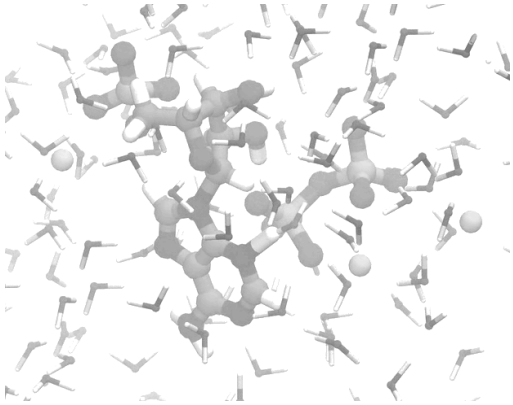
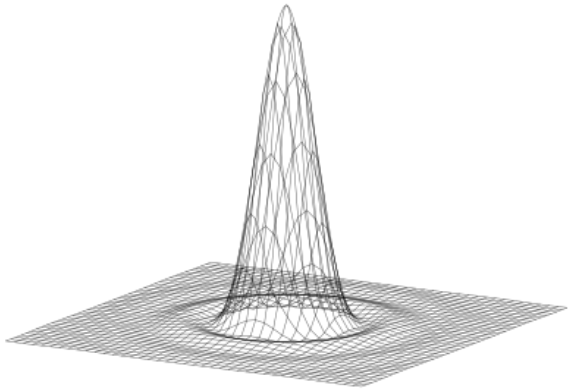
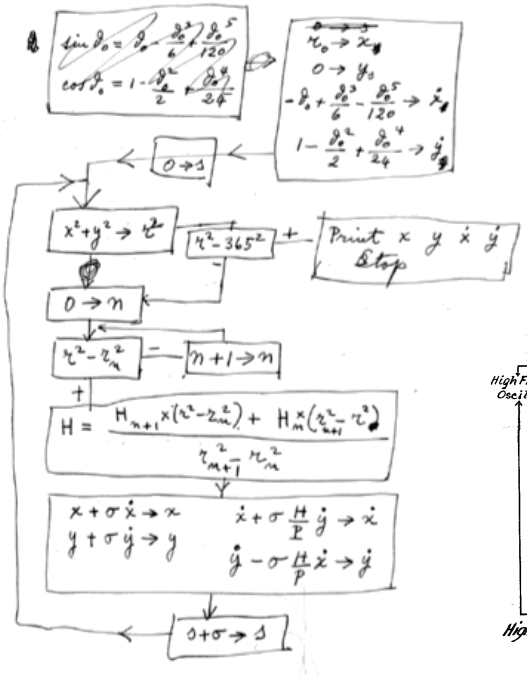
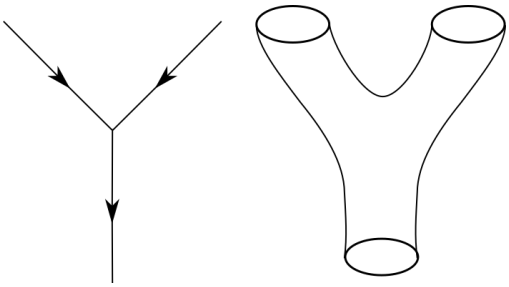
The XXIXth IUPAP Conference on Computational Physics

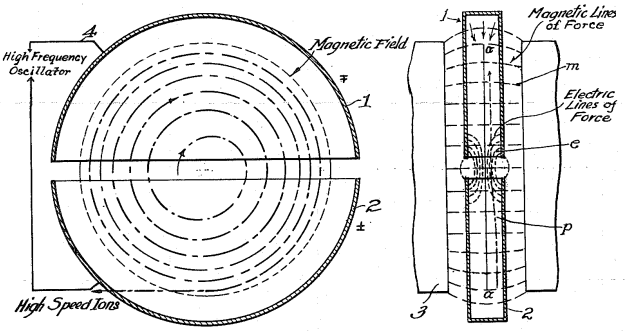
CCP2017











Paris, 9-13 July 2017

Welcome to CCP2017

We are delighted to welcome you to the XXIXth IUPAP Conference in Computational Physics at the Campus Jussieu, UPMC, ideally located in the center of Paris. Attendees can look forward to three and a half days of exciting and stimulating talks covering all fields of computational physics. These include nine plenary lectures in the main auditorium of the conference center. The Young Scientific Prize 2017 of the IUPAP C20 commission will be awarded on this occasion to Glen Evenbly. The conference is followed by one half-day spin-off meeting on the history of simulation.

The IUPAP Conference in Computational Physics (CCP) is a series of conferences held annually under the auspices of the International Union of Pure and Applied Physics (IUPAP) on the basis of endorsement by its Commission on Computational Physics (C20). The application of computation is ever increasing and far-reaching in all aspects of science and so in physics. It is a major building block of the modern day science. This 29th edition will present the latest techniques and discoveries to the computational scientists working in various branches in physics and closely related areas.

The proceedings of the conference will be published in the open access Journal of Physics: Conference Series (JPCS) from IOPscience. The book of abstract can be downloaded for free from the conference website.

CCP2017 is grateful to its local host UPMC and to the sponsoring institutions for their support and to all participants for contributing to a rich scientific program.

Scientific Topics

Education

Astrophysics

Nuclear, Particle and Fields Physics

Atomic, Molecular and Optical Physics

Quantum Many Body Physics

Classical Statistical Mechanics

Fluid Dynamics: from Macro- to Nano-fluidics

Chemical Physics

Soft Matter and Biophysics

Materials Science

Energy Storage and Production

Geosciences and Climate Modeling

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Monday 10.07

Plenary session – Auditorium (PLN-1)
Chair : S. Baroni

08:50-09:00	Welcome *A. M. Saitta, R. Spezia, R. Vuilleumier (UPMC)*
09:00-10:00	**Plenary** - Materials discovery and scientific design by computation: what does it take? *G. Galli (U. of Chicago)*
10:00-11:00	**Plenary** - Multiscale Lattice Boltzmann Simulations at the Physics-Biology Interface *S. Succi (CNR, Rome)*
Coffee break	
11:30-12:30	**Plenary** - The Quantum Way of Doing Computations *R. Blatt (Universität Innsbruck)*

Lunch

Materials Sciences – Room 108/44-45 (MS-1)
Chair: G. Galli

14:00-14:40	**Keynote** - Car and Parrinello meet Green and Kubo: simulating heat transport from ab initio equilibrium molecular dynamics. *S. Baroni (SISSA, Trieste)*
14:40-15:05	Phonon-phonon interactions in semiconductors and in bismuth, and their effect on the electronic and thermal transport. *N. Vast (Laboratoire des Solides Irradiés)*
15:05-15:30	Quantum model of optical properties and thermal emission of superradiant electronic excitations. *A. Vasanelli (CNRS, Univ. Paris 7)*
Coffee break	
16:00-16:25	Quantum effect on site preference and diffusion of interstitial hydrogen in face-centered cubic metals. *H. Kimizuka (Osaka University)*
16:25-16:50	Structural and dynamical properties of methane hydrate under high pressure via Raman spectroscopy and first-principles molecular dynamics including nuclear quantum effects. *S. Schaack (INSP, UPMC)*
16:50-17:15	Regulation of structure and thermoelectric properties of the smallest SnTe nanowires via encapsulation within single-walled carbon nanotubes. *A. Vasylenko (Dept. Of Physics, Warwick)*
17:15-17:40	Multiscale modelling of nanoscale materials and electronic transport. *W. Wenzel (Karlsruhe Institute of Technology)*

Classical Statistical Mechanics – Room 105/44-54 (CSM-1)
Chair: S. Succi

14:00-14:40	**Keynote** - Scalable and efficient first-principles based Monte Carlo simulations on high performance computers *Y. W. Li (Oak Ridge National Laboratory)*
14:40-15:05	Wang-Landau algorithm with the control of accuracy *L. Shchur (Landau Institute for Theor. Phys.)*
15:05-15:30	Large deviations for equilibrium and non–equilibrium processes *A. Hartmann (Univ. of Oldenburg)*
Coffee break	
16:00-16:25	Computations of self-assembly of rod-like particles on a plane *Y. Tarasevich (Astrakhan State University)*
16:25-16:50	Vapor nucleation under extreme confinement. *S. Meloni (Univ. of Rome "Sapienza")*
16:50-17:15	Nucleation to percolation: crack growth in random spring ladder *P. Ray (The Institute of Mathematical Sciences)*

Chemical Physics – Room 106/44-45 (CP-1)
Chair: B. Peters

14:00-14:40	**Keynote** - Modelling Supramolecular Polymers *B. Sundaram (JNCASR, India)*
14:40-15:05	SFG spectroscopy of Silica/water interfaces by DFT-MD simulations *S. Pezzotti (LAMBE, Evry)*
15:05-15:30	Improving Solubility in Supercritical CO2: Theoretical Studies of CO2-philic Compounds and Solubilizers *F. Ingrosso (SRSMC, Nancy)*
Coffee break	
16:00-16:25	Simplifying calculations of IR and Raman spectra from DFT-based molecular dynamics simulations *D. R. Galimberti (LAMBE, Evry)*
16:25-16:50	Vibrational energy relaxation at water interfaces from ab initio molecular dynamics simulations *D. Lesnicki (University Mainz)*
16:50-17:15	All-trans, all-cis and mixed isomers of azobenzene star: A multiscale simulation study *M. Koch (Technische Universität Dresden)*
17:15-17:40	Hidden Beneath the Surface: Origin of the Observed Enantioselective Adsorption on PdGa(111) *D. Passerone (EMPA, Switzerland)*

Quantum Many Body Physics – Room 107/44-54 (QMB-1)
Chair: M. Casula

14:00-14:40	**Keynote** - Cluster multipole theory for anomalous Hall effect in antiferromagnets *R. Arita (RIKEN Center for Emergent Matter Science)*
14:40-15:05	Spin-Charge Coupling in Unconventional Superconductors: Insights from Diffusion Monte Carlo *A. Narayan (Materials Theory, ETH Zurich)*
15:05-15:30	Doping dependence of charge order in electron-doped cuprate superconductors *S. Feng (Beijing Normal University)*
Coffee break	
16:00-16:25	Carbon nanotubes as excitonic insulators *M. Rontani (CNR, Modena)*
16:25-16:50	Recent Advances in Thermally-Assisted-Occupation Density Functional Theory (TAO-DFT) *J.-D. Chai (National Taiwan University)*
16:50-17:15	Dephasing and disorder effects in the topological systems *X. C. Xie (Peking University)*
17:15-17:40	Nature of Quasi-Particle Excitations in the Spin-1/2 Square-Lattice Heisenberg Antiferromagnet *H. Shao (Boston University and Beijing Computational Science Research Center)*

Atomic, Molecular and Optical Physics
Room 109/44-54 (AMOP-1)
Chair: F. Werner

14:00 - 14:40	**Keynote** - Towards controlled description of correlated fermions: diagrammatic Monte Carlo for the Hubbard model. *E. Kozik (King's College London)*
14:40 - 15:05	C++QED: a framework for simulating open quantum dynamics – the first ten years *A. Vukics (Centre for Physics of the Hungarian Academy of Sciences)*
15:05 - 15:30	Numerical simulation of sympathetic cooling in radiofrequency ion traps for studies on antimatter *N. Sillitoe (Laboratoire Kastler Brossel)*
Coffee break	

Poster session – Patio, 18:00-20:00

Tuesday 11.07

Plenary session – Auditorium (PLN-2)
Chair : R. Vuilleumier

09:00-10:00	**Plenary** - Nuclear Physics as Precision Science *Ulf-G Meißner (Universität Bonn and Forschungszentrum Jülich)*
10:00-11:00	**Plenary** - Numerical Relativity in the Era of Multi-Messenger Astronomy *M. Campanelli (Rochester Institute of Technology)*
Coffee break	
11:30-12:30	**Plenary** - Multiscale characterization of macromolecular dynamics *C. Clementi (Rice University)*

Lunch

Materials Science – Room 108/44-45 (MS-2)
Chair: B. Sundaram

13:50-14:15	Absence of spin edge polarization of acenes in the long-chain limit M. Casula (CNRS, UPMC)
14:15-14:40	Accurate ground-state correlation energies within the RPA and beyond: Theory and applications to molecules and zeolites *D. Rocca (Laboratoire CRM2)*
14:40-15:05	Electronic and Structural Properties of K-doped NiO Mott-Insulator : Quantum Monte Carlo Study *H. Shin (Argonne National Laboratory)*
15:05-15:30	Development of a joint refinement model for the one-electron reduced density matrix using different data sets *S. Gueddida (CentraleSupélec Paris)*
Coffee break	
16:00-16:25	Interplay between morphology and properties of core-shell Fe@Au nanoparticles *M. Benoit (CEMES, Toulouse)*
16:25-16:50	UV-Visible Absorption Spectra of Silver Clusters from TDDFT Calculations *R. Schira (Institut Lumière Matière, Grenoble)*
16:50-17:15	On the coordination of the Zn(II) ion in bistriflimide-based Ionic Liquids: Structural and dynamics properties at varying nature of the cation *F. Sessa (Università di Roma "La Sapienza")*
17:15-17:40	Unraveling the Icosahedral geometry of a light lanthanoid ion in a protic ionic liquid: a combined Molecular Dynamics and EXAFS study *A. Serva (Università di Roma "La Sapienza")*

Classical Statistical Mechanics – Room 105/44-54 (CSM-2)
Chair: L. Shchur

13:50-14:15	Deep Learning for Fatigue Estimation on the Basis of Multimodal Human-Machine Interactions *N. Gordienko (National Technical University of Ukraine)*
14:15-14:40	Non-canonical spin glass of polyhedral spin models on quasi-regular lattices *T. Surungan (Hasanuddin University, Indonesia)*
14:40-15:05	Synchronisation of Conservative Parallel Discrete Event Simulations in Small World Network *L. Ziganurova (Science Center in Chernogolovka, Moscow)*
15:05-15:30	GPU accelerated population annealing algorithm and its application to first- and second-order phase transitions – *L. Barash (Landau Institute for Theoretical Physics)*
Coffee break	
16:00-16:25	Phase transitions in evolutionary space games *E. Burovski (State University Higher School of Economics, Moscow)*
16:25-16:50	Contour analysis of multi-affine nanostructure AZO thin films *S. Hosseinabadi (Islamic Azad University, Tehran, Iran)*
16:50 - 17:15	Melting transition of skyrmion lattice in a two-dimensional chiral magnet *Y. Nishikawa (The University of Tokyo)*
17:15 - 17:40	Effect of temperature specification on simulated ergodicity *R. Ocaya (University of the Free State, South Africa)*

Chemical Physics – Room 106/44-45 (CP-2)
Chair: G. Ciccotti

14:00 - 14:40	**Keynote** - Rare Events Methods, Reaction Coordinates, and Useful Rate Theories *B. Peters (University of California, Santa Barbara)*
14:40 - 15:05	Ab initio molecular dynamics simulations of RNA nucleotides in hydrothermal prebiotic environment *A. Pérez Villa (IMPMC, UPMC)*
15:05 - 15:30	Open Boundary / Grand-Canonical Adaptive Resolution Simulations of Ionic Liquids *C. Krekeler (Freie Universität Berlin)*
Coffee break	
16:00 - 16:25	On the dynamics through a conical intersection *F. Agostini (University Paris-Sud, University Paris-Saclay)*
16:25 - 16:50	Nuclear quantum effects in molecular dynamics simulations *H. Dammak (Centrale Supélec)*
16:50 - 17:15	Estimating thermodynamic expectations and free energies in expanded ensemble simulations: systematic variance reduction through conditioning *M. Athenes (CEA, France)*
17:15 - 17:40	Free energies of solvation and binding, and solvent positions around any molecule in few minutes by rigorous liquid state théories *M. Levesque (ENS, UPMC)*

Quantum Many Body Physics – Room 107/44-54 (QMB-2)
Chair: H.-Q. Lin

13:50-14:15	Ab initio approach to strong correlations in lanthanide compounds: from localized magnets to heavy-fermions. – *L. Pourovskii (Ecole Polytechnique)*
14:15-14:40	Simulations of electron energy loss spectra with turboEELS *O. Motornyi (Ecole Polytechnique)*
14:40-15:05	Controlled summation of diagrammatic series for the unitary Fermi gas: bold diagrammatic Monte Carlo, large-order asymptotics and conformal-Borel transformation – *F. Werner (Laboratoire Kastler Brossel, ENS)*
15:05-15:30	Towards exascale simulations of quantum superfluids far from equilibrium *P. Magierski (Warsaw University of Technology)*
Coffee break	
16:00-16:25	Assessing theoretical spectroscopy from novel first-principle approaches *S. Backes (Ecole Polytechnique)*
16:25-16:50	Off-Diagonal Expansion Quantum Monte Carlo *I. Hen (University of Southern California, Los Angeles)*
16:50-17:15	Dynamics of nuclear fission within the time-dependent generator coordinate method *D. Regnier (Institut de Physique Nucléaire d'Orsay)*

17:16-17:40	Connected Determinant Diagrammatic Monte Carlo: polynomial-time complexity thanks to the fermionic sign *R. Rossi (Laboratoire de Physique Statistique de l'ENS)*

Soft Matter and Biophysics – Room 109/44-54 (SMB-1)
Chair: C. Clementi

14:00-14:40	**Keynote** - Molecular simulations of membrane sensing and remodeling *G. Hummer (MPI Biophysics, Goethe Univ. Frankfurt)*
14:40-15:05	Electron Transfer in Organic and Biological Materials *A. Carof (University College London)*
15:05-15:30	Protein adaptation to high temperatures does not necessary require enhanced mechanical stability *G. Stirnemann (IBPC, Paris)*
Coffee break	
16:00-16:25	The challenge for Gram-negative bacteria: Towards in-silico screening of antibiotics for fast permeation through nanopores M. Ceccarelli (University of Cagliari, Italy)
16:25-16:50	Finding protein folding funnels in random networks M. Kikuchi (Osaka University)
16:50-17:15	Theoretical studies on stability and dynamics of protein complex by a coarse-grained model H. Nagao (Kanazawa University)
17:15-17:40	Weak Nanoscale Chaos And Anomalous Relaxation in DNA A. Mazur (IBPC, Paris)

Poster session – Patio, 18:00-19:30

Gala Dinner – La Coupole, 20:00-22:00

Wednesday 12.07

Plenary session – Auditorium (PLN-3)
Chair : J. Adler

09:00-10:00	**Plenary** - Potential Energy Surfaces and Berry Phases beyond the Born-Oppenheimer Approximation: A New Approach to Non-Aadiabatic Dynamics *E.K.U. Gross Max Planck Institute, Halle)*
10:00-11:00	**Plenary** - Theoretical Physics is More than Equations: The African School for Electronic Structure Methods and Applications *R. M. Martin (University of Illinois at Urbana Champaign, Stanford University)*
Coffee break	
11:30-12:30	**YSP2017 award** - Tensor Network Renormalization *Glen Brian Evenbly (University of Sherbrooke)*

Lunch

Materials Science – Room 108/44-45 (MS-3)
Chair: M. Lazzeri

14:15-14:40	Chemisorption of Hydroxides on Carbon and Boron Nitride Nanomaterials from Ab Initio Calculations *B. Grosjean (École Normale Supérieure, Paris)*
14:40-15:05	Multiscale Modeling of the Insertion and Diffusion of H-3 and Cl-36 in UNGG Graphite *Christoph Lechner (EDF R&D)*
15:05-15:30	Molecular dynamics modeling of graphite and graphene melting *N. Orekhov (Moscow Institute of Physics and Technology)*
Coffee break	
16:00-16:25	Atomistic Simulations of the Assembly of Large Gold Nanocrystals *J. Richardi (UPMC, Paris)*
16:25-16:50	On the oxidation state of titanium in titanium dioxide *S. Manzhos (National University of Singapore)*
16:50-17:15	Ab initio study of inorganic perovskites: towards the prediction of PbZr_1-x_Ti_x_O_3 (PZT) IR spectrum *Y. Peperstraete (Synchrotron SOLEIL)*
17:15-17:40	Study of the ferroelectric properties of epitaxially strained SrTaO2N by means of DFT all-electrons first principles calculations. *Roberto Alonso (Conicet, Argentina)*

Nuclear, Particle and Fields Physics – Room 105/44-54 (NPFP-1)
Chair: G. B. Evenbly

14:00-14:40	**Keynote** - Machine Learning from the proton structure to Higgs pair production at the LHC *J. Rojo (Vrije University, Amsterdam)*
14:40-15:05	Transformed Lattice Rules for Feynman Loop Integrals *E. de Doncker (Western Michigan University)*
15:05-15:30	ATLAS Track reconstruction at the energy frontier *A. Kastanas (KTH Royal Institute of Technology)*
Coffee break	
16:00-16:25	The new ATLAS Fast Calorimeter Simulation *H. Ahmed (University of Edinburgh)*
16:25-16:50	Statistical and systematic errors in the analysis of multiple datasets *O. Selyugin (Universite de Liege)*
16:50-17:15	Novel methods in track-based alignment to correct for time-dependent distortions of the ATLAS Inner Detector *Oscar Estrada (CERN)*
17:15-17:40	Primary Vertex Reconstruction with the ATLAS experiment *D. Casper (CERN)*

Classical Statistical Mechanics – Room 107/44-54 (CSM-3)
Chair: E. Trizac

13:50-14:15	Random Field Ising Model with Conserved Kinetics: Super-Universality Violation, Logarithmic Growth Law and the Generalized Tomita Sum Rule *V. Banerjee (Indian Institute of Technology, Delhi)*
14:15-14:40	Improving and testing the population annealing Monte Carlo algorithm *Martin Weigel (Coventry University)*

Quantum Many Body Physics – Room 107/44-54 (QMB-3)
Chair: T. Xiang

14:40-15:05	Coupled Electron-Ion Monte Carlo study of hydrogen under extreme conditions *Markus Holzmann (CNRS, Université Grenoble-Alpes)*
15:05-15:30	Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of multireference perturbation theory *Y. Garniron (IRSAMC)*
Coffee break	
16:00-16:25	Importance of correlation effects for theoretical description of pressure induced electronic transitions: IMT, ETT, CLC. *I. Abrikosov (Linköping University, Sweden)*

16:25-16:50	Proposal of a new fully uncontracted multi-reference perturbation theory *E. Giner (MPI for Solid State Research)*
16:50-17:15	Diagrammatic extensions of DMFT: Nonlocal interactions and nonlocal corrélations *E. van Loon (Radboud University, Nijmegen)*

Soft Matter and Biophysics – Room 109/44-54 (SMB-2)
Chair: G. Hummer

14:15-14:40	Conformational dynamics of the human Guanylate binding protein 1 from Hamiltonian replica exchange MD simulations and FRET experiments *B. Barz (Jülich Research Centre, University Düsseldorf)*
14:40-15:05	Mesoscale Hydrodynamic Simulation of Microswimmers *R. Winkler (Forschungszentrum)*
15:05-15:30	Monte Carlo simulation for pattern formation of run-and-tumble chemotactic bacteria *S. Yasuda (University of Hyogo)*
Coffee break	
16:00-16:25	Transition to network synchronization in neuronal cultures: modelling the activity bursts with an adaptive 2D dynamical model *P. Monceau (Université Paris-Diderot)*
16:25-16:50	Viscoelastic hydrodynamic interactions and anomalous CM diffusion in polymer melts: influence of thermostat and simulation box *H. Meyer (Institut Charles Sadron)*

FLuid dynamics : from macro to nano – Room 109/44-54 (FD-1)
Chair: D. Passerone

16:50-17:15	Numerical investigation on spreading behavior of falling droplet on inclined surface *S. Pati (National Institute of Technology Silchar, India)*
17:15 - 17:40	Solidification of a simple liquid near wall in high-speed lubrication flows *Shugo Yasuda (University of Hyogo)*

Energy Storage and Production – Room 106/44-45 (ESP-1)
Chair: R. Spezia

14:00 - 14:40	**Keynote** - Understanding Ionic liquids role in energy application from calculations *B. Kirchner (University of Bonn)*
14:40 - 15:05	Modelling Nanoporous Graphene Based Supercapacitors *T. Méndez Morales (Maison de la Simulation – CEA)*
15:05 - 15:30	Confinement Effects on an Electron Transfer Reaction in Nanoporous Carbon Electrodes *Z. LI (CEA – UPMC – RS2E)*
Coffee break	

Chemical Physics – Room 106/44-45 (CP-3)
Chair: M. Salanne

16:00-16:25	Analysis of local bond-orientational order for liquid gallium at ambient pressure *T.-M. Wu (National Chiao-Tung University)*
16:25-16:50	Interlayer binding of bilayer blue phosphorus: quantum Monte Carlo study *J. Ahn (Konkuk University)*

Thursday 13.07 Morning

Materials Science – Room 108/44-45 (MS-4)
Chair: M.-L. Bocquet

09:00-09:40	**Keynote** - Embedded many-body perturbation theories for organic optoelectronics *X. Blase (Institut Néel)*
09:40-10:05	Optical properties of single-molecule junctions *Herve Bulou (IPCM, Strasbourg)*
10:05-10:30	On screening in organic semi conductors *S. Gueddida (CentraleSupélec Paris)*
Coffee break	
11:00-11:25	Buckled monolayer of GaAs under transverse electric field *B. Prasad (National Institute of Technology, Surat)*
11:25-11:50	Numerical analysis of Brillouin zone integration methods *A. Levitt (MATHERIALS)*

FLuid dynamics : from macro to nano – Room 109/44-54 (FD-2)
Chair: B. Rotenberg

09:00-09:40	**Keynote** - Hydration friction in nano-confinement: from bulk via interfacial to dry friction *R. Netz (TU Berlin)*
09:40-10:05	Molecular dynamics simulations of diffusio-osmotic flow driven by chemical potential gradient *H. Yoshida (ENS, Paris, Toyota Central R&D Labs., Inc.)*
10:05-10:30	Multiscale modelling of ion adsorption and electrokinetic phenomena in porous oxides. *J.-F. Dufrêche (ICSM, Marcoule)*
Coffee break	
11:00-11:25	Transient hydrodynamic finite size effects in simulations under periodic boundary conditions *A. Asta (Phenix, UPMC)*
11:25-11:50	Design criteria for underwater superhydrophobicity: a rare-event molecular dynamics study *Matteo Amabili (University of Rome "La Sapienza")*

Geosciences and Climate Modelling – Room 105/44-54 (Geo-1)
Chair: A. Vasanelli

09:00-09:40	**Keynote** - Towards high-resolution climate models *C. Schär, (ETH Zurich)*
09:40-10:05	Bridging the Scale Hierarchy Problem in Biogeochemical Models *F. Paparella (New York University Abu Dhabi)*
10:05-10:30	Hierarchies of complexity in Earth System Modeling *V. Balaji (Princeton University)*
Coffee Break	
11:00-11:25	Importance of a fully anharmonic treatment of equilibrium isotope fractionation properties of dissolved ionic species as evidenced by Li+(aq) *M. Méheut (Géosciences Environnement Toulouse)*
11:25-11:50	Investigating the properties of silicate and carbonate melts at Earth's mantle conditions by molecular dynamics simulation *Nicolas Sator (UPMC, Paris)*

Quantum Many Body Physics – Room 107/44-54 (QMB-4)
Chair: S. Biermann

09:00-09:40	**Keynote** - Gapless Spin-Liquid Ground State in the S=1/2 Kagome Antiferromagnet *T. Xiang (Chinese Academy)*
09:40-10:05	Quantum spin phases emerged from the interplay between strong correlation and spin-orbital coupling *J. Li (Nanjing University)*
10:05 - 10:30	Short-time quantum critical dynamics for Ising model in a transverse field *D. Yao, (Sun Yat-Sen University)*
Coffee break	

Energy Storage and Production – Room 107/44-54 (ESP-2)
Chair: B. Kirchner

11:00-11:25	Proton Mobility in Protic Ionic Liquids: New Results from Theoretical Calculations *E. Bodo (University of Rome "La Sapienza")*
11:25 - 11:50	Comparative Density Functional Theory - Density Functional Tight Binding study of fullerene derivatives: effects of addends, buckyball size, and crystallinity on properties affecting solar cell functionality *S. Manzhos (National University of Singapore)*

Astrophysics – Room 106/44-45 (Astro)
Chair: P. Ray

09:00-09:40	**Keynote** - Gravitational waves: The new frontier of astrophysics *P. Ajith (International Centre for Theoretical Sciences)*
09:40-10:05	Simulation of magnetorotational processes in core-collapsed supernovae *S. Moiseenko (Space Research Institute, Russia)*
10:05 - 10:30	Modeling of Fragmentation and Density Stratification in the Process of Shock Interaction with Molecular Clouds on Grids with Very Large Resolution *B. Rybakin (Lomonosov Moscow State)*
Coffee break	

Education – Room 106/44-45 (Educ)
Chair: R. Martin

11:00-11:25	Groundstates of liquid crystals with colloids: a project for undergraduate students *J. Adler (Technion - Israel Institute of Technology)*
11:25 - 11:50	Toolkit-based approach to undergraduate training in molecular dynamics *Richard Ocaya (University of the Free State)*
11:50 - 12:15	Time evolution of the unstable soliton solution for dust acoustic waves with trapped électrons *S. Phibanchon (Faculty of Education, Burapha Univeristy)*

Concluding Remarks – Room 108/44-45

12:30-12:45	Conclusions *A. M. Saitta, R. Spezia, R. Vuilleumier*

Thursday 13.07 Afternoon : Spin-off meeting on the history of simulation

Amphitheater Charpak
Chair : D. Borgis and E. Vanden-Eijnden

14:00-14:45	The Birth, Rise and Triumph of Molecular Dynamics *J.-P. Hansen (Cambridge – UPMC)*
14 :45-15 :30	Electronic Structure Computation from the first years after the advent of quantum mechanics to challenges today *R. Martin (University of Illinois)*
Coffee break	
16 :00-16 :45	How has Molecular Simulation contributed to the dream of Theoretical physics? An attempt at an historical reconstruction *G. Ciccotti (Univerity of Rome « La Sapienza »)*
16 :45-17 :15	Round Table *D. Borgis (Maison de la simulation – ENS), E. Vanden-Eijnden (New York University)*

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P1. Propagation of Dust-Ion Acoustic (DIA) waves in multi-species plasma with Cairn's distributed electrons, quantum effects in inertia less electrons and ions
Kalita Bhaben Chandra, Das Samiran

P2. Investigation of dust ion acoustic (DIA) solitons in multicomponent plasma with relativistic ions and Cairns distributed électrons
Das Samiran, B.C. Kalita

P3 The role of the order of perturbation and its determination in the process of enforcing discrete Korteweg-de-Vries solitons to modified Korte-de-Vries solitons as means of continuum hypothesis in a multi component dusty plasma
Kalita Bhaben

P4 Complexity Cmp and Time's Arrow
Rajilic Zoran

Nuclear, Particle and Fields Physics

P5. Computational studying energy and spectral parameters of hadronic (pionic) atoms with account of the strong pion-nuclear interaction
Dubrovskaya Yuliya

P6. Computational studying the hyperfine and electroweak interaction and parity violation in heavy finite Fermi-systems: Advanced Code
Khetselius Olga

P7. Confinement and Chiral Phase Transition in Dual QCD Formulation.
Punetha Garima

P8. SU(3) Dual QCD formulation and quark-hadron phase transition
Punetha Garima

P9. Implications of general lepton mass matrices in the standard model for Neutrinoless Double Beta Decay parameter m_{ee}
Sharma Samandeep

Atomic, Molecular and Optical Physics

P10. Advanced computational approach to studying Rydberg and autoionization resonances in spectra of heavy lanthanides and actinides
Ternovsky Valentin

P11. Advanced computational approach to nonlinear dynamics of laser systems with elements of a chaos
Ternovsky Valentin

P12. Advanced relativistic model potential approach to computing the radiation transition characteristics for atoms and multicharged ions
Buyadzhi Vasily

P13. Advanced computational approach in electron-collisional spectroscopy of atoms and multicharged ions in plasmas
Buyadzhi Vasily

P14. Cooperative laser electron-gamma-nuclear phenomena in dynamics and spectroscopy of molecules: Advanced Computational Code
Glushkov Alexander

P15. New relativistic computational energy approach to heavy Fermi-systems in a super strong field: AC Stark and multi-photon resonances
Glushkov Alexander

P16. Advanced computational code to « shake-up » and NEET effects in laser electron-gamma-nuclear spectroscopy of atoms and ions
Khetselius Olga

P17. Modulation of Intense Femtosecond Laser Pulse by a strong magnetic field
Shu Xiaofang

P18. Superexchange Interatomic Coulombic decay by Fano-ADC-Stieltjes method
Votavov· Petra

P19. Projectile Charge Effect on Electron and Positron Impact Single Ionization Cross Sections of Plasma Relevant Molecular Targets
Singh Prithvi

P20. Computer simulation of the interaction of fullerene with nanographene
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P21. Ab- initio calculation of the electronic gap, the refractif index of (PbTe), (SrTe) and Lead strontium telluride alloys (Pb1-xSrxTe).
Sifi Chahra, Chouit Fairouz, Sifi Chahra

Quantum Many Body Physics

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Miyahara Shin

P23. Enhancement of superconducting correlations by charge and spin ordering in coupled electron and spin systems
Farkasovsky Pavol

P24. Quantum Monte Carlo calculations of elastic properties of one-dimensional carbon chain
Hong Iuegyun

P25. Determination of energies dan wave functions of a quantum many-body system by the finite difference time domain (FDTD) with the Hartree Fock (HF) approximation
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P30. The SAPBC method on local, non-cluster updates algorithms of Monte Carlo simulation: A study on more convergence of spin correlation at critical temperature.
Najafi Amin

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P32. Mean squared displacement of dust particles in 2-dimensional strongly coupled Yukawa liquids exposed to an external magnetic field
Masheyeva Ranna

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Yu Chengxin

P34. Ion acoustic solitary waves with high relativistic thermal ions and non-thermal electrons and thermal positrons in plasma
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P35. Computational Model Of Calcium And IP3 Dynamics: A Finite Difference Method Approach
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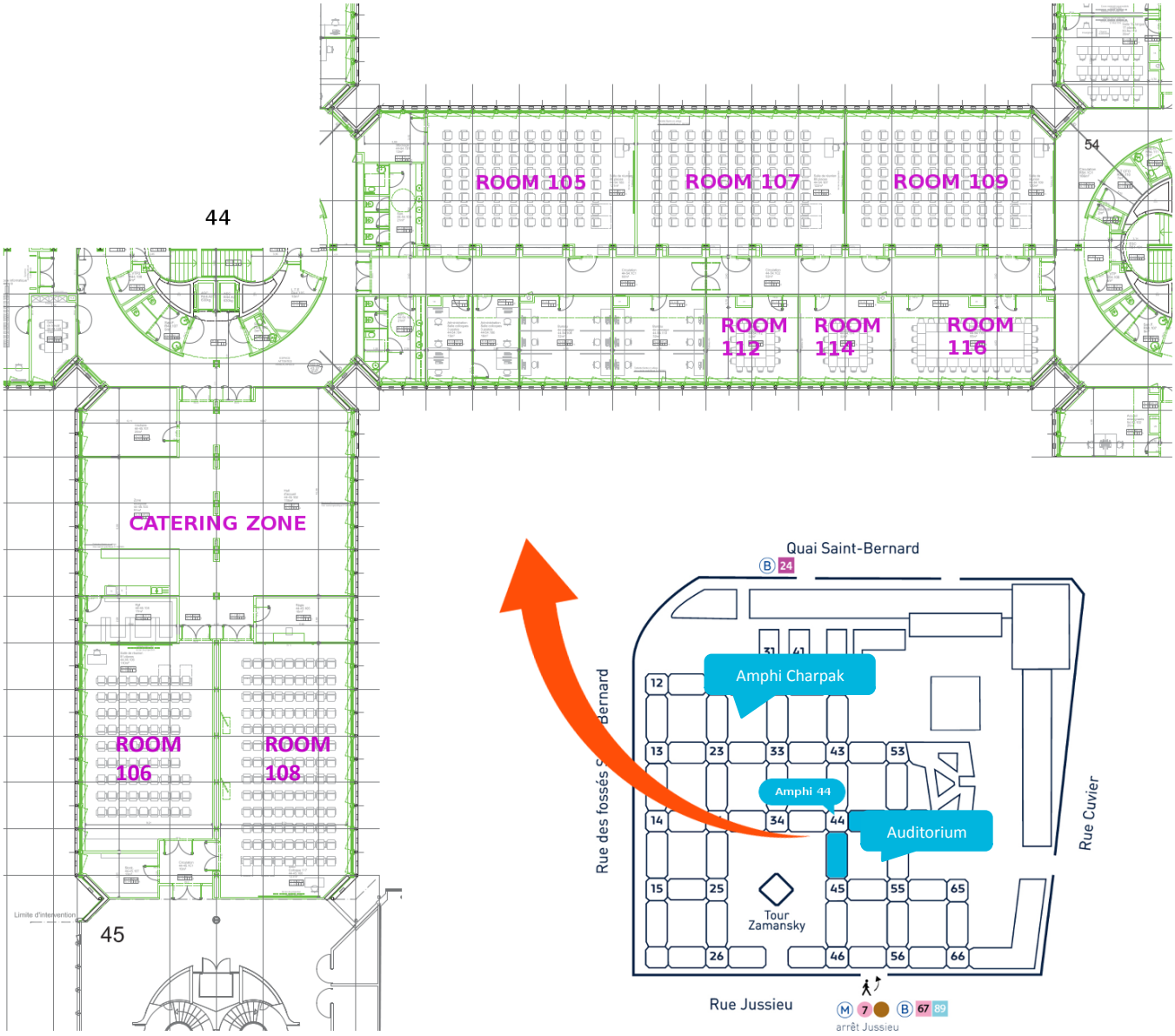

Auditorium

Plenary sessions, Morning coffee breaks

Patio 44-54

Welcome, Poster session, Lunch boxes, Afternoon coffee breaks

Rooms 106/44-45, 108/44-45, 105/44-54, 107/44-54, 109/44-54, Catering zone

Parallel sessions, Afternoon coffee breaks

Amphitheater Charpak

Thursday afternoon spin-off meeting on the history of simulation

Sunday 09.07	17:00-20:00	Patio	**Registration**
Monday 10.07	08:50-09:00	Auditorium	**Welcome**
	09:00-10:00	Auditorium	**Plenary Lecture** Materials discovery and scientific design by computation: what does it take? *G. Galli (U. of Chicago)*
	10:00-11:00	Auditorium	**Plenary Lecture** Multiscale Lattice Boltzmann Simulations at the Physics-Biology Interface *S. Succi (CNR, Rome)*
	11:00-11:30	Hall	**Coffee Break**
	11:30-12:30	Auditorium	**Plenary Lecture** The Quantum Way of Doing Computations *R. Blatt (Universität Innsbruck)*
	12:30-14:00	Patio	**Lunch**
	14:00-15:30	Conference center	**Parallel Sessions**
	15:30-16:00	Catering zone Patio	**Coffee Break**
	16:00-17:40	Conference center	**Parallel Sessions**
	18:00-20:00	Patio	**Poster session**
Tuesday 11.07	09:00-10:00	Auditorium	**Plenary Lecture** Nuclear Physics as Precision Science *Ulf-G Meißner (Universität Bonn and Forschungszentrum Jülich)*
	10:00-11:00	Auditorium	**Plenary Lecture** Numerical Relativity in the Era of Multi-Messenger Astronomy *M. Campanelli (Rochester Institute of Technology)*
	11:00-11:30	Hall	**Coffee Break**
	11:30-12:30	Auditorium	**Plenary Lecture** Multiscale characterization of macromolecular dynamics *C. Clementi (Rice University)*
	12:30-13:50	Patio	**Lunch**
	13:50-15:30	Conference center	**Parallel Sessions**
	15:30-16:00	Catering zone Patio	**Coffee Break**
	16:00-17:40	Conference center	**Parallel Sessions**
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	20:00-22:00	La Coupole	**Gala dinner**
Wednesday 12.07	09:00-10:00	Auditorium	**Plenary Lecture** Potential Energy Surfaces and Berry Phases beyond the Born-Oppenheimer Approximation: A New Approach to Non-Aadiabatic Dynamics *E.K.U. Gross Max Planck Institute, Halle)*
	10:00-11:00	Auditorium	**Plenary Lecture** Theoretical Physics is More than Equations: The African School for Electronic Structure Methods and Applications *R. M. Martin (University of Illinois at Urbana Champaign, Stanford University)*
	11:00-11:30	Hall	**Coffee Break**
	11:30-12:30	Auditorium	**YSP2017 Award Ceremony** Tensor Network Renormalization *Glen Brian Evenbly (University of Sherbrooke)*
	12:30-13:50	Patio	**Lunch**
	13:50-15:30	Conference center	**Parallel Sessions**
	15:30-16:00	Catering zone Patio	**Coffee Break**
	16:00-17:40	Conference center	**Parallel Sessions**
Thursday 13.07	09:00-10:30	Conference center	**Parallel Sessions**
	10:30-11:00	Catering zone Patio	**Coffee Break**
	11:00-12:15	Conference center	**Parallel Sessions**
	12:30-12-45	Room 108/44-45	**Concluding Remarks**
	12:45-14:00	Patio	**Lunch**
	14:00-17:15	Amphi. Charpak	**Spin-off meeting on the history of simulations**