

# XXVII IUPAP Conference on Computational Physics

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## Editorial

The 27th IUPAP Conference on Computational Physics, CCP2015, was held in the heritage city Guwahati, in the eastern part of India, next to the mighty river Brahmaputra, during December 2-5, 2015. The Conference on Computational Physics is organized annually under the auspices of Commission 20 (C20) of the IUPAP (International Union of Pure and Applied Physics). This is the first time it has been held in India. Almost 300 participants from 25 countries convened at the auditorium and lecture halls at the Indian Institute of Technology Guwahati for four days. Thirteen plenary speakers, fifty six invited speakers, three presnters from the computer industries and two hundred and eight contributory participants covered a broad range of topics in computational physics and related areas. Thirty eight women participated in CCP2015 and seven of them presented invited talks. This volume of Journal of Physics: Conference Series contains the proceedings of the scientific contributions presented at the Conference.

The main purpose of the meeting was to discuss the progress, opportunities and challenges of common interest to physicists engaged in computational research. Computational physics has taken giant leaps during the lat few years, not only because of the enormous increases in computer power but especially because of the development of new methods and algorithms. Computational physics now represents a third leg of research alongside analytical theory and experiments. A meeting such as CCP, must have sufficient depth in different areas and at the same time should be broad and accessible. The topics covered in this conference were: Materials/Condensed Matter Theory and Nanoscience, Strongly Correlated Systems and Quantum Phase Transitions, Quantum Chemistry and Atomic Physics, Quantum Chromodynamics, Astrophysics, Plasma Physics, Nuclear and High Energy Physics, Complex Systems: Chaos and Statistical Physics, Macroscopic Transport and Mesoscopic Methods, Biological Physics and Soft Materials, Supercomputing and Computational Physics Teaching, Computational Physics and Sustainable Energy.

As organizers and editors of these Proceedings, we are very pleased with the number and the quality of the papers provided by the participants. The papers cover a good cross-section of what was presented at the meeting. We are sure that these will represent the state of the computational physics today. The remainder of this Preface contains lists detailing the organizational structure of CCP2015, endorsers and sponsors of the meeting, plenary and invited talks, and a presentation of the 2015 IUPAP C20 Young Scientist Prize.

Finally, we would like to express our sincere thanks to our sponsors and endorsers: C20 Commission of International Union of Pure and Applied Physics (IUPAP); Division of Computational Physics, American Physical Society (APS); European Physicsl Society (EPS);



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Association of Asia Pacific Physical Societies (AAAPS), Intel Software; Nvidia; Fujitsu; Netweb Technologies; The Institute of Mathematical Sciences Chennai, and finally Indian Institute of Technology Guwahati. We are grateful to the organizing committee, the International Advisory Board, the local organizing committee and participants who helped in making CCP2015 a success.

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## IUPAP Young Scientist Award

The 2014 IUPAP Young Scientist Prize for Computational Physics was awarded during CCP2015 at IIT Guwahati by the C20 Commission to Professor Mathieu Salanne of Université Pierre et Marie Curie, Paris, France, as Dr Salanne could not attend the CCP2014, 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.

The 2015 Young Scientist Prize awarded to Dr. Wei-Min Wang at Laser-plasma physics of the Institute of Physics, Chinese Academy of Sciences, China for his significant achievements in computational plasma physics with applications to advanced schemes of inertial confined fusion and novel laser-plasma based particle accelerators and radiation sources. However, the prize was not presented to Dr. Wang at the CCP2015 because of his inability to attend CCP2015.

For further information on the Prize and the nomination process, please see information online at <http://phycomp.technion.ac.il/~C20/prizes.html>

## Endorsers and Sponsors of CCP2015

The organizations who sponsor or endorse CCP2015 are listed below:

- 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)
- Intel Software
- Nvidia
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- Netweb Technologies
- The Institute of Mathematical Sciences, Chennai, India
- Indian Institute of Technology Guwahati, India

We would like to take this opportunity to thank all the sponsors for their generous support, which was critical to the success of CCP2015.

## Plenary Presentations

A total of 13 plenary talks were presented over the four days of the meeting. The title of the presentation with presenters affiliation are listed below:

- Annette Zippelius, University of Goettingen, Germany, *Dense Granular Flow of Frictional Particles*
- Barry I. Schneider, National Institute of Standards and Technology, USA, *How Novel Algorithms and Access to High Performance Computing Platforms are Enabling Scientific Progress in Atomic and Molecular Physics*
- Carlo Massimo Casciola, University of Rome La Sapienza, Italy, *Energy fluxes, scale energy and turbulent separation*
- Gabriel Kotliar, Rutgers University, USA, *Understanding Strongly Correlated Materials thru Theory Algorithms and High Performance Computers*

- Hans J. Herrmann, ETH Zurich, Switzerland, *Packing of wires in cavities and growing surfaces*
- Luca Baiotti, Osaka University, Japan, *Numerical relativity for binary neutron-star mergers*
- Norbert Attig, Juelich Supercomputing Centre, Germany, *Impacts of Current Hardware and Software Developments on Simulation Sciences*
- Richard Martin, Illinois State University, USA, *Undergraduate Computational Physics Education: Uneven History and Promising Future*
- Shyam S Rai, Indian Institute of Science Education and Research Pune, India, *Imaging Earths Interior through Noise Interferometry*
- Steve Gottlieb, Indiana University, USA, *Lattice Field Theory Applications in High Energy and Nuclear Physics*
- Turab Lookman, Los Alamos National Laboratory, USA, *Information-driven approach to materials discovery and design*
- William Goddard, California Institute of Technology, USA, *In silico predictions of 3D structures and binding sites for GPCRligand complexes*
- Yutaka Ishikawa, RIKEN Advanced Institute for Computational Science, Japan, *An Overview of the Next Flagship Supercomputer in Japan*

### Industry Sessions

- Austin Cherian, INTEL Software
- Ashok Chaudhary, FUJITSU
- Gaurav Mishra, NVIDIA
- Rama Kishan V Malladi, INTEL Software

### Parallel and Poster Sessions

The parallel sessions were organized as eleven 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, 56 invited talks and almost 100 contributed presentations were given. Poster sessions with almost 100 presenters were held during the conference. The invited talks are listed below:

#### Statistical Physics, Complex system and Non-linear Dynamics

- Jian-Sheng Wang, National University of Singapore, Singapore, *Computational methods for quantum thermal transport in nanostructures*
- Mathis Plapp, Ecole Polytechnique, Palaiseau, France, *Phase-field models for the growth and evolution of complex structures*
- Pinaki Chaudhuri, IMSc Chennai, India, *Onset of flow in soft glasses: linking percolation to flow*
- Sitabhra Sinha, IMSc Chennai, India, *Chaos, Complexity and Computation: Patterns in oscillatory media*
- Smarajit Karmakar, TIFR Hyderabad, India, *Short-time  $\beta$ -relaxation in glass-forming liquids is cooperative in nature*

- Wolfram Janke, Institut für Theoretische Physik, Germany, *Finite-Size Scaling at the Droplet Condensation-Evaporation Transition*

### Soft materials and Polymer Physics

- Michael Bachmann, University of Georgia, *Statistical Analysis of Transitions in Finite Polymer Systems*
- Rajarshi Chakrabarti, IIT Bombay, India, *Single polymer chain with internal friction*
- Sumesh P Thampi, IIT Madras, India, *Intrinsic free energy in active nematics*
- Takahiro Hatano, University of Tokyo, Japan, *Critical slowing down at jamming transition*
- Tanja Schilling, University of Luxembourg, Luxembourg, *Percolation in colloidal model systems*

### Computational Biological Physics

- Birgit Strodel, Structural Biochemistry Research Centre Juelich, Germany, *Thermodynamics and kinetics of amyloid aggregation from atomistic simulations*
- Durba Sengupta, NCL Pune, India, *Association at the membrane: Do lipophobic effects mediate membrane protein assembly?*
- Prabal Kumar Maiti, IISc Bangalore, India, *Effect of Dendrimer in HIV-1 inhibition*
- Sanjoy Bandyopadhyay, IIT Kharagpur, India, *Correlated conformational features and hydration dynamics of protein-DNA complexes*

### Quantum many body and strongly correlated systems

- Federica Agostini, Max-Planck-Institut Halle, Germany, *Electron-Nuclear Correlation: A Time-Dependent Perspective*
- Hong-Gang Luo, Lanzhou University, China, *Phase diagram of one-dimensional t-J model with long-range dipolar interactions*
- Kedar S. Damle, TIFR Mumbai, India, *Sign-free Quantum Monte Carlo simulation of certain frustrated quantum magnets*
- Mark Jarrell, Louisiana State University, USA, *Typical Medium Dynamical Cluster Simulations of Interacting and Strongly Disordered Systems*
- Silke Biermann, École Polytechnique, France, *Screened exchange dynamical mean field theory*
- Wei Ku, Brookhaven National Lab, USA, *Spin/Orbital Correlation and Itinerancy-Enhanced Quantum Fluctuation in Iron-Based Superconductors*

### Material and Nano Sciences

- A Marco Saitta, UPMC, France, *Reaction networks and free-energy landscapes via a novel topological approach: ab initio Miller-like experiments and beyond*
- G. P. Das, IACS Kolkata, India, *Substrate induced modulation of physical and chemical properties of quasi two-dimensional nanostructures*
- Priya Mahadevan, SNBNCBS Kolkata, India, *The dilute magnetic semiconductors: A playground for the ZaanenSawatzky-Allen phase diagram*
- Rajeev Ahuja, Uppsala University, Sweden, *Materials for Li & Na Batteries : A Computational Materials Science Point of View*
- Stefano Sanvito, Trinity College Dublin, Ireland, *The magnetic genome project*
- Yuan-Ping Feng, NUS, Singapore, *2D Materials and Devices for Spintronics: First-principles Studies*

### Atomic, Molecular and Optical Physics

- Dibakar Roy Chowdhury, Mahindra Ecole Centrale Hyderabad, India, *Near field coupled Metamaterials for Terahertz Wavelengths*
- E. Krishnakumar, TIFR Mumbai, India, *Dynamics of Electron - Molecule Resonances: A Challenge to Computational Physics*
- Gagan Kumar, IIT Guwahati, India, *Terahertz guided wave devices using plasmonic metamaterials*
- Gautam Vemuri, Indiana University, USA, *Realization of a PT-symmetric dimmer in coupled semiconductor lasers*
- Harishankar Ramachandran, IIT Madras, India, *Modelling Dielectric Structures with Bends using the Beam Propagation Method*
- Harshawardhan Wanare, IIT Kanpur, India, *Interplay between light and magnetic field in inducing anisotropy in atomic systems*
- Satrajit Adhikari, IACS Kolkata, India, *Beyond Born-Oppenheimer Theories: Diabatic PESs for Spectroscopic & Scattering Processes*

### Astrophysics, Plasma, Gravitation and Cosmology

- Adam Amara, ETH Zurich, Switzerland, *Information from Cosmology Experiments*
- Ganesh Rajaraman, IPR Gandhinagar, India, *Strongly correlated classical plasmas under external forcing and dissipation - examples using molecular dynamics approach*
- Parameswaran Ajith, ICTS Bangalore, India, *Towards gravitational-wave astronomy*
- Pankaj Joshi, TIFR Mumbai, India, *Gravitational Collapse, Black Holes and Space-time Singularities in Einstein Gravity*
- Tarun Souradeep, IUCAA Pune, India, *Bayesian Cosmological inference beyond statistical isotropy*

### High energy, Nuclear and Particle Physics

- Andreas Juettner, University of Southampton, UK, *Flavour physics and lattice QCD*
- Nilmani Mathur, TIFR Mumbai, India, *Heavy quark physics using large scale simulations*
- Pushan Majumdar, IACS Kolkata, India, *Lattice QCD simulations using the OpenACC platform*
- Satyaki Bhattacharya, Saha Institute of Nuclear Physics, India, *Multivariate techniques in analysis of the LHC data*
- Yoshinobu Kuramashi, University of Tsukuba, Japan, *Tensor Network scheme for lattice gauge theories*

### Fluid Dynamics, Oceanography, Geophysics and Climate modeling

- Gautam Biswas, IIT Guwahati, India, *Simulation of Multi-Fluid System: Understanding Drop Impact*
- L. S. Luo, Old Dominion University, USA, *Multiscale Modeling and Simulation of Gaseous Microflows*
- Prasad Perlekar, TIFR Hyderabad, India, *Two and three-dimensional binary-fluid turbulence*
- Rajeev Bhatla, Banaras Hindu University, India, *Simulation of different phases of Indian summer monsoon using Regional Climate Model*
- Ronojoy Adhikari, IMSc Chennai, India, *Computation of many-body hydrodynamic interactions in active colloidal suspensions*

- Tapan K Sengupta, IIT Kanpur, India, *Non-equilibrium thermodynamics of Rayleigh-Taylor instability*
- Tapan Mukerji, Stanford University, USA, *Computational Rock Physics: Imaging and Process Modeling at the Pore Scale*

### Computational Physics Education

- Ananda Dasgupta, IISER Kolkata, India, *Open Source Computation in Physics Education*
- KPN Murthy, University of Hyderabad, India, *Non-Boltzmann Ensembles and Monte Carlo Simulation*
- Scott A Lathrop, University of Illinois, USA, *Expanding Access to Computational Science Education*

### Software and Hardware development

- Prabhu Ramachandran, IIT Bombay, India, *Extensible, reusable, and reproducible computing: a case study of PySPH*
- Scott A. Klasky, ORNL, USA, *SIRIUS: Science-driven Data Management for Multi-tiered Storag*