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Dr. Christian Caron
Springer Heidelberg
Physics Editorial Department I
Tiergartenstrasse 17
69121 Heidelberg/Germany
christian.caron@springer.com

Mauro Ferrario Giovanni Ciccotti Kurt Binder

Computer Simulations in Condensed Matter Systems: From Materials to Chemical Biology Volume 1

Springer

Editors

Professor Mauro Ferrario
Dipartimento di Fisica
Università di Modena e Reggio Emilia
Via Campi, 213/A
41100 Modena, Italy
E-mail: mauro.ferrario@unimore.it

Professor Kurt Binder
Institut für Physik
Universität Mainz
Staudinger Weg 7
55128 Mainz, Germany
E-mail: kurt.binder@uni-mainz.de

Professor Giovanni Ciccotti
Dipartimento di Fisica, INFN
Università di Roma La Sapienza
Piazzale Aldo Moro 2
00185 Roma, Italy
E-mail: giovanni.ciccotti@roma1.infn.it

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Preface

The school that was held at the Ettore Majorana Foundation and Center for Scientific Culture (EMFCSC), Erice (Sicily), in July 2005, aimed to provide an up-to-date overview of almost all technical advances of computer simulation in statistical mechanics, giving a fair glimpse of the domains of interesting applications. Full details on the school programme and participants, plus some additional material, are available at its Web site, `http://cscm2005.unimore.it`

Computer simulation is now a very well established and active field, and its applications are far too numerous and widespread to be covered in a single school lasting less than 2 weeks. Thus, a selection of topics was required, and it was decided to focus on perspectives in the celebration of the 65th birthday of Mike Klein, whose research has significantly pushed forward the frontiers of computer simulation applications in a broad range, from materials science to chemical biology. Prof. M. L. Klein (Dept. Chem., Univ. Pennsylvania, Philadelphia, USA) is internationally recognized as a pioneer in this field; he is the winner of both the prestigious Aneesur Rahman Prize for Computational Physics awarded by the American Physical Society, and its European counterpart, the Berni J. Alder CECAM Prize, given jointly with the European Physical Society. The festive session held on July 23rd, 2005, highlighting these achievements, has been a particular focus in this school. In the framework of the EMFCSC International School of Solid State Physics Series, the present school was the 34th course of its kind.

However, this school can be considered as being the third (and perhaps last?) event in a series of comprehensive schools on computer simulation, 10 years after the COMO Euroconference on "Monte Carlo and Molecular Dynamics of Condensed Matter systems," and 20 years after the VARENNA Enrico Fermi Summer School on "Molecular Dynamics of Statistical Mechanical Systems." Comparing the topics emphasized upon in these schools, both the progress in achieving pioneering applications to problems of increasing complexity, and the impressive number of new methodological developments are evident. While the focus of the Varenna School was mostly on Molecular Dynamics (MD) and its applications from simple to complex fluids, the Como school included both Monte Carlo (MC) simulations of lattice systems (from

quantum problems to the advanced analysis of critical phenomena in classical systems like the simple Ising model), and the density functional theory of electronic structure up to the Car-Parrinello ab initio Molecular Dynamics techniques (CPMD). At the Erice school, a new focus was put on the paradigma of "Multiscale Simulation", i.e. the idea to combine different methods of simulation on different scales of length and time in a coherent fashion. This method allow us to clarify the properties of complex materials or biosystems where a single technique (like CPMD or MD or MC etc.) due to excessive needs of computer resources is bound to fail. Good examples presented at this school for such multiscale simulation approaches included MD studies of polymers coupled with a solvent, which is described only in a coarse-grained fashion by the lattice Boltzmann technique and hybrid quantum mechanical/molecular mechanics (QM/MM) methods for CPMD simulations of biomolecules, etc.

As a second "leitmotif," emphasis has been put on rapidly emerging novel simulation techniques. Techniques that have been dealt with at this school include the methods of "transition path sampling" (i.e. a Monte Carlo sampling not intending to clarify the properties of a state in the space of thermodynamic variables, but the properties of the dominating paths that lead "in the course of a transition" from one stable state to another), density of state methods (like Wang-Landau sampling and multicanonical Monte Carlo, allowing an elegant assessment of free energy differences and free energy barriers, etc.) and so on. These techniques promise substantial progress with famous "grand challenge problems" like the kinetics of protein folding, as well as with classical ubiquitous problems like the theory of nucleation phenomena. Other subjects where significant progress in methodological aspects was made included cluster algorithms for off-lattice systems, evolutionary design in biomedical physics, construction of coarse-grained models describing the self-assembly and properties of lipid layers or of liquid crystals under confinement and/or shear, glass simulations, novel approaches to quantum chemistry, formulation of models to correctly describe the essence of dry friction and lubrication, rare event sampling, quantum Monte Carlo methods, etc. The diversity of this list vividly illustrates the breadth and impact that simulation methods have today.

While the most simple MC and MD methods have been invented about 50 years ago (the celebration of the 50th anniversary of the Metropolis algorithm was held in 2003, the 50th anniversary of the Alder-Wainwright spectacular first discovery by MD of the (then unexpected) phase transition in the hard sphere fluid is due in 2007), even the "second generation" of scientists, who started out 30-40 years ago as "simulators" are now already the "old horses" of the field, either close to the end of their scientific career, or, in the best case, near it. Thus, we can clearly observe that the task of developing the computer simulation methodology is further taken over with vigor by the "third generation" of well-established younger scientists who have emerged in the field. Because two of the organizers of the school (KB, GC) do belong to the "old horse" category, it was clearly necessary to get an energetic younger

co-organizer involved (MF), and we also felt it was the appropriate time that the most senior experts need not give the main lectures of the school, but rather the younger generation who are now most actively driving forward the frontier of research. Of course, it was crucial to involve the very valuable experience and knowledge of our senior colleagues into the school as well, and we are very glad that so many of them have accepted our invitation to give one-hour seminars providing tutorial introductions to various advanced research topics, which is at the heart of the research interests of the speakers. In this way, it was possible to produce an exciting event on the forefront of research on computer simulation in condensed matter, in a very stimulating and interactive atmosphere, with plenty of fruitful discussions.

It is with great pleasure that we end this preface with several acknowledgments. This school, of which the lecture notes are collected here, could not have taken place without the generous support of the European Community under the Marie Curie Conference and Training Courses, Contract No. MSCF-CT-2003-503840. We are grateful to the coordinators of this program, Michel Mareschal and Berend Smit, for their help in securing this support. We also wish to thank the CECAM secretaries, Emmanuelle Crespeau and Emilie Bernard.

We thank the Ettore Majorana Foundation and Centre for Scientific Culture in Erice, Sicily, for providing their excellent facilities to hold this school, and also Giorgio Benedek, Director of the International School of Solid State Physics, for the opportunity to hold our school as its 34th course: for his enthusiastic support during the school, and for his personal scientific participation. We are particularly grateful to him for providing the beautiful facilities of Erice.

MF thanks Davide Calanca, INFM-S3, Modena, for his valuable help in setting up the Web site of the school.

We thank the director of the physics department of the University of Rome "La Sapienza", Guido Martinelli, and the Administrative Secretary of the Department, Mrs. Maria Vittoria Marchet and her assistant, Mrs. Maria Proietto, for helping us in the difficult duty of managing all the financial matters. Mrs. Fernanda Lupinacci deserves grateful appreciation for her devoted and untiring presence and skillful help in overcoming all practical difficulties related to the organizational needs, and for providing a hospitable atmosphere to all the participants.

We are very grateful to Daan Frenkel, Mike Klein, and Peter Nielaba for their very valuable input when setting up the scientific program of the school, to all the lecturers, for their willingness to engage in the endeavor, and to all the participants, for their engagement and enthusiasm.

May 2006

Mauro Ferrario
Giovanni Ciccotti
Kurt Binder

Contents

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LNP 704 Computer Simulations in Condensed Matter Systems: From Materials to Chemical Biology Volume 2

List of Contributors

Jerry B. Abrams
Dept. of Chemistry
New York University
New York, NY 10003, U.S.A.
jerry.abrams@nyu.edu

Ali Alavi
University of Cambridge
Chemistry Department
Lensfield Road
Cambridge CB2 1EW, U.K.
asa10@cam.ac.uk

Axel Arnold
Max-Planck-Institut
für Polymerforschung
Ackermannweg 10
55128 Mainz, Germany
and
Frankfurt Institute for
Advanced Studies (FIAS)
Johann Wolfgang Goethe-Universität
Frankfurt/Main, Germany
arnolda@mpip-mainz.mpg.de

Kurt Binder
Institut fuer Physik
Universitaet Mainz
Staudinger Weg 7
D-55099 Mainz-Germany
Kurt.Binder@uni-mainz.de

Peter G. Bolhuis
van 't Hoff Institute for Molecular
Sciences
University of Amsterdam
Nieuwe Achtergracht 166
1018 WV Amsterdam
The Netherlands
bolhuis@science.uva.nl

Sara Bonella
NEST Scuola Normale Superiore
Piazza dei Cavalieri 7
It-56126 Pisa
s.bonella@sns.it

David M. Ceperley
Department of Physics and NCSA
University of Illinois at
Urbana-Champaign
Urbana IL 61801, U.S.A.
david.ceperley@uiuc.edu

Giovanni Ciccotti
Dipartimento di Fisica
Università "La Sapienza"
Piazzale Aldo Moro
2 00185 Roma, Italy
giovanni.ciccotti@roma1.infn.it

David F. Coker
Department of Chemistry
Boston University
590 Commonwealth Avenue
Boston, MA 02215, U.S.A.
coker@bu.edu

Christoph Dellago
Faculty of Physics
University of Vienna
Boltzmanngasse 5
1090 Wien, Austria
Christoph.Dellago@univie.ac.at

Evelyn Dittmer
Institut für Mathematik II
Freie Universität Berlin
Arnimallee 2–6
14195 Berlin, Germany
dittmer@math.fu-berlin.de

Ron Elber
Department of Computer Science
Cornell University
4130 Upson Hall
Ithaca NY 14853
ron@cs.cornell.edu

Mauro Ferrario
Dipartimento di Fisica
Università di Modena e
Reggio Emilia
Via G. Campi 213/A
I-41100 Modena-Italy
Mauro.Ferrario@unimore.it

Daan Frenkel
FOM Institute for Atomic
and Molecular Physics (AMOLF)
Kruislaan 407
1098 SJ Amsterdam
The Netherlands
frenkel@amolf.nl

Phillip L. Geissler
Department of Chemistry
University of California
at Berkeley
94720 Berkeley, CA, U.S.A.
geissler@cchem.berkeley.edu

Christian Holm
Max-Planck-Institut für
Polymerforschung
Ackermannweg 10
55128 Mainz, Germany
and
Frankfurt Institute for
Advanced Studies (FIAS)
Johann Wolfgang Goethe-Universität
Frankfurt/Main, Germany
c.holm@fias.uni-frankfurt.de

Illia Horenko
Institut für Mathematik II
Freie Universität Berlin
Arnimallee 2–6
14195 Berlin, Germany
horenko@math.fu-berlin.de

Jürg Hutter
Physical Chemistry Institute
University of Zurich
Winterthurerstrasse 190
8057 Zurich, Switzerland
hutter@pci.unizh.ch

Marcella Iannuzzi
Physical Chemistry Institute
University of Zurich
Winterthurerstrasse 190
8057 Zurich, Switzerland
marcella@pci.unizh.ch

Raymond Kapral
Chemical Physics Theory Group
Department of Chemistry
University of Toronto
Toronto, ON M5S 3H6, Canada
rkapral@chem.utoronto.ca

Alessandro Laio
Statistical and Biological Physics
SISSA – International School for Advanced Studies
Via Beirut 2
34100, Trieste, Italy
Laio@sissa.it

Erik Luijten
Department of Materials Science and Engineering
Frederick Seitz Materials Research Laboratory
University of Illinois at Urbana-Champaign
Urbana, Illinois 61801, U.S.A.
luijten@uiuc.edu

Bernward A.F. Mann
Max-Planck-Institut für Polymerforschung
Ackermannweg 10
55128 Mainz, Germany
mann@mpip-mainz.mpg.de

Glenn J. Martyna
T.J. Watson Research Center
International Business Corporation
P.O. Box 218, Yorktown Heights
NY 10598, USA
martyna@us.ibm.com

Eike Meerbach
Institut für Mathematik II
Freie Universität Berlin
Arnimallee 2–6
14195 Berlin, Germany
meerbach@math.fu-berlin.de

Marcus Müller
Institut für Theoretische Physik
Georg-August-Universität
37077 Göttingen, Germany
mmueller@theorie.physik.uni-goettingen.de

Michele Parrinello
Computational Science
Dept. of Chemistry and Applied Biosciences
ETH Zurich. c/o USI Campus
Via Buffi 13
6900 Lugano, Switzerland
parrinello@phys.chem.ethz.ch

Juan J. de Pablo
Department of Chemical and Biological Engineering
University of Wisconsin-Madison
Madison Wisconsin 53706-1691, U.S.A.
depablo@engr.wisc.edu

Carlo Pierleoni
Department of Physics
University of L'Aquila
Polo di Coppito, Via Vetoio
L'Aquila, 67010, Italy
carlo.pierleoni@aquila.infn.it

Christof Schütte
Institut für Mathematik II
Freie Universität Berlin
Arnimallee 2–6
14195 Berlin, Germany
schuette@math.fu-berlin.de

Alex J.W. Thom
University of Cambridge
Chemistry Department
Lensfield Road
Cambridge CB2 1EW, U.K.
ajwt3@cam.ac.uk

Simon Trebst
Microsoft Research and Kavli Institute for Theoretical Physics
University of California
Santa Barbara, CA 93106, U.S.A.
trebst@kitp.ucsb.edu

Matthias Troyer
Theoretische Physik
ETH Zürich
CH-8093 Zürich, Switzerland
troyer@comp-phys.org

Mark E. Tuckerman
Courant Institute
of Mathematical Sciences
New York University
New York, NY 10003, U.S.A.
mark.tuckerman@nyu.edu

Eric Vanden-Eijnden
Courant Institute
of Mathematical Sciences
New York University
New York, NY 10012
eve2@cims.nyu.edu

Joost VandeVondele
Department of Chemistry
University of Cambridge
Lensfield Road
Cambridge CB2 1EW, U.K.
jv244@hermes.cam.ac.uk

Rodolphe Vuilleumier
Laboratoire de Physique
Théorique de la Matière
Condensée, Tour 24-25
$2^{\text{ème}}$ étage c.c. 121
Universitè Pierre
et Marie Curie
4 place Jussieu
F-75005 Paris, France
rodolphe.vuilleumier-
@lptmc.jussieu.fr

N.B. Wilding
Department of Physics
University of Bath
Bath, BA2 7AY, United Kingdom
N.B.Wilding@Bath.ac.uk