B. Smit, FEBS Letters, **568** (2004) 15-18
4. *Chain Length Dependencies of the Bending Modulus of Surfactant Monolayers,* L. Rekvig, B. Hafskjold, and B. Smit Phys. Rev. Lett. **92** (2004) 116101
5. *Elastic properties of 2D colloidal crystals from video microscopy,* K. Zahn, A. Wille, G. Maret, S. Sengupta, P. Nielaba, Phys. Rev. Lett. **90**, (2003) 155506.

Appendix B:List of proposed Steering Committee members

AUSTRIA	Christophe Dellago	University of Vienna
BELGIUM:	Jean-Paul Ryckaert	Universite Libre de Bruxelles
BULGARIA	Andrey Milchev	Acad. of Sciences
CYPRUS	Epameinondas Leontidis	University of Cyprus
CZECH REPUBLIC	Ivo Nezbeda	Acad. Sciences
DENMARK:	Ole Mouritsen	University of Copenhagen
FINLAND:	Kari Laasonen	University of Oulu
FRANCE:	Daniel Borgis	U. d'Evry-Val-d'Essonne
GERMANY:	Helmut Grubmüller	Max-Planck-Institut Göttingen
GREECE:	Vlasis Mavrantzas	University of Patras
ICELAND:	Hannes Jonsson	University of Reykjavik
IRELAND:	Donal McKernan	University of Dublin
ITALY:	Davide Galli	University of Milano
NETHERLANDS:	Marjolein Dijkstra	Universiteit Utrecht
NORWAY:	Bjoern Hafskjold	University of Trondheim
POLAND:	Bogdan Lesyng	Warsaw University
PORTUGAL:	Patricia Faisca	Universidade de Lisboa
SPAIN:	Santiago Lago	University of Sevilla
SWEDEN:	Lennart Nilsson	Karolinska Institutet
SWITZERLAND:	Wanda Andreoni	IBM Zurich Research Lab.
UNITED KINGDOM:	Mark Rodger	University of Warwick

Appendix C: CONTRIBUTING RESEARCHERS LISTED BY COUNTRY[1]

Austria		
Boresch	Stefan	University of Vienna
Dellago	Christoph	University of Vienna
Hafner	Jürgen	University of Vienna
Kahl	Gerhard	Technical University of Vienna
Kresse	Georg	University of Vienna
Neumann	Martin	University of Vienna
Posch	Harald	University of Vienna
Steinhauser	Othmar	University of Vienna
Vesely	Franz	University of Vienna
von Grünberg	Hans-Hennig	University of Graz
Belgium		
Ausloos	Marcel	ULG (Liège)
Baus	Marc	ULB (Bruxelles)
Boon	Jean-Pierre	ULB (Bruxelles)
Champagne	Benoit	FUNDP (Namur)
Cornil	Jerome	University of Mons-Hainaut
Damman	Pascal	UMH
De Coninck	Joel	UMH (Mons)
De Maeyer	Marc	KUL (Leuven)
Gaspard	Pierre	ULB (Bruxelles)
Gonze	Xavier	Universite Catholique de Lovaine
Hou	Marc	ULB (Bruxelles)
Indekeu	Joseph	KUL (Leuven)
Lamoen	Dirk	University of Antwerp
Lazzaronni	Roberto	UMH (Mons)
Lensink	Marc	ULB (Bruxelles)
Malek Mansour	Mamad	ULB (Bruxelles)
Mareschal	Michel	Universite Libre de Bruxelles,
Nies	Erik	KUL (Leuven)
Ryckaert	Jean-Paul	Université Libre de Bruxelles
Van Helden	Jacques	ULB (Bruxelles)
Vandenbroeck	Christian	LUC (Limburg)
Vercauteren	Daniel P.	Laboratoire PCI-FUNDP
Bulgaria		
Milchev	Andrey	Bulgarian Academy of Science, Institute of Physical Chemistry
Cyprus		
Archontis	Georgios	Department of Physics, University of Cyprus
Leontidis	Epameinondas B.	Department of Chemistry, University of Cyprus.
Spyros	Skourtis	Department of Physics, University of Cyprus
Czech Republic		
Kolafa	Jiri	Institute of Chemical Technology, Prague
LISAL	Martin	Prague Institute of Chemical Technology
Nezbeda	Ivo	E. Hala Lab of Thermodyn., Acad. Sci.
Prochazka	Karel	Charles Universtiy
Denmark		
Besold	Gerhard	MEMPHYS - Center for Biomembrane Physics
Hansen	Flemming Y.	The Technical University of Denmark
Ipsen	John H.	The University of Southern Denmark
Jacobsen	Karsten Wedel	NULL
Mouritsen	Ole G.	MEMPHYS, University of Southern Denmark
Sperotto	Maria Maddalena	Biocentrum, DTU
Toxværd	Søren	University of Copenhagen
Finland		
Hakkinen	Hannu	University of Jyväskylä
Juffer	Andre	Department of Biochemistry, University of Oulu
Karttunen	Mikko	Helsinki University of Technology
Laasonen	Kari	University of Oulu
Mattila	Kimmo	
Nyronen	Tommi	
Peräkylä	Mikael	University of Kuopio
Vattulainen	Ilpo	, Helsinki University of Technology
France		
Athènes	Manuel	SRMP, CEA/Saclay
Barmes	frederic	CECAM
Barrat	Jean-Louis	University of Lyon
Baschnagel	Jörg	University of Strasbourg
Bernu	Bernard	
Biben	Thierry	CNRS
Blase	Xavier	Université Claude Bernard-Lyon 1
Bocquet	Marie-Laure	Ecole Normale Supérieure de Lyon
Bocquet	Lydéric	Université Claude Bernard-Lyon 1
Bopp	Philippe A.	Universite Bordeaux 1
Borgis	Daniel	Université Evry vel d'Essonne
Boutin	Anne	CNRS
Caillol	Jean Michel	
Cartailler	Thierry	
Chipot	Christophe	CNRS
Dean	David	, University Paul Sabatier, Toulouse
Descamp	Marc	
Dong	Wei	Ecole Normale Supérieure de Lyon
Fuchs	Alain	University of Paris-Sud
Gaigeot	Marie-Pierre	Université Evry vel d\'Essonne
Guillot	Bertrand	
Hinsen	Konrad	Laboratoire Léon Brillouin (CEA-CNRS)
Hynes	James	Ecole Normale Superieure Paris

[1] On the website www.SimBioMa.cecam.fr the most recent number of participating groups can be found.

Karplus	Martin	Chimie Biophysique ISIS, Strasbourg
Kneller	Gerald	Universite d'Orleans / CNRS
Kob	Walter	Universite Montpellier II
Lavery	Richard	
Lesveque	Dominique	
Lorente	Nicolas	Universite Paul Sabatier Toulouse
Maggs	Tony	
Maillet	Jean-Bernard	CEA-DAM
Marchi	Massimo	
Meyer	Hendrik	Institut Charles Sadron (CNRS)
Millot	Claude	
Morineau	Denis	CNRS UMR6626 University of Rennes
Mounir	Tarek	CNRS / Université Henri-Poincaré
Pasturel	Alain	CNRS
Pellenq	Roland	
Pontikis	Vassilis	CEA
Ramirez	Rosa	Université Evry vel d'Essonne
Sanejouand	Yves-Henri	Ecole Normale Supérieure de Lyon
Sautet	Philippe	Ecole Normale Supérieure de Lyon
Sayede	Adlane	Universite d'Artois
Simonson	Thomas	Dept of Biology, Ecole Polytechnique
Smit	Berend	CECAM
Tanguy	Döme	Ecole des Mines de Saint-Etienne
Trizac	Emmanuel	Laboratoire de Physique Theorique et Modeles Statistiques
TURQ	Pierre	Université Pierre et Marie Curie
Victor	Jean-Marc	
Viot	Pascal	,Universite PAris VI
Vuilleumier	Rodolphe	Université Pierre et Marie Curie
Wittmer	Joachim P.	Institut Charles Sadron, Strasbourg
XU	Hong	LPMD, Univ. Metz
Zerah	Gilles	Commisariat à l\'Energie Atomique,
Germany		
Binder	Kurt	Universität Mainz
Christian	Fleck	Albert-Ludwig University Freiburg
Dederichs	Peter	IFF, Forschungszentrum Juelich
Dietrich	Siegfried	Max-Planck-Institut für Metallforschung
Duenweg	Burkhard	Max-Planck-Institut fuer Polymerforschung
Everaers	Ralf	MPI fuer Physik komplexer Systeme
Fuchs	Matthias	Fachbereich fuer Physik, Universitaet Konstanz,
Gompper	Gerhard	FZ Juelich
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