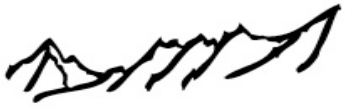
ÉCOLE DE PHYSIQUE des HOUCHES



UNIVERSITE JOSEPH FOURIER

SCIENTIFIC REPORT

First Les Houches school in computational physics : soft condensed matter June 20th-July 1st, 2011

Organizers : J-L. Barrat, R. Everaers, W. Krauth

Lecturers :J. Baschnagel, T. Biben, R. Everaers, W. Kob, I. Pagonabarraga

Seminar speakers : W. Krauth, P. Kestener

Technical support and practical works: O. Benzerara, C. Calugaru, E. Quemener

SUPPORTED BY

Centre Blaise Pascal, Ecole Normale Supérieure de Lyon ENS DE LYON 	***Maison de la Modélisation et de la Simulation, Nanosciences et Environnement, Université Joseph Fourier, Grenoble*** MaiMoSiNE
EUROPEAN SCIENCE FOUNDATION SETTING SCIENCE AGENDAS FOR EUROPE	cecam Centre Européen de Calcul Atomique et Moléculaire

SUMMARY

The school received more than 70 applications before the deadline set to March 15th . While the organizers originally intended to limit the number of students to 40 for practical reasons, the quality of the applications lead to increase this number to 48. The participants also included 2 research engineers from Lyon and Strasbourg who provided technical and pedagogical support for the practical work, 5 lecturers and 2 organizers .

The school took place during two weeks of intense work for the students and lecturers. The vast majority of participants were first or second year PhD. Students from all countries, and the lecturers had a very pedagogical approach starting from the basics and taking the students trough the details of the methods used in simulation of soft matter. The courses were given in part in the form of powerpoint presentation, but also to a large extent on the blackboard, a formulation that was The courses were supplemented by practical work supervized by the lecturers and two staff members. The interaction about practical work was created trough a wikispace were the content of the courses and exercises were posted. A standardized computation environment in the form of a ‘’virtual machine’’ was provided for students using their own laptop, Extra laptops were provided by Centre Blaise Pascal for the students who did not bring their own.

The content of the lectures is described in detail below. They were completed by 10 presentations given by participants, and two research seminars of 1.30 each. Many of the students will make use of the credits provided by the school to validate master courses or graduate courses required by their graduate school.

The wiki space is accessible on http://houches2011.no-ip.org (login: jbarrat ; passwd: 12994521) A satisfaction poll was realized after the school. The poll is accessible on http://www.cbp.ens-lyon.fr/tiki-index.php?page=EvaluationForm. The results are commented in the ‘’IMPACT’’ section below.

Finally, we note that the school was generously supported by ESF, but also by the Rhône-Alpes node of CECAM, by the Ecole des Houches itself, and that it was granted the label ‘’predoc school’’ which corresponds to a reduced accommodation rate. This support made it possible to offer the students a full accommodation at a very low cost of 350 euros (for full board during two weeks). Moreover, all master students and all students coming from overseas or from less developed countries were fully supported for their accommodation.

SCIENTIFIC CONTENT

Lecture 1 : *Introduction to Monte-Carlo and Molecular Dynamics*,

Walter Kob

1) *Monte Carlo Technique*

- master equations and detailed balance
- the Monte Carlo Method

2) *Molecular Dynamics*

- Basic idea and various issues
- The Verlet algorithm

3) *Practical Issues*

- potential and forces
- periodic boundary conditions
- neighbor lists
- random number generators

4) *Advanced techniques*

- simulation at constant pressure, temperature
- Gibbs ensemble technique
- rare events

Lecture 2 : *Soft Matter on a Lattice : From generic properties to semi-quantitative models*,

Ralf Everaers

1) *Generic Polymer models / Monte Carlo techniques*

- Exact Enumeration
- Simple Sampling
- Dynamic Algorithms / Importance Sampling
- Dimerization
- Configurational Bias, Rosenbluth, PERM
- Performance of the different algorithms for simulating self-avoiding walks

2) *1d Poland-Sheraga model of cooperatively folding biopolymers*
3) *2d Lattice models of biomembranes*
4) *3d Lattice models of biopolymers*

- Generic aspects of protein folding
- A semi-quantitative lattice model of RNA and DNA melting, folding & association

Lecture 3 : *Molecular simulation approaches to polymer systems*,

J. Baschnagel

This course intends to give an introduction to molelcular simulation approaches of polymer systems. The computational study of the physical properties of polymers is challenging because of the extremely broad spectra of length and time scales governing their structure and dynamics. Therefore, the simulation models used in current research are obtained by some kind of coarse-graining procedure, designed to eliminate fast degrees of freedom. The resulting models can address phenomena over a specific window of time and length scales. This model-building step can take different levels of complexity, ranging from chemicallly realistic models over generic bead-spring models to coarse-grained representations of polymer systems inspired by self-consistent field theory or similar theoretical concepts and also tohierachical models encompassing many interconnected levels. After a brief introduction to polymer physics, serving as a justification for the coarse-graining idea, the course will discuss each level of modeling alluded to above, present adapted simulation strategies, and give example applications.

Lecture 4 : *Coarse-grained dynamics*,

Ignacio Pagonnabaraga

In these lectures I will describe the physical basis of kinetic based coarse grained methods to describe the dynamics of materials in the mesoscale. In particular, I will analyze the relationship between lattice gases and the lattice Boltzman approaches. I will explore the flexibility that these approaches offer to model a variety of complex fluids, including binary mixtures, colloidal

suspensions and electrolytes.

I will also address kinetically based methods which build on the knowldege of molecular modelling. In particular, MPCD combine the insight of Bird's approach to the Boltzmann equation with the knowledge developed in past decades on molecular modelling. Understanding the basic collision process from a more general perspective, MPCD can be applied to dense fluid systems, in regimes far beyond those which can be covered with the original Boltzmann equation. Momentum conserving thermostats (like dissipative particle dynamics or lowe-anderson thermostat) offer natural alternatives to model coarse grained fluids, and constitutive natural venues to explore the dynamics of complex fluids in the mesoscale . I will analyze critically the different approaches, their potentialities and limitations discussing representative examples.

Lecture 5 : *Phase field models*,

Thierry Biben

Phase field models are very efficient tools to investigate the dynamics of a system undergoing a phase transition, or simply to solve a problem with free boundaries (moving interfaces for example). They are essentially based on two ingredients: the phase-field, a local order parameter field, and the corresponding dynamical equations. The goal of this lecture is to give an overview of the wide range of problems that can be treated with these models and to provide a practical experience on the way to design phase field models and to avoid the main dangers. We shall thus illustrate the different parts of the lecture with examples, and use the problem of the dendric growth as a basic example.

Outline :
1 - Introduction: why and when is it interesting to use phase-field models?
2 - The Phase-Field:
a - Interfaces: Phase equilibrium, the square gradient theory and surface tension.
b - Allen-Cahn and Cahn-Hilliard equations.
3 - Conservation equations.
4 - An elementary example: Dendritic growth and implementation.
5 - Control of the model.
a - The Sharp Interface limit.
b - The "smooth interface problem" and possible solution.
6 - Various examples involving hydrodynamics, elasticity or heat transfer.

SEMINARS

Melting of hard disks

Werner KRAUTH, Département de Physique, Ecole Normale Supérieure, Paris

The hard-disk model has exerted outstanding influence on computational physics and statistical mechanics. Decades ago, hard disks were the first system to be studied by Markov-chain Monte Carlo methods and by molecular dynamics. It was in hard disks, through numerical simulations, that a two-dimensional melting transition was first seen to occur even though such systems cannot develop long-range crystalline order. Scores of theoretical, computational, and experimental works have analysed this fundamental melting transition, without being able to settle its nature.
The first-order melting scenario between a liquid and a solid (as in three dimensions), and the

Kosterlitz, Thouless, Halperin, Nelson and Young (KTHNY) scenario with an intermediate hexatic phase separated by continuous transitions from the liquid and the solid have been mainly focussed upon. Recently, we showed by large-scale simulations using the powerful Event-chain Monte Carlo algorithm that the hard-disk system indeed possesses a narrow hexatic phase, where orientational order is maintained across large samples while positional order is short-ranged. However, in difference with the KTHNY scenario, the liquid-hexatic phase transition is proven to be first-order. In this talk, I will give a general introduction to the field, present the new (and also the old) algorithms, and then discuss results, insights and possible generalizations.

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An overview of modern GPU computing : from architectures to applications.

Pierre KESTENER, de la Simulation, Saclay

PRESENTATIONS BY PARTICIPANTS

THURSDAY, June 30th		**CHAIR: RALF EVERAERS**	
10.40-11.00 am	Mechanisms of DNA Oligonucleotide Hybridization.	Dan Hinckley	Department of Chemical and Biological Engineering University of Wisconsin-Madison
11.00-11.20	Hydrodynamic interactions of 2 vesicles in a linear creeping shear flow	Pierre-Yves Gires	Laboratoire Interdisciplinaire de Physique Université Joseph Fourier, Grenoble
11.20-11.40	Testing non-equilibrium statistical mechanics in a 1D driven model	Milos Knezevic	Physics Department, University of Belgrad
11.40-12.00	"Early Stage aggregation studies of human amylin in solution"	Sadanand Singh	Department of Chemical and Biological Engineering University of Wisconsin-Madison
12.00-12.20	Non-affine droplets and shear deformation in a crystalline solid	Tamoghna Das	S.N.Bose National Centre for Basic Sciences, Kolkata
FRIDAY, July 1st		**CHAIR: JOERG BASCHNAGEL**	
9.-9.20am	Synthesis and characterisation of new biobased high-performance polyamide. Use of molecular modeling as a properties investigation tool	Thibaut Cousin	Institut des Matériaux Polymères, INSA Lyon
9.20-9.40	Surface effects of EMIM/FSI on LiFePO4	Volker Lesch	Department of physical chemistry, University of Münster
9.40-10.00	Coarse-grained modelling of DNA burnt-bridges motors	Peter Sulc	University of Oxford
10.-10.20	Dynamic Self Assembly of Photo-Switchable Nanoparticles	Prateek Kumar Jha	Chemical and Biological Engineering

			Northwestern University
10.20-10.40	Models of flowing amorphous media	Kirsten Martens	University of Lyon 1

IMPACT

The reactions and comments of the student, directly during the school and in the poll, indicated that they felt the event will be important for the development of their PhD thesis and corresponds to a real need. Numerical methods, as compared to theory or lab work, receive comparatively little attention in the curriculum of most students in physics and chemistry. The lectures given exposed them to the theoretical basis of the methods, but also to the more technical aspects which they could effectively put into practice during the afternoons. This scheme proved quite effective, especially with a relatively limited number of lecturers who were given enough time to get into the details of their topic.

We note that in spite of the fact that at least two similar schools are organized regularly in Europe (one in Amsterdam, and one by CCP5 in the UK) the number of applications and the level of applicants were excellent, which shows the need for such events.

The impact on the student is best summarized by quoting the answers obtained from the poll, which are summarized below. The list of questions is rather longs, with answers in the range 0 (strongly disagree) to 4 (strongly agree). The average of the 38 answers collected (out of 48) is given below for some of the most relevant questions (a complete response is available from the organizers on request):

The Summer School broadened my understanding of concepts and principles in the field of Computational physics and soft matter : 3.58/4
The Summer School improved my ability to carry out original research in the field of Computational physics and soft matter: 3.05/4
The Summer School taught me techniques directly applicable to my career: 3.25/4
The School helped me to meet new people working in my field: 3.37/4
The instructors explained the material well: 3.27/4
The practical work sessions were important for the learning process in the summer School: 3.05/4
The cost of the School was reasonable: 3.77/4
The Summer School was well organized: 3.68/4
Overall, the Summer School met my expectations: 3.47/4

Overall the satisfaction of the students apperas to have been quite high, with as only weak point the connection of the school to the internet with an insufficient bandwidth.

FINAL PROGRAM

	8.30-8.45	8h45-10h15	10h45-12h15	14h-16h	17h15-19h	20h45-22h
Monday, June 20th				Arrival	Arrival	
Tuesday, June 21st	Introduction	KOB 1	EVERAERS 1		KOB 2	
Wednesday, June 22nd		BASCHNAGEL 1	KOB 3	Practical work	BIBEN 1	
Thursday June 23rd		BASCHNAGEL 2	KOB 4	Practical work	EVERAERS 2	
Friday June 24th		BIBEN 2	BASCHNAGEL 3	Practical work	PAGONABARRAGA 1	KRAUTH
Saturday June 25th		PAGONABARRAGA 2	EVERAERS 3			
Monday June 27th		PAGONABARRAGA 3	EVERAERS4	Practical work	KOB 5	KESTENER
Tuesday June 28th		BASCHNAGEL 4	EVERAERS 5	Practical work	BIBEN 3	
Wednesday June 29th		BASCHNAGEL 5	BIBEN 4	Practical work	PAGONABARRAGA 4	
Thursday June 30th		BIBEN 5	Presentations by participants		PAGONABARRAGA 5	
Friday July 1st		Presentations by participants	Presentations by participants		Departure	

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