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Boston University

XXVI IUPAP Conference on Computational Physics (CCP2014)

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26th IUPAP Conference on Computational Physics

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1. Editorial

The 26th IUPAP Conference on Computational Physics, CCP2014, was held in Boston, Massachusetts, during August 11-14, 2014. Almost 400 participants from 38 countries convened at the George Sherman Union at Boston University for four days of plenary and parallel sessions spanning a broad range of topics in computational physics and related areas.

The first meeting in the series that developed into the annual Conference on Computational Physics (CCP) was held in 1989, also on the campus of Boston University and chaired by our colleague Claudio Rebbi. The express purpose of that meeting was to discuss the progress, opportunities and challenges of common interest to physicists engaged in computational research. The conference having returned to the site of its inception, it is interesting to reflect on the development of the field during the intervening years. Though 25 years is a short time for mankind, computational physics has taken giant leaps during these years, not only because of the enormous increases in computer power but especially because of the development of new methods and algorithms, and the growing awareness of the opportunities the new technologies and methods can offer. Computational physics now represents a "third leg" of research alongside analytical theory and experiments in almost all subfields of physics, and because of this there is also increasing specialization within the community of computational physicists. It is therefore a challenge to organize a meeting such as CCP, which must have sufficient depth in different areas to hold the interest of experts while at the same time being broad and accessible. Still, at a time when computational research continues to gain in importance, the CCP series is critical in the way it fosters cross-fertilization among fields, with many participants specifically attending in order to get exposure to new methods in fields outside their own.

As organizers and editors of these Proceedings, we are very pleased with the high quality of the papers provided by the participants. These articles represent a good cross-section of what was presented at the meeting, and it is our hope that they will not only be useful individually for their specific scientific content but will also represent a historical snapshot of the state of computational physics that they represent collectively.

The remainder of this Preface contains lists detailing the organizational structure of CCP2014, endorsers and sponsors of the meeting, plenary and invited talks, and a presentation of the 2014 IUPAP C20 Young Scientist Prize.

We would like to take the opportunity to again thank all those who contributed to the success of CCP214, as organizers, sponsors, presenters, exhibitors, and participants.

Anders Sandvik, David Campbell, David Coker, Ying Tang

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3. IUPAP Young Scientist Price

The 2014 IUPAP Young Scientist Prize for Computational Physics was awarded at CCP2014 by the C20 Commission to Professor Mathieu Salanne of Université Pierre et Marie Cure, Paris, France, in recognition of his development of appropriate methods to allow realistic atomistic

simulation of molten salts and ionic liquids in situations of relevance to electrochemistry. For further information on the Prize and the nomination process, please see information on line at `http://phycomp.technion.ac.il/~C20/prizes.html`.

4. Endorsers and Sponsors of CCP2014

4.1. Endorsers

CCP2014 was endorsed by the following professional organizations

- The International Union of Pure and Applied Physics (IUPAP)
- The American Physical Society (APS)
- The European Physical Society (EPS)
- The Association of Asia Pacific Physical Societies (AAAPS)

4.2. Sponsors

CCP2014 was sponsored financially by the IUPAP, APS, and the following universities in the Boston area

- Boston University
- Boston College
- Clark University
- Harvard University (Institute for Applied Computational Science)
- Northeastern University
- University of Massachusetts Amherst
- University of Massachusetts Boston

as well as by these corporations

- Intel Corporation
- Cambridge University Press
- Elsevier
- Institute of Physics Publishing
- American Institute of Physics Publishing

We would like to take this opportunity to thank all the sponsors for their generous support, which was critical to the success of CCP2014.

To secure IUPAP sponsorship, the organizers have provided assurance that CCP2014 will be conducted in accordance with IUPAP principles as stated in the ICSU document *Universality of Science* (sixth edition, 1989) regarding the free circulation of scientists for international purposes. In particular, no bona fide scientist will be excluded from participation on the grounds of national origin, nationality, or political considerations unrelated to science.

5. Plenary Presentations

A total of 15 plenary talks were presented over the four days of the meeting. They were formally organized into two sections, with presenters and titles as follows (in order of appearance):

General Computational Physics

- Sauro Succi (IAC-CNR, Italy), *Lattice Boltzmann simulations of complex flows across scales: turbulence, soft- glasses and quark-gluon plasmas*
- Yuko Okamoto (Nagoya University, Japan), *Enhanced configurational sampling methods for spin systems and biomolecular systems*
- Nandini Trivedi (Ohio State University, USA), *Topology and Correlations driving new materials, phases and phenomena*
- Helmut Katzgraber (Texas A&M University, USA), *Four decades of frustration in spin-glass physics: Advances and applications*
- A. Peter Young (University of California, Santa Cruz, USA), *Numerical Studies of the Quantum Adiabatic Algorithm*
- Ursula Rothlisberger (Ecole Polytechnique Federale de Lausanne, Switzerland), *Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Simulations of Biological Systems: From Understanding to Control*
- Brian Granger (California Polytechnic State University, USA), *Open source tools for exploratory and reproducible computational physics*
- Steven Louie (University of California, Berkeley, and Lawrence Berkeley National Lab, USA), *GW-based Methods for ab initio Studies of Electronic Excited-State Phenomena in Condensed Matter*
- Steven White (University of California, Irvine, USA), *Solving frustrated magnetic systems with the density matrix renormalization group*
- Luigi Del Debbio (University of Edinburgh, UK), *Recent progress in simulations of gauge theories on the lattice: QCD at the physical point and new strongly-interacting dynamics beyond the Standard Model*
- Romeel Davé (University of the Western Cape, South Africa), *Simulations of Galaxy Formation*

Enabling Technologies for Computational Science

- John Danskin (NVIDIA), *The Physics of Computation and GPU Architecture*
- Karl Schulz (Intel), *Enabling Technology Trends in High Performance Computing*
- Thomas Sterling (Center for Research in Extreme Scale Technologies, Indiana University, USA), *Computational Physics at Extreme Scale*
- James Sexton (IBM), *A Vision for Data Centric Systems*

6. Parallel and Poster Sessions

The parallel sessions were organized as ten different tracks with a mix of invited (30 minute) and contributed (15 minute) talks, and one session on General Computational Physics with eight contributed talks. In total, 52 invited talks and almost 100 contributed presentations were given. A poster session with almost 100 presenters was held during the first evening of the conference. The invited talks are listed below.

Statistical Physics

- Mark Newman, (University of Michigan, USA), *Large-scale structure in networks*
- Lenka Zdeborova, (CEA Saclay and CNRS, France), *Module detection in networks: phase transitions and optimal algorithms*
- Werner Krauth, (ENS Paris, France), *Rejection-free, Irreversible, and Infinitesimal Monte Carlo Algorithms and Melting in two dimensions*
- Salvatore Torquato (Princeton University, USA), *New Algorithm to Generate Jammed Sphere Packings*
- Youjin Deng (University of Science and Technology of China), *Universal amplitudes in the canonical ensemble*
- Koji Hukushima (University of Tokyo, Japan), *Equilibrium-state simulations of some (spin) glass models in finite dimensions*

Soft Matter and Biological Physics

- Mark Robbins (Johns Hopkins University, USA), *Welding and healing of polymer interfaces: Strength from entanglements*
- Marcus Müller, (Georg-August-Universität, Germany), *Studying the kinetics of copolymer self-assembly*
- Ivet Bahar, (University of Pittsburgh, USA), *Structure-Encoded Dynamics of Proteins: Learning from Network Models and Experiments*
- Normand Mousseau (Université de Montréal, Canada), *Computational challenges for the study of amyloid processes*
- Marina Guenza (University of Oregon, USA), *A coarse-graining method that preserves the free energy, structural correlations, and thermodynamic state of polymer melts from the atomistic to the mesoscale*
- Celeste Sagui (North Carolina State University, USA), *Free energy methods for biomolecular simulations*

Materials Science and Nanoscience

- Markus Eisenbach (Oak Ridge National Laboratory, USA), *Magnetic Materials at finite Temperatures: thermodynamics and combined spin and molecular dynamics derived from first principles calculations*
- Lin-lin Wang (Ames Laboratory, USA), *Computational Modeling of Transition-Metal Alloyed Nanoparticles in Working Condition*
- Hsin Lin (National University of Singapore), *Topological Crystalline Insulators: A New Phase of Quantum Matter*
- Caterina Cocchi (Humboldt-Universität zu Berlin, Germany), *From Molecules to Organic Crystals: Optical Excitations from First Principles*
- Volodymyr Turkowski (University of Central Florida, USA), *Development and application of DFT+DMFT and TDDFT+DMFT techniques for nanosystems*
- Luca Ghiringhelli, (Fritz Haber Institute, Germany), *Big Data of Materials Science - Critical Role of the Descriptor*

Fluid Dynamics

- Monika Nitsche (University of New Mexico, USA), *Vortex Shedding and Low Order Models*
- George Karniadakis (Brown University, USA), *Microscopic theory of Brownian motion: Effects of memory and confinement*
- Marc Gerritsma (TU Delft, The Netherlands), *Structure preserving discretizations for computational physics*
- Chun Liu, (Penn State University, USA), *Energetic Variational Approaches in Complex Fluids*

Quantum Many-Body Physics

- Ribhu Kaul (University of Kentucky, USA), *Deconfined quantum criticality in SU(N) magnets*
- Boris Svistunov (University of Massachusetts Amherst, USA), *Diagrammatic Monte Carlo for Fermionic and Fermionized Systems*
- Federico Becca (CNR and SISSA, Trieste, Italy), *Variational wave functions for strongly-correlated models*
- Philippe Corboz (University of Amsterdam, The Netherlands), *Recent progress in simulating strongly correlated systems with tensor network methods*
- Tao Xiang (Institute of Physics, Chinese Academy of Sciences, China), *Renormalization of quantum many-body systems by the projected entangled simplex states*
- Corinna Kollath (University of Bonn, Germany), *Spreading of correlations in strongly correlated (dissipative) quantum gases*

Quantum Computing

- David Clader (Johns Hopkins University, USA), *Preconditioned quantum linear system algorithm*
- Bryan Clark (University of Illinois at Urbana-Champaign, USA), *The cost of simulating quantum mechanics on a quantum computer*
- Sergio Boixo (Google, USA), *Experiments with the D-Wave prototype*

Lattice Field Theory

- Taku Izubuchi (RIKEN, Japan, and BNL Research Center, USA), *Lattice QCD calculations for particle physics*
- Aida El-Khadra (University of Illinois at Urbana-Champaign, USA), *Lattice QCD and Quark Flavor Physics*
- John Negele (MIT, USA), *Understanding the Structure of Nucleons using Lattice QCD*
- William Detmold (MIT, USA), *Dark Nuclei*
- Simon Catterall, (Syracuse University, USA), *Supersymmetry on a lattice*
- Frithjof Karsch (Brookhaven National Laboratory, USA), *Conserved charge fluctuations in strong interaction matter*

Novel Computing Paradigms

- Thomas Cheatham (University of Utah, USA), *Molecular dynamics simulation of nucleic acids: Convergence, reproducibility, assessment/validation, and data dissemination enabled by GPUs on XSEDE and Blue Waters*
- Ying-jer Kao (National Taiwan University, Taipei, Taiwan), *Uni10: the Universal Tensor Network Library*
- Martin Berzins (University of Utah, USA), *Multiscale and Multiphysics Computations on Present and Future Architectures*
- Erik Schnetter (Perimeter Institute, Canada), *Automated Code Generation for Solving PDEs on Modern HPC Architecture*
- Norbert Attig (Jülich Supercomputing Centre, Germany), *The Path to Exascale: A European Perspective*
- Lars Korsterke (Texas Advanced Computing Center, USA), *Heterogeneous computing. What is it and do we need it?*

Astrophysics

- Mike Boylan-Kolchin (University of Maryland, USA), *The Local Universe as a Dark Matter Laboratory*
- Claude-Andre Faucher-Giguere (Northwestern University, CIERA, USA), *The Universe on a computer: Cosmological simulations of galaxy formation*
- Christian David Ott (Caltech, USA), *Petascale Simulations of Core-Collapse Supernovae*
- Deirdre Shoemaker (Georgia Tech, USA), *Numerical Relativity and Gravitational Waves*

Computational Physics Education

- Ruth Chabay (North Carolina State University, USA), *Computation and Conceptual Understanding in Introductory Physics*
- Francisco Esquembre, (Universidad de Murcia, Spain), *Facilitating programming computational physics simulations for tablets*
- Beate Schmittmann (Iowa State University, USA), *K-12 outreach and student recruitment with computational science*
- Spencer Wheaton (University of Cape Town, South Africa), *Infusing Computational Physics throughout the Undergraduate Curriculum*
- Shobhana Narasimhan (Jawaharlal Nehru Centre for Advanced Scientific Research, India), *Teaching Density Functional Theory through Experiential Learning: Examples from the Developing World*