

CCP2014

XXVI IUPAP Conference on Computational Physics
August 11-14 ▪ Boston, USA

Program and Information



BOSTON
UNIVERSITY

Sponsors of CCP2014



Welcome to CCP2014

Dear Participants,

It is my great pleasure to welcome you to the XXVI IUPAP Conference on Computational Physics and to Boston University.

The CCP series marks the start of its second quarter-century by returning to Boston, the city of its inception. The 1989 conference led to an annual Physics Computing conference, which in 1997 was renamed the CCP. The organizers understood the need for a broad meeting where researchers working on computational methods and applications in different areas of physics could come together and discuss progress, opportunities and challenges of common interest.

Today, computational research continues to gain in importance and hardly any field of science can progress successfully without some aspect of computation or large-scale data processing. There are now many specialized meetings focusing on different branches of computational physics, but there is also a role for a broad meeting series such as CCP, where researchers can be informed and inspired to adapt methods across fields. Such a conference also sends a message to the scientific community and funding agencies that research investments in computational methods and hardware can deeply impact many different areas.

In organizing CCP2014, we have strived for both breadth and depth. Accessible plenary sessions showcase progress and challenges in different areas of computational physics and enabling technologies. In the more specialized parallel oral and poster sessions there are opportunities to reach deeper into various disciplines, but I hope and believe that these sessions will also attract participants engaged in research outside the immediate topics presented. This way the meeting can achieve its goal of facilitating communication and collaboration across subfields.

On behalf of the Local Organization Committee, the Program Committee, and the International Advisory Board, I thank you for attending CCP2014 and look forward to an exciting meeting.



Anders Sandvik, Chair of CCP2014

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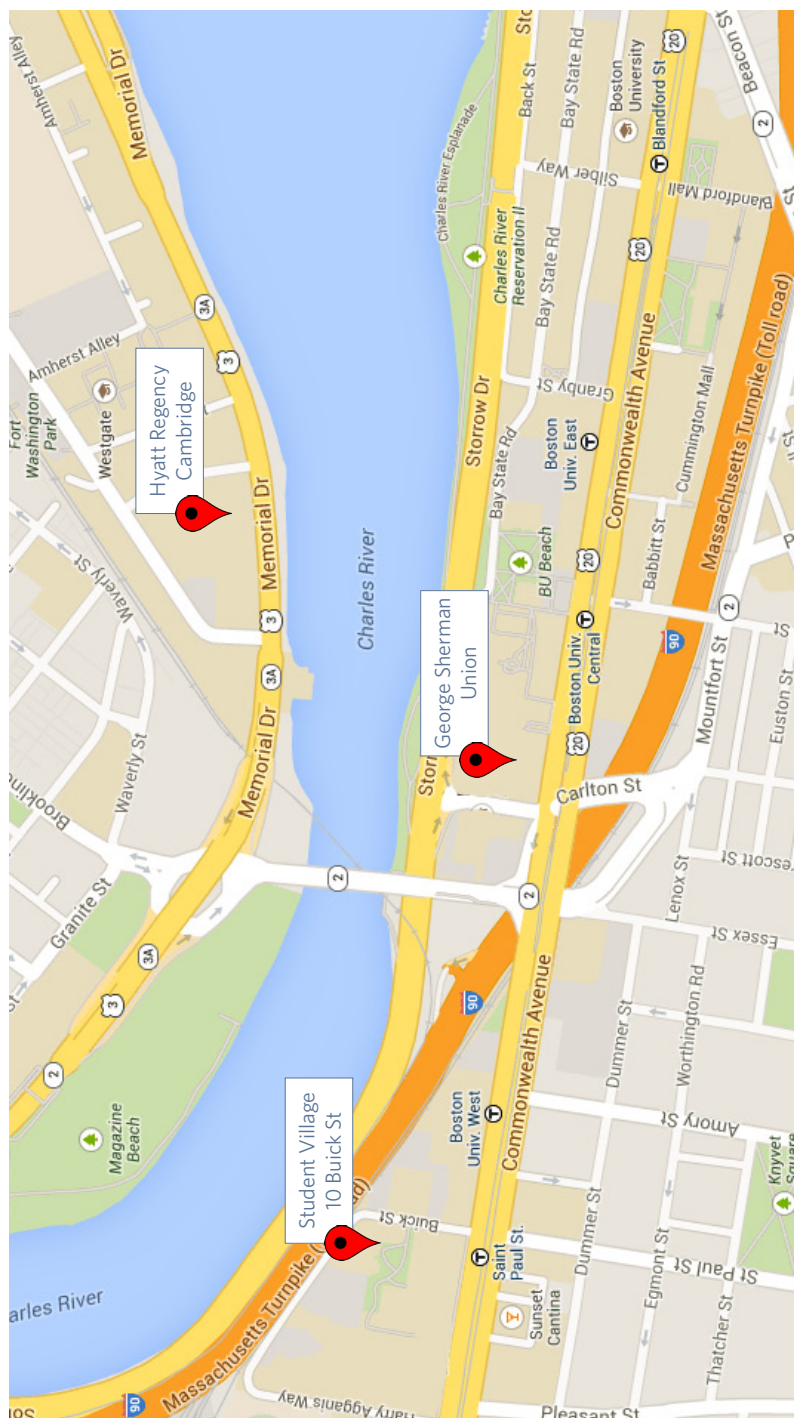
Novel hardware and software paradigms

Barry Schneider (*NIST*), Chair
Richard Brower (*Boston University*), Vice Chair
Mark Jarrell (*Louisiana State University*)
Jim Sexton (*IBM*)

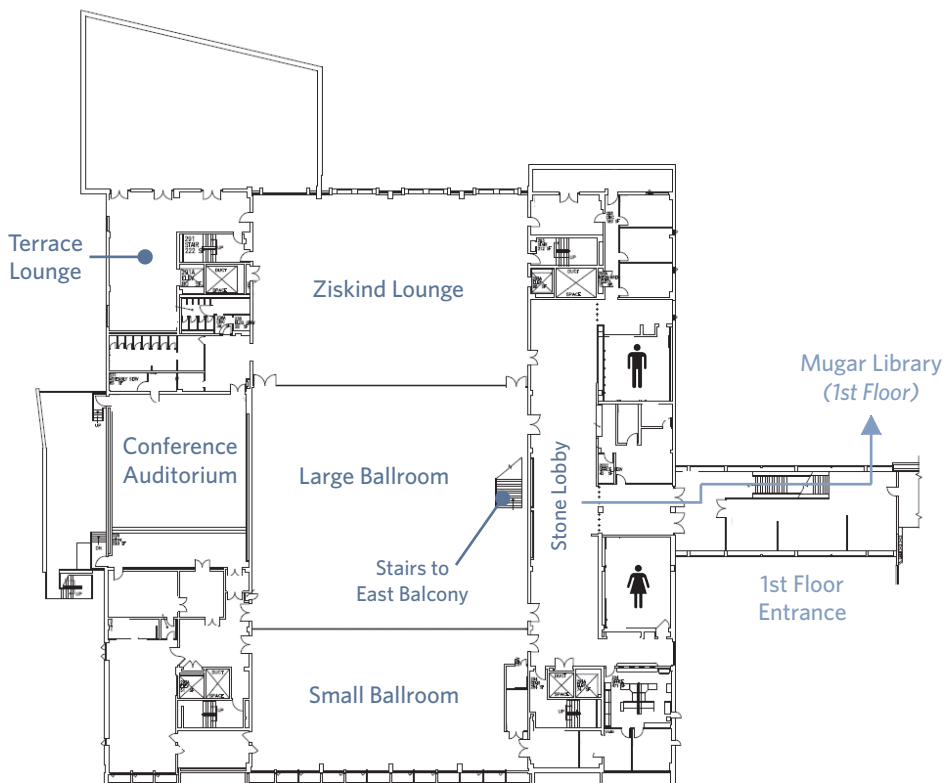
Computational physics education

Wolfgang Christian (*Davidson College, USA*), Chair
Harvey Gould (*Clark University*), Vice Chair
Nithaya Chetty (*The University of Kwazulu-Natal, South Africa*)

CCP2014 venue: Boston University George Sherman Union



George Sherman Union (GSU)
775 Commonwealth Avenue
Second Floor



The **East Balcony** is accessible from inside the Large Ballroom. Go up the stairs at the back of the ballroom; the room will be on your right.

The **Terrace Lounge** and **Conference Auditorium** are through the Ziskind Lounge.

Mugar 205 is located in Mugar library. From the conference venue (Stone Lobby), go down the stairs, continue ahead on the first floor, then take a left into Mugar Library. There will be a staircase/elevator on your right. Go up to the second floor and take a right. Mugar 205 will be at the end of the hall.

Program Overview

Morning

| | Sunday | Monday | Tuesday | Wednesday | Thursday |
|-------|--------|---------------------------|----------------------------|---------------------------------|-------------------------|
| 7:30 | | Registration | | | |
| 7:45 | | | | | |
| 8:00 | | | | | |
| 8:15 | | | | | |
| 8:30 | | | Plenary <i>Danskin</i> | Plenary <i>Katzgraber</i> | Parallel Sessions |
| 8:45 | | | | | |
| 9:00 | | Welcome | | | |
| 9:15 | | Plenary <i>Succi</i> | Plenary <i>Schulz</i> | Plenary <i>Young</i> | |
| 9:30 | | | | | |
| 9:45 | | | | | |
| 10:00 | | Break | Break | Break | |
| 10:15 | | | | | |
| 10:30 | | Plenary <i>Okamoto</i> | Plenary <i>Sterling</i> | Plenary <i>Rothlisberger</i> | Plenary <i>Louie</i> |
| 10:45 | | | | | |
| 11:00 | | | | | |
| 11:15 | | Plenary <i>Trivedi</i> | Plenary <i>Sexton</i> | Plenary <i>Granger</i> | Plenary <i>White</i> |
| 11:30 | | | | | |
| 11:45 | | | | | |
| 12:00 | | Lunch | Lunch | Lunch | Lunch |
| 12:15 | | | | | |
| 12:30 | | | | | |
| 12:45 | | | | | |
| 13:00 | | | | | |
| 13:15 | | | | | |

Session and Event Locations

Plenary sessions are located in the [Large Ballroom](#).

The **poster session** is located in the [Small Ballroom](#), [Large Ballroom](#), and [Ziskind Lounge](#).

Breaks are located in the [Ziskind Lounge](#).

The **Welcome Reception** is located in the [Ziskind Lounge](#).

The **Banquet** is located in the [Trustee Center](#) (1 Silber Way, 9th floor, Ballroom).

Program Overview

Afternoon/Evening

| | Sunday | Monday | Tuesday | Wednesday | Thursday |
|-------|-------------------|--|-------------------|-------------------|------------------------------|
| 13:30 | Registration | Parallel Sessions | Parallel Sessions | Parallel Sessions | Plenary <i>Del Debbio</i> |
| 13:45 | | | | | Plenary <i>Dave</i> |
| 14:00 | | | | | |
| 14:15 | | | | | |
| 14:30 | | | | | |
| 14:45 | | | | | Closing |
| 15:00 | | | | | |
| 15:15 | | Break | Break | Break | |
| 15:30 | | | | | |
| 15:45 | | Parallel Sessions | Parallel Sessions | Parallel Sessions | |
| 16:00 | | | | | |
| 16:15 | | | | | |
| 16:30 | | | | | |
| 16:45 | | | | | |
| 17:00 | | | | | |
| 17:15 | | | | | |
| 17:30 | Welcome Reception | Poster Session | | | |
| 17:45 | | | | | |
| 18:00 | | | | | |
| 18:15 | | | | | |
| 18:30 | | Banquet Reception 18:30-19:00 Dinner 19:00-21:00 | | | |
| 18:45 | | | | | |
| 19:00 | | | | | |
| 19:15 | | | | | |
| 19:30 | | | | | |
| 19:45 | | | | | |
| 20:00 | | | | | |
| 20:15 | | | | | |
| 20:30 | | | | | |
| 20:45 | | | | | |

Overview of Parallel Sessions

| Monday, Parallel Sessions 1, 13:30-15:15 | | | | |
|--|----------------------------|-----------------------|----------------------------|-----------|
| Auditorium | Small Ballroom | Terrace Lounge | East Balcony | Mugar 205 |
| Materials Science | Soft Matter | Fluid Dynamics | Quantum Many-Body | |
| Monday, Parallel Sessions 2, 15:45-17:30 | | | | |
| Auditorium | Small Ballroom | Terrace Lounge | East Balcony | Mugar 205 |
| Soft Matter | Statistical Physics | Fluid Dynamics | Computing Paradigms | |

| Tuesday, Parallel Sessions 1, 13:30-15:15 | | | | |
|---|----------------------------|------------------|----------------------------|-----------------------------|
| Auditorium | Small Ballroom | Terrace Lounge | East Balcony | Mugar 205 |
| Soft Matter | Statistical Physics | General | Quantum Many-Body | Lattice Field Theory |
| Tuesday, Parallel Sessions 2, 15:45-17:30 | | | | |
| Auditorium | Small Ballroom | Terrace Lounge | East Balcony | Mugar 205 |
| Materials Science | Statistical Physics | Education | Computing Paradigms | Lattice Field Theory |

| Wednesday, Parallel Sessions 1, 13:30-15:15 | | | | |
|---|----------------------------|--------------------------|--------------------------|-----------|
| Auditorium | Small Ballroom | Terrace Lounge | East Balcony | Mugar 205 |
| Materials Science | Statistical Physics | Astrophysics | Quantum Many-Body | |
| Wednesday, Parallel Sessions 2, 15:45-17:30 | | | | |
| Auditorium | Small Ballroom | Terrace Lounge | East Balcony | Mugar 205 |
| Materials Science | Computing Paradigms | Quantum Computing | Education | |

| Thursday, Parallel Sessions, 8:30-10:15 | | | | |
|---|--------------------|-----------------------------|---------------------|-----------|
| Auditorium | Small Ballroom | Terrace Lounge | East Balcony | Mugar 205 |
| Materials Science | Soft Matter | Lattice Field Theory | Astrophysics | |

Daily Schedules

Session Locations

Plenary sessions are located in the **Large Ballroom**.

The **poster session** is located in the **Small Ballroom**, **Large Ballroom**, and **Ziskind Lounge**.

Breaks are located in the **Ziskind Lounge**.

Monday, August 11

| | |
|-------------|---|
| 7:30-9:00 | Registration |
| 9:00-9:15 | Welcome Anders Sandvik, <i>Chair of CCP2014</i> Robert Brown, <i>President of Boston University</i> Alex Hansen, <i>Chair of IUPAP's C20 Commission</i> |
| 9:15-10:00 | Plenary Session: Computational Physics 1 <i>Chair: Anders Sandvik</i> Sauro Succi , <i>IAC-CNR (Italy)</i> Lattice Boltzmann simulations of complex flows across scales: turbulence, soft-glasses and quark-gluon plasmas |
| 10:00-10:30 | Break |
| 10:30-11:15 | Plenary Session: Computational Physics 2 <i>Chair: David Coker</i> Yuko Okamoto , <i>Nagoya University (Japan)</i> Enhanced configurational sampling methods for spin systems and biomolecular systems |
| 11:15-12:00 | Nandini Trivedi , <i>Ohio State University (USA)</i> Topology and Correlations driving new materials, phases and phenomena |
| 12:00-13:30 | Lunch |
| 13:30-15:15 | Parallel Sessions 1 Materials Science and Nanoscience 1, <i>Conference Auditorium</i> Soft Matter and Biological Physics 1, <i>Small Ballroom</i> Fluid Dynamics 1, <i>Terrace Lounge</i> Quantum Many-Body Physics 1, <i>East Balcony</i> |
| 15:15-15:45 | Break |
| 15:45-17:30 | Parallel Sessions 2 Soft Matter and Biological Physics 2, <i>Conference Auditorium</i> Statistical Physics 1, <i>Small Ballroom</i> Fluid Dynamics 2, <i>Terrace Lounge</i> Novel Computing Paradigms 1, <i>East Balcony</i> |
| 17:30-19:30 | Poster Session |

Monday, Parallel Sessions 1

| Materials Science and Nanoscience 1 | |
|-------------------------------------|---|
| Location: Conference Auditorium | Chairperson: Markus Eisenbach |
| 13:30-14:00 | Invited Talk: Luca Ghiringhelli , <i>Fritz Haber Institute of the Max Planck Society (Germany)</i> , Big Data of Materials Science - Critical Role of the Descriptor |
| 14:00-14:30 | Invited Talk: Lin-lin Wang , <i>Ames Laboratory (USA)</i> , Computational Modeling of Transition-Metal Alloyed Nanoparticles in Working Condition |
| 14:30-14:45 | Hossein Mosallaei , <i>Northeastern University (USA)</i> , Novel Materials Enabled with Core-Shell Dielectric-Plasmonic Particles |
| 14:45-15:00 | Theodore Einstein , <i>Physics & CMTC, University of Maryland (USA)</i> , Characterizing Capture Zone Distributions (CZD) in Island Growth on Surfaces: Simulations Confront Experiments |
| 15:00-15:15 | Vlad Sokhan , <i>National Physical Laboratory (UK)</i> , Electronically coarse-grained simulations in materials science |

| Soft Matter and Biological Physics 1 | |
|--------------------------------------|---|
| Location: Small Ballroom | Chairperson: Joerg Rottler |
| 13:30-14:00 | Invited Talk: Mark Robbins , <i>Johns Hopkins University (USA)</i> , Welding and healing of polymer interfaces: Strength from entanglements |
| 14:00-14:30 | Invited Talk: Marcus Mueller , <i>Georg-August-Universität, Institute for Theoretical Physics (Germany)</i> , Studying the kinetics of copolymer self-assembly |
| 14:30-14:45 | Alexander Wagner , <i>North Dakota State University (USA)</i> , Towards a computational modeling of structure formation in colloidal drying |
| 14:45-15:00 | Chandan Dasgupta , <i>Indian Institute of Science</i> , Complex Rheology of Nematogenic Fluids: Connection to Elastic Turbulence |
| 15:00-15:15 | Lampros Mountrakis , <i>University of Amsterdam (Netherlands)</i> , Looking into the transport of blood cells in flows without walls |

| Fluid Dynamics 1 | |
|--------------------------|--|
| Location: Terrace Lounge | Chairperson: Emily Ryan |
| 13:30-14:00 | Invited Talk: Monika Nitsche , <i>University of New Mexico (USA)</i> , Vortex Shedding and Low Order Models |
| 14:00-14:30 | Invited Talk: George Karniadakis , <i>Brown University (USA)</i> , Microscopic theory of Brownian motion: Effects of memory and confinement |
| 14:30-14:45 | Alex Hansen , <i>Norwegian University of Science and Technology</i> , A Monte Carlo Algorithm for Immiscible Two-Phase Flow in Porous Media |
| 14:45-15:00 | Junxue Ren , <i>Wright State University (USA)</i> , PIC Algorithm with Multiple Poisson Equation Solves during One time Step |
| 15:00-15:15 | Nils Moschuerer , <i>LMU Munich (Germany)</i> , Adaptive-Particle-Refinement for PIC Simulations |

| Quantum Many-Body Physics 1 | |
|-----------------------------|---|
| Location: East Balcony | Chairperson: Nikolai Prokofiev |
| 13:30-14:00 | Invited Talk: Ribhu Kaul , <i>University of Kentucky (USA)</i> , Deconfined quantum criticality in SU(N) magnets |
| 14:00-14:30 | Invited Talk: Boris Svistunov , <i>University of Massachusetts, Amherst (USA)</i> , Diagrammatic Monte Carlo for Fermionic and Fermionized Systems |
| 14:30-14:45 | George Batrouni , <i>Institut Non-Linéaire de Nice, University of Nice (France)</i> , Competition between the Haldane insulator, superfluid and supersolid phases in the one-dimensional Bosonic Hubbard Model |
| 14:45-15:00 | Karine Piacentini Coelho da Costa , <i>University of Massachusetts, Amherst (USA); University of Sao Paulo (Brazil)</i> , Critical Exponents of the Superfluid-Bose-Glass Transition in Three Dimensions |
| 15:00-15:15 | Yu-cheng Lin , <i>National Chengchi University (Taiwan)</i> , Neel to valence-bond-solid phase transitions in correlated valence-bond states |

Monday, Parallel Sessions 2

| Soft Matter and Biological Physics 2 | |
|--------------------------------------|---|
| Location: Conference Auditorium | Chairperson: Celeste Sagui |
| 15:45-16:15 | Invited Talk: Ivet Bahar , <i>University of Pittsburgh (USA)</i> , Structure-Encoded Dynamics of Proteins: Learning from Network Models and Experiments |
| 16:15-16:45 | Invited Talk: Normand Mousseau , <i>Université de Montréal (Canada)</i> , Computational challenges for the study of amyloid processes |
| 16:45-17:00 | Ming-chya Wu , <i>National Central University (Taiwan)</i> , Correlated vibrations in ion-pair dynamics in mechanoactivation identifies functional domains of force-dependent titin kinase |
| 17:00-17:15 | Christopher Roland , <i>North Carolina State University (USA)</i> , Investigating rare events with nonequilibrium work measurements: transition and reaction rates |

| Statistical Physics 1: Networks | |
|---------------------------------|--|
| Location: Small Ballroom | Chairperson: Jonathan Machta |
| 15:45-16:15 | Invited Talk: Mark Newman , <i>University of Michigan (USA)</i> , Large-scale structure in networks |
| 16:15-16:45 | Invited Talk: Lenka Zdeborova , <i>CEA Saclay and CNRS (France)</i> , Module detection in networks: phase transitions and optimal algorithms |
| 16:45-17:00 | Florent Krzakala , <i>Ecole Normale Supérieure (France)</i> , Belief-Propagation Guided Monte-Carlo Sampling |
| 17:00-17:15 | Lev Shchur , <i>Landau Institute for Theoretical Physics (Russia)</i> , Relation of Parallel Discrete Event Simulations algorithms with the physical models |
| 17:15-17:30 | Bruce Boghosian , <i>Tufts University (USA)</i> , Asset exchange and the origin of Pareto's Law of wealth distribution |

Monday, Parallel Sessions 2, continued

| Fluid Dynamics 2 | |
|--------------------------|--|
| Location: Terrace Lounge | Chairperson: James Adler |
| 15:45-16:15 | Invited Talk: Marc Gerritsma , <i>TU Delft (Netherlands)</i> , Structure preserving discretizations for computational physics |
| 16:15-16:45 | Invited Talk: Chun Liu , <i>Penn State University (USA)</i> , Energetic Variational Approaches in Complex Fluids |
| 16:45-17:00 | Christopher Amey , <i>University of Massachusetts, Amherst (USA)</i> , Persistent Patterns and Mixed Phase Space Dynamics |
| 17:00-17:15 | Blair Perot , <i>University of Massachusetts, Amherst (USA)</i> , Numerical Investigation of the Decay Rate of Isotropic Turbulence |
| 17:15-17:30 | Duncan McGregor , <i>Oregon State University (USA)</i> , Modelling Arcs in Magnetohydrodynamic Generator Channels |

| Novel Computing Paradigms 1 | |
|-----------------------------|---|
| Location: East Balcony | Chairperson: Martin Berzins |
| 15:45-16:15 | Invited Talk: Thomas Cheatham , <i>University of Utah (USA)</i> , Molecular dynamics simulation of nucleic acids: Convergence, reproducibility, assessment/validation, and data dissemination enabled by GPUs on XSEDE and Blue Waters |
| 16:15-16:45 | Invited Talk: Ying-jer Kao , <i>National Taiwan University</i> , Uni10: the Universal Tensor Network Library |
| 16:45-17:00 | Joshua Anderson , <i>University of Michigan (USA)</i> , Monte Carlo and Molecular Dynamics simulations of soft matter in the GPU era |
| 17:00-17:15 | Jens Glaser , <i>University of Michigan (USA)</i> , Strong Scaling of a Molecular Dynamics code on 1000's of GPUs |
| 17:15-17:30 | Hyun Lim , <i>South Dakota State University (USA)</i> , A Parallel Implementation of the Time-Decomposition Approach for the time-dependent Dirac Equation |

Tuesday, August 12

| | |
|----------------------------|---|
| 8:30-9:15 9:15-10:00 | Plenary Session: Enabling Technologies for Computational Science 1 <i>Chair: Richard Brower</i> John Danskin , <i>NVIDIA</i> The Physics of Computation and GPU Architecture Karl Schulz , <i>Intel</i> Enabling Technology Trends in High Performance Computing |
| 10:00-10:30 | Break |
| 10:30-11:15 11:15-12:00 | Plenary Session: Enabling Technologies for Computational Science 2 <i>Chair: Norbert Attig</i> Thomas Sterling , <i>CREST, Indiana University (USA)</i> Computational Physics at Extreme Scale James Sexton , <i>IBM</i> A Vision for Data Centric Systems |
| 12:00-13:30 | Lunch |
| 13:30-15:15 | Parallel Sessions 1 Soft Matter and Biological Physics 3, <i>Conference Auditorium</i> Statistical Physics 2, <i>Small Ballroom</i> General Computational Physics 1, <i>Terrace Lounge</i> Quantum Many-Body Physics 2, <i>East Balcony</i> Lattice Field Theory 1, <i>Mugar 205</i> |
| 15:15-15:45 | Break |
| 15:45-17:30 | Parallel Sessions 2 Materials Science and Nanoscience 2, <i>Conference Auditorium</i> Statistical Physics 3, <i>Small Ballroom</i> Computational Physics Education 1, <i>Terrace Lounge</i> Novel Computing Paradigms 2, <i>East Balcony</i> Lattice Field Theory 2, <i>Mugar 205</i> |
| 18:30-21:00 | Banquet Dinner speech: Claudio Rebbi, <i>Boston University (USA)</i> The early days of the Division of Computational Physics |

Tuesday, Parallel Sessions 1

| Soft Matter and Biological Physics 3 | |
|--------------------------------------|---|
| Location: Conference Auditorium | Chairperson: Marcus Mueller |
| 13:30-14:00 | Invited Talk: Marina Guenza , <i>University of Oregon (USA)</i> , A coarse-graining method that preserves the free energy, structural correlations, and thermodynamic state of polymer melts from the atomistic to the mesoscale |
| 14:00-14:30 | Invited Talk: Celeste Sagui , <i>North Carolina State University (USA)</i> , Free energy methods for biomolecular simulations |
| 14:30-14:45 | Thomas Salez , <i>(CNRS/ESPCI)</i> , A direct quantitative measure of surface mobility in a glassy polymer |
| 14:45-15:00 | Xizhong An , <i>Northeastern University (China)</i> , MPFEM modeling and mechanism analysis on the compaction of binary granular system |
| 15:00-15:15 | Guangjie Shi , <i>University of Georgia (USA)</i> , Protein Folding of the HOP Model: A Parallel Wang-Landau Study |

Tuesday, Parallel Sessions 1, continued

| Statistical Physics 2: Jamming, Hard Spheres | |
|--|---|
| Location: Small Ballroom | Chairperson: Alex Hansen |
| 13:30-14:00 | Invited Talk: Werner Krauth , <i>ENS Paris (France)</i> , Rejection-free, Irreversible, and Infinitesimal Monte Carlo Algorithms and Melting in two dimensions |
| 14:00-14:30 | Invited Talk: Salvatore Torquato , <i>Princeton University (USA)</i> , New Algorithm to Generate Jammed Sphere Packings |
| 14:30-14:45 | Masaharu Isobe , <i>Nagoya Institute of Technology (Japan)</i> , Nucleation of Hard Spheres in local Monte Carlo, Event-Chain Monte Carlo, and Molecular Dynamics |
| 14:45-15:00 | Chandan Dasgupta , <i>Indian Institute of Science</i> , Short-time relaxation in glass-forming liquids from dynamics in a meta-basin of the potential energy landscape |
| 15:00-15:15 | Ronald Dickman , <i>Universidade Federal de Minas Gerais (Brazil)</i> , Inconsistencies in steady state thermodynamics |

| General Computational Physics 1 | |
|---------------------------------|--|
| Location: Terrace Lounge | Chairperson: Jan Tobochnik |
| 13:30-13:45 | Panos Argyrakis , <i>University of Thessaloniki (Greece)</i> , Network of the FP7 collaboration projects |
| 13:45-14:00 | Larry Engelhardt , <i>Francis Marion University (USA)</i> , Quantum spin simulations made simple |
| 14:00-14:15 | Guiping Zhang , <i>Renmin University of China</i> , Effects of contact and strain on electronic transport properties of graphene: exact and renormalized transfer matrix method |
| 14:15-14:30 | Zine El Abidine Chaoui , <i>University of Setif (Algeria)</i> , An optimized analytic model for charged particle transport in water |
| 14:30-14:45 | Nikita Kirnosov , <i>University of Arizona (USA)</i> , Non-BO calculations of rovibrational states of systems with Coulomb interactions using explicitly correlated all-particle Gaussian functions |
| 14:45-15:00 | Mitsuyoshi Tomiya , <i>Seikei University (Japan)</i> , Scar State on Time-evolving Wavepacket |
| 15:00-15:15 | Joan Adler , <i>Technion (Israel)</i> , Efficient simulated annealing of segmented telescopes by invoking their analogy with SOS models |

| Quantum Many-Body Physics 2 | |
|-----------------------------|--|
| Location: East Balcony | Chairperson: Chisa Hotta |
| 13:30-14:00 | Invited Talk: Federico Becca , <i>National Council for Research (CNR) and SISSA (Italy)</i> , Variational wave functions for strongly-correlated models |
| 14:00-14:30 | Invited Talk: Philippe Corboz , <i>Institute for Theoretical Physics, University of Amsterdam (Netherlands)</i> , Recent progress in simulating strongly correlated systems with tensor network methods |
| 14:30-14:45 | Roger Melko , <i>University of Waterloo (Canada)</i> , Quantum Kagome Ice |
| 14:45-15:00 | Wenan Guo , <i>Beijing Normal University (China)</i> , Novel quantum glass of bosons in a random potential in two dimensions |
| 15:00-15:15 | Thomas Lang , <i>Boston University (USA)</i> , Mott Transitions of Correlated Fermions from SU(2) to SU(N) |

| Lattice Field Theory 1 | |
|------------------------|--|
| Location: Mugar 205 | Chairperson: Claudio Rebbi |
| 13:30-14:00 | Invited Talk: Taku Izubuchi , <i>RIKEN BNL Research Center (USA)</i> , TBD |
| 14:00-14:30 | Invited Talk: Aida El-Khadra , <i>University of Illinois (USA)</i> , Lattice QCD and Quark Flavor Physics |
| 14:30-14:45 | Steven Gottlieb , <i>Indiana University (USA)</i> , Electromagnetic effects of the light hadron spectrum |
| 14:45-15:00 | Oliver Witzel , <i>Boston University (USA)</i> , Lattice-QCD determination of B-meson decay constants and semileptonic form factors |
| 15:00-15:15 | Stefan Krieg , <i>Forschungszentrum Juelich (Germany)</i> , From quarks to hadrons and back: spectral and bulk properties of strongly interacting matter from Lattice QCD |

Tuesday, Parallel Sessions 2

| Materials Science and Nanoscience 2 | |
|-------------------------------------|---|
| Location: Conference Auditorium | Chairperson: Theodore L Einstein |
| 15:45-16:15 | Invited Talk: Hsin Lin , <i>Graphene Research Centre and Department of Physics, National University of Singapore</i> , Topological Crystalline Insulators: A New Phase of Quantum Matter |
| 16:15-16:30 | Zenan Qi , <i>Boston University (USA)</i> , Strain Engineering of Graphene Hexagon and Nanobubbles |
| 16:30-16:45 | Vladimir Stegailov , <i>JIHT RAS (Russia)</i> , Graphite melting: atomistic kinetics resolves long-standing controversy |
| 16:45-17:00 | Jenni Portman , <i>Michigan State University (USA)</i> , Evidence of stacking disorder induced gap opening in the ground state of 1T-TaS ₂ |
| 17:00-17:15 | Hiroaki Nakamura , <i>National Institute for Fusion Science (Japan)</i> , A Binary-Collision-Approximation Simulation Study on the Dependence of Noble Gas Absorption upon Crystal Orientation of Tungsten |
| 17:15-17:30 | Abdiravuf Dzhurakhalov , <i>University of Antwerp (Belgium)</i> , Computer simulation of the interaction of ringlike carbon clusters with nanographene |

Tuesday, Parallel Sessions 2, continued

| Statistical Physics 3: Spin Models | |
|------------------------------------|--|
| Location: Small Ballroom | Chairperson: Lev Shchur |
| 15:45-16:15 | Invited Talk: Youjin Deng , <i>University of Science & Technology of China</i> , Universal amplitudes in the canonical ensemble |
| 16:15-16:30 | Pablo Serna , <i>University of Murcia (Spain)</i> , Loop models with crossings |
| 16:30-16:45 | Robert Swendsen , <i>Carnegie Mellon University (USA)</i> , Solving the inverse Ising model with multi-spin interactions |
| 16:45-17:00 | Wolfhard Janke , <i>University of Leipzig (Germany)</i> , Non-Standard Finite-Size Scaling at First-Order Phase Transition |
| 17:00-17:15 | Edyta Malolepsza , <i>Boston University (USA)</i> , Generalized ensemble method applied to study systems with strong first order transition |
| 17:15-17:30 | Patrick Malsom , <i>University of Cincinnati (USA)</i> , The limitations of the Onsager-Machlup functional |

| Computational Physics Education 1 | |
|-----------------------------------|--|
| Location: Terrace Lounge | Chairperson: Wolfgang Christian |
| 15:45-16:15 | Invited Talk: Ruth Chabay , <i>North Carolina State University (USA)</i> , Computation and Conceptual Understanding in Introductory Physics |
| 16:15-16:45 | Invited Talk: Francisco Esquembre , <i>Universidad de Murcia (Spain)</i> , Facilitating programming computational physics simulations for tablets |
| 16:45-17:15 | Invited Talk: Beate Schmittmann , <i>Iowa State University (USA)</i> , K-12 outreach and student recruitment with computational science |
| 17:15-17:30 | Jan Tobochnik , <i>Kalamazoo College (USA)</i> , The Computational Physics Section of the American Journal of Physics |

| Novel Computing Paradigms 2 | |
|-----------------------------|---|
| Location: East Balcony | Chairperson: Thomas Cheatham |
| 15:45-16:15 | Invited Talk: Martin Berzins , <i>University of Utah (USA)</i> , Multiscale and Multiphysics Computations on Present and Future Architectures |
| 16:15-16:45 | Invited Talk: Erik Schnetter , <i>Perimeter Institute (Canada)</i> , Automated Code Generation for Solving PDEs on Modern HPC Architectures |
| 16:45-17:00 | Xavier Saez , <i>Barcelona Supercomputing Center (Spain)</i> , First experience with Particle-in-cell Plasma Physics code on ARM-based HPC systems |
| 17:00-17:15 | Elise de Doncker , <i>Western Michigan University (USA)</i> , Scalable Software for Multivariate Integration on Hybrid Platforms |
| 17:15-17:30 | Yasunari Zempo , <i>Hosei University (Japan)</i> , Real-Time and Real-Space Program Tuned in K-Computer |

| Lattice Field Theory 2 | |
|------------------------|---|
| Location: Mugar 205 | Chairperson: Richard Brower |
| 15:45-16:15 | Invited Talk: John Negele , <i>Massachusetts Institute of Technology (USA)</i> , Understanding the Structure of Nucleons using Lattice QCD |
| 16:15-16:45 | Invited Talk: William Detmold , <i>MIT (USA)</i> , Dark Nuclei |
| 16:45-17:00 | Sergey Syritsyn , <i>RIKEN BNL Research Center (USA)</i> , Nucleon Structure on a Lattice at the Physical Point |
| 17:00-17:15 | Venkitesh Ayyar , <i>Duke University (USA)</i> , Semimetal-Insulator transition without a fermion bilinear condensate |

Wednesday, August 13

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|-------------|--|
| 8:30-9:15 | Plenary Session: Computational Physics 3 <i>Chair: Wolfhard Janke</i> Helmut Katzgraber , <i>Texas A&M University (USA)</i> Four decades of frustration in spin-glass physics: Advances and applications |
| 9:15-10:00 | A. Peter Young , <i>University of California, Santa Cruz (USA)</i> Numerical Studies of the Quantum Adiabatic Algorithm |
| 10:00-10:30 | Break |
| 10:30-11:15 | Plenary Session: Computational Physics 4 <i>Chair: David Campbell</i> Ursula Rothlisberger , <i>Ecole Polytechnique Federale de Lausanne (Switzerland)</i> Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Simulations of Biological Systems: From Understanding to Control |
| 11:15-12:00 | Brian Granger , <i>California Polytechnic State University (USA)</i> Open source tools for exploratory and reproducible computational physics |
| 12:00-13:30 | Lunch |
| 13:30-15:15 | Parallel Sessions 1 Materials Science and Nanoscience 3, <i>Conference Auditorium</i> Statistical Physics 4, <i>Small Ballroom</i> Astrophysics 1, <i>Terrace Lounge</i> Quantum Many-Body Physics 3, <i>East Balcony</i> |
| 15:15-15:45 | Break |
| 15:45-17:30 | Parallel Sessions 2 Materials Science and Nanoscience 4, <i>Conference Auditorium</i> Novel Computing Paradigms 3, <i>Small Ballroom</i> Quantum Computing 1, <i>Terrace Lounge</i> Computational Physics Education 2, <i>East Balcony</i> |

Wednesday, Parallel Sessions 1

| Materials Science and Nanoscience 3 | |
|-------------------------------------|--|
| Location: Conference Auditorium | Chairperson: Volodymyr Turkowski |
| 13:30-14:00 | Invited Talk: Caterina Cocchi , <i>Humboldt-Universität zu Berlin (Germany)</i> , From Molecules to Organic Crystals: Optical Excitations from First Principles |
| 14:00-14:15 | Rodion Belosludov , <i>IMR, Tohoku University (Japan)</i> , Computation Modelling of Thermodynamic Properties of Nanoporous Materials toward Gas Storage and Separation |
| 14:15-14:30 | Stephanie Valleau , <i>Harvard University (USA)</i> , Electromagnetic study of the chlorosome antenna complex of <i>Chlorobaculum tepidum</i> |
| 14:30-14:45 | Huan Tran , <i>University of Connecticut (USA)</i> , Designing Organotin Polymers For Energy Storage Applications |
| 14:45-15:00 | Sahar Sharifzadeh , <i>Boston University (USA)</i> , Understanding the Photophysical Properties of Organic Polycrystalline Films |
| 15:00-15:15 | Ilnur Saitov , <i>Joint Institute for High Temperatures (Russia)</i> , First principle calculation of shocked xenon reflectivity |

| Statistical Physics 4: Spin Models | |
|------------------------------------|--|
| Location: Small Ballroom | Chairperson: Wolfhard Janke |
| 13:30-14:00 | Invited Talk: Koji Hukushima , <i>University of Tokyo (Japan)</i> , Equilibrium-state simulations of some (spin) glass models in finite dimensions |
| 14:00-14:15 | Wenlong Wang , <i>University of Massachusetts, Amherst (USA)</i> , Population annealing Monte Carlo: An effective simulation for spin glasses |
| 14:15-14:30 | Tasrief Surungan , <i>Hasanuddin University (Indonesia)</i> , Spin glass behavior of the antiferromagnetic Heisenberg model on scale free network |
| 14:30-14:45 | Elmar Bittner , <i>ITP, Heidelberg University (Germany)</i> , MuCa vs WL: A tight race |
| 14:45-15:00 | Alexandra Valentim , <i>Universidade Federal do Paraná (Brazil)</i> , Exploring Replica-Exchange Wang-Landau sampling in higher-dimensional parameter space |
| 15:00-15:15 | Raul Toral , <i>Institute for Cross-Disciplinary Physics and Complex Systems (Spain)</i> , Weighted-ensemble Brownian dynamics simulation: Sampling of rare events in non-equilibrium systems |

| Astrophysics 1: Cosmology and Galaxy Formation | |
|--|--|
| Location: Terrace Lounge | Chairperson: Romeel Davé |
| 13:30-14:00 | Invited Talk: Mike Boylan-Kolchin , <i>University of Maryland (USA)</i> , The Local Universe as a Dark Matter Laboratory |
| 14:00-14:30 | Invited Talk: Claude-andre Faucher-Giguere , <i>Northwestern/CIERA (USA)</i> , The Universe on a computer: Cosmological simulations of galaxy formation |
| 14:30-14:45 | Claudio Gheller , <i>CSCS (Switzerland)</i> , Numerical cosmology on the GPU with Enzo and Ramses |
| 14:45-15:00 | Robert Hohlfield , <i>Boston University (USA)</i> , Instability of Counterrotating Flow in an Astrophysical Disk |
| 15:00-15:15 | Ke-jung Chen , <i>University of California, Santa Cruz (USA)</i> , Cosmic Impact of the First Binaries |

| Quantum Many-Body Physics 3 | |
|-----------------------------|--|
| Location: East Balcony | Chairperson: Adrian Feiguin |
| 13:30-14:00 | Invited Talk: Tao Xiang , <i>Institute of Physics, Chinese Academy of Sciences (China)</i> , Renormalization of quantum many-body systems by the projected entangled simplex states |
| 14:00-14:30 | Invited Talk: Corinna Kollath , <i>University of Bonn (Germany)</i> , Spreading of correlations in strongly correlated (dissipative) quantum gases |
| 14:30-14:45 | Chisa Hotta , <i>University of Tokyo (Japan)</i> , Grand canonical analysis in one and two dimension: A route to measuring bulk properties in an applied field |
| 14:45-15:00 | Adrian Del Maestro , <i>University of Vermont (USA)</i> , A quantum Monte Carlo method to compute entanglement entropies of interacting bosons in the spatial continuum |
| 15:00-15:15 | Edwin Stoudenmire , <i>Perimeter Institute (Canada)</i> , Corner Contributions to Entanglement Entropy in Critical Systems |

Wednesday, Parallel Sessions 2

| Materials Science and Nanoscience 4 | |
|-------------------------------------|---|
| Location: Conference Auditorium | Chairperson: Lin-lin Wang |
| 15:45-16:15 | Invited Talk: Volodymyr Turkowski , <i>University of Central Florida (USA)</i> , Development and application of DFT+DMFT and TDDFT+DMFT techniques for nanosystems |
| 16:15-16:30 | Kenichi Asano , <i>Osaka University (Japan)</i> , Trions and Biexcitons in Semiconducting Single-Wall Carbon Nanotubes |
| 16:30-16:45 | Georgios Tritsarlis , <i>Harvard University (USA)</i> , On the possibility of photocatalytic water splitting on rutile TiO ₂ (110): a theoretical study |
| 16:45-17:00 | David A. Strubbe , <i>Massachusetts Institute of Technology (USA)</i> , Photoisomerization dynamics of solar thermal fuels with TDDFT excited-state forces |
| 17:00-17:15 | Iskakova Kulpash , <i>Kazakh National Pedagogical University (Kazakhstan)</i> , The modeling of the energy levels GaAs |
| 17:15-17:30 | Bin Hwang , <i>Michigan State University (USA)</i> , Effective transient states for nonequilibrium systems under ultrafast control pulses |

Wednesday, Parallel Sessions 2, continued

| Novel Computing Paradigms 3 | |
|-----------------------------|--|
| Location: Small Ballroom | Chairperson: Ying-Jer Kao |
| 15:45-16:15 | Invited Talk: Norbert Attig , <i>Julich Supercomputing Centre (Germany)</i> , The Path to Exascale: A European Perspective |
| 16:15-16:45 | Invited Talk: Lars Korsterke , <i>Texas Advanced Computing Center (USA)</i> , Heterogeneous computing. What is it and do we need it? |
| 16:45-17:00 | Feng Chen , <i>Brown University (USA)</i> , GPU Spectral Method and Stable Parareal Method for Large-scale Computational Science |
| 17:00-17:15 | Patrick Dreher , <i>North Carolina State University (USA)</i> , Proof of Concept Implementation of a Cloud Computing Infrastructure within a Supercomputer Architecture |
| 17:15-17:30 | Charles Still , <i>Lawrence Livermore National Laboratory (USA)</i> , Estimating the Impact of Future Advanced Architectures on ASC Multiphysics Codes |

| Quantum Computing 1 | |
|--------------------------|---|
| Location: Terrace Lounge | Chairperson: Edward Farhi |
| 15:45-16:15 | Invited Talk: David Clader , <i>Johns Hopkins University (USA)</i> , Preconditioned quantum linear system algorithm |
| 16:15-16:45 | Invited Talk: Bryan Clark , <i>University of Illinois at Urbana Champaign (USA)</i> , The cost of simulating quantum mechanics on a quantum computer |
| 16:45-17:15 | Invited Talk: Boixo Sergio , <i>Google (USA)</i> , Experiments with the DWave prototype |
| 17:15-17:30 | Jonathan Moussa , <i>Sandia National Labs (USA)</i> , Maximum entropy quantum simulation |
| 17:30-17:45 | Debasish Banerjee , <i>ITP, Uni Bern (Switzerland)</i> , Measurement driven quantum dynamics |

| Computational Physics Education 2 | |
|-----------------------------------|---|
| Location: East Balcony | Chairperson: Harvey Gould |
| 15:45-16:15 | Invited Talk: Spencer Wheaton , <i>University of Cape Town (South Africa)</i> , Infusing Computational Physics throughout the Undergraduate Curriculum |
| 16:15-16:45 | Invited Talk: Shobhana Narasimhan , <i>Jawaharlal Nehru Centre for Advanced Scientific Research (India)</i> , Teaching Density Functional Theory through Experiential Learning: Examples from the Developing World |
| 16:45-17:00 | Wolfgang Christian , <i>Davidson College (USA)</i> , Parallel Programming Using Easy Java Simulations |
| 17:00-17:15 | Rachele Dominguez , <i>Randolph-Macon College (USA)</i> , The role of computational physics in the liberal arts curriculum |
| 17:15-17:30 | Werner Krauth , <i>ENS Paris (France)</i> , Statistical Mechanics: Algorithms and Computations - A High-Level Massive Open Online Course (2014) |

Thursday, August 14

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|-------------|---|
| 8:30-10:15 | Parallel Sessions Materials Science and Nanoscience 5, <i>Conference Auditorium</i> Soft Matter and Biological Physics 4, <i>Small Ballroom</i> Lattice Field Theory 3, <i>Terrace Lounge</i> Astrophysics 2, <i>East Balcony</i> |
| 10:15-10:30 | Break |
| 10:30-11:15 | Plenary Session: Computational Physics 5 <i>Chair: Arun Bansil</i> Steven Louie , <i>University of California, Berkeley; Lawrence Berkeley National Lab (USA)</i> GW-based Methods for ab initio Studies of Electronic Excited-State Phenomena in Condensed Matter |
| 11:15-12:00 | Steven White , <i>University of California, Irvine (USA)</i> Solving frustrated magnetic systems with the density matrix renormalization group |
| 12:00-13:30 | Lunch |
| 13:30-14:15 | Plenary Session: Computational Physics 6 <i>Chair: Claudio Rebbi</i> Luigi Del Debbio , <i>University of Edinburgh (UK)</i> Recent progress in simulations of gauge theories on the lattice: QCD at the physical point and new strongly-interacting dynamics beyond the Standard Model |
| 14:15-15:00 | Romeel Davé , <i>University of the Western Cape (South Africa)</i> Simulations of Galaxy Formation |
| 15:00-15:15 | Closing |

Thursday, Parallel Sessions 1

| Materials Science and Nanoscience 5 | |
|-------------------------------------|--|
| Location: Conference Auditorium | Chairperson: Hsin Lin |
| 8:30-9:00 | Invited Talk: Markus Eisenbach , <i>Oak Ridge National Laboratory (USA)</i> , Magnetic Materials at finite Temperatures: thermodynamics and combined spin and molecular dynamics derived from first principles calculations |
| 9:00-9:15 | Van An Dinh , <i>Osaka University (Japan)</i> , Origin of ferromagnetism in GaMnAs: A hybrid density functional study |
| 9:15-9:30 | Tiago de Campos , <i>Universidade de São Paulo (Brazil)</i> , Diagonalization of very large dense electronic structure matrices: an out-of-core iterative method |
| 9:30-9:45 | Qiao-neng Guo , <i>Zhengzhou University (China)</i> , Temperature dependence of tensile properties of nano-Cu films: Molecular dynamics simulation |
| 9:45-10:00 | Xavier Andrade , <i>Harvard University (USA)</i> , Application of compressed sensing to electronic structure simulations |

Thursday, Parallel Sessions 1, continued

| Soft Matter and Biological Physics 4 | |
|--------------------------------------|---|
| Location: Small Ballroom | Chairperson: Alfredo Alexander-Katz |
| 8:30-8:45 | Shanadeen Begay , <i>Boston University (USA)</i> , The Thermodynamics and Structure of Methionine Enkephalin using the Statistical Temperature Molecular Dynamics-CHARMM algorithm |
| 8:45-9:00 | Xizhong An , <i>Northeastern University (China)</i> , Radical Tessellation and Microstructure Characterization of Binary and Ternary Hard Sphere Crystals |
| 9:00-9:15 | Zhenlu Cui , <i>Fayetteville State University (USA)</i> , Mesoscale structures and Rheology of Active Liquid Crystals |
| 9:15-9:30 | Amandeep Sangha , <i>UT/ORNL Center for Molecular Biophysics (USA)</i> , Lignin polymerization in plant cell walls: Monolignol binding, oxidation and radical coupling reactions |
| 9:30-9:45 | Nikolaos Papadimitriou , <i>National Center for Scientific Research "Demokritos" (Greece)</i> , Study of Ceramide Bilayers with Molecular Dynamics Simulations |
| 9:45-10:00 | Sunita Negi , <i>University of Delhi (India)</i> , Probing temperature dependent conformation change of Calmodulin protein using Molecular Dynamics simulations |
| 10:00-10:15 | Christopher Cooper , <i>Boston University (USA)</i> , Implicit-solvent model using Python and GPUs for proteins interacting with charged surfaces |

| Lattice Field Theory 3 | |
|--------------------------|---|
| Location: Terrace Lounge | Chairperson: Anna Hasenfratz |
| 8:30-9:00 | Invited Talk: Simon Catterall , <i>Syracuse University (USA)</i> , Supersymmetry on a lattice |
| 9:00-9:30 | Invited Talk: Frithjof Karsch , <i>Brookhaven National Laboratory (USA)</i> , Conserved charge fluctuations in strong interaction matter |
| 9:30-9:45 | Evan Weinberg , <i>Boston University (USA)</i> , Targeting the Conformal Window: Measuring the O^{++} Scalar |
| 9:45-10:00 | Rajamani Narayanan , <i>Florida International University (USA)</i> , Polyakov loops in two dimensional QCD |

| Astrophysics 2: Compact Objects and Gravitational Waves | |
|---|--|
| Location: East Balcony | Chairperson: TBD |
| 8:30-9:00 | Invited Talk: Christian David Ott , <i>Caltech (USA)</i> , Petascale Simulations of Core-Collapse Supernovae |
| 9:00-9:30 | Invited Talk: Deirdre Shoemaker , <i>Georgia Tech (USA)</i> , Numerical Relativity and Gravitational Waves |
| 9:30-9:45 | Hyun Lim , <i>South Dakota State University (USA)</i> , A Time Parallalizable Numerical Approach for the Semilinear Wave Equation |
| 9:45-10:00 | R K Chhajlani , <i>Vikram University (India)</i> , Self-gravitational Instability in Interstellar Molecular Clouds with polarized dust and neutral collisions |

Poster Session

Monday, 17:30-19:30

| 1 Statistical Physics (Ziskind Lounge) | |
|--|--|
| 1 | Lukas Einkemmer , <i>University of Innsbruck (Austria)</i> , A Hamiltonian splitting for the Vlasov-Maxwell system |
| 2 | Adriana Gomes Dickman , <i>Pontifícia Universidade Católica de Minas Gerais (Brazil)</i> , Simulation of an epidemic model with vector transmission |
| 3 | Lucila Alvarez Zuzek , <i>IFIMAR-CONICET (Argentina)</i> , Theory and simulations of Epidemics in partially overlapped Multiplex Networks |
| 4 | Sitangshu Bikas Santra , <i>Indian Institute of Technology Guwahati</i> , Random rotational sandpile model: Crossover from rotational to stochastic universality class |
| 5 | Amin Najafi , <i>Islamic Azad University (Iran)</i> , The study of Binder Cumulant's behavior in two-dimensional anisotropic of Ising models with foreign-neighbor interactions by SAPBC method |
| 6 | Gonzalo Suarez , <i>IFIMAR-CONICET (Argentina)</i> , Transport with hard-core interaction in a chain of asymmetric cavities. |
| 7 | Ronald Dickman , <i>Universidade Federal de Minas Gerais (Brazil)</i> , Intrinsic convergence properties of entropic sampling algorithms |
| 8 | Zhenjiu Wang , <i>Beijing Normal University (China)</i> , Phase transitions in A nonlinear XY model with symmetry-breaking field in two dimensions |
| 9 | Manabu Hasegawa , <i>University of Tsukuba (Japan)</i> , Functionality limit of classical simulated annealing |
| 10 | Henio Rego , <i>CPS/Boston University and IFMA (USA)</i> , Percolation-Like Complexity in a 2 Dimensional Long Range SIR O-Lattice Model |
| 11 | Antonina Fedorova; Michael Zeitlin , <i>IPME RAS (Russia)</i> , Pattern Formation: From Local Hidden Symmetries to Global Dynamics |
| 12 | Atsunari Katsuki , <i>Nihon University (Japan)</i> , Numerical simulation of dune morphology deformed by multiple flow conditions |
| 13 | Altan Allawala , <i>Brown University (USA)</i> , Equal-time PDF of the stochastically forced Lorenz-63 attractor using a Fokker-Planck description |
| 14 | Zheng Zhu; Andrew Ochoa , <i>Texas A&M University (USA)</i> , Efficient sampling of ground-state configurations for quasi-two-dimensional Ising spin glasses |
| 15 | Nagendra Panduranga , <i>Boston University (USA)</i> , k-Core percolation in interdependent networks |
| 16 | Na Xu , <i>Boston University (USA)</i> , Dynamics of 2D Ising Model in linearly varying magnetic field |
| 17 | Bolun Chen , <i>Boston College (USA)</i> , Scaling of spiking neural network for mammalian olfaction |
| 18 | Alejandro Lage Castellanos , <i>Universidad de la Habana (Cuba)</i> , Bayesian inference of epidemics on networks via Belief Propagation |
| 19 | Alejandro Lage Castellanos , <i>Universidad de la Habana (Cuba)</i> , Region graph approximations to free energy in finite dimensional spin glasses. |

| 2 Soft Matter and Biological Physics (Ziskind Lounge) | |
|---|---|
| 1 | Shourjya Sanyal , <i>University College Dublin (Ireland)</i> , Simulations On The Designing Rationale of FRET Based Uni-Molecular Probes |
| 2 | Amid Ranjesh Siahkal , <i>University of Maribor (Slovenia)</i> , Computer simulation of domain patterns in randomly perturbed Nematic liquid crystal |
| 3 | Emine Deniz Tekin , <i>University of Turkish Aeronautical Association (Turkey)</i> , Molecular Dynamics Simulation of Self-Assembled Peptide-Amphiphiles |
| 4 | Freddie Salsbury , <i>Wake Forest University (USA)</i> , All-atom GPU-enabled simulations of therapeutic nucleic acids and their effects on DNA-binding proteins |
| 5 | Julio Rocha , <i>UFMG (Brazil)</i> , Identifying transitions in finite systems by means of partition function zeros and microcanonical inflection-point analysis: A comparison for elastic flexible polymers |
| 6 | Danh-Tai Hoang , <i>Asia Pacific Center for Theoretical Physics (Korea)</i> , Conserved rule for pancreatic islet organization |
| 7 | Muhammad Anwar , <i>University of Luxembourg</i> , Crystallization mechanism in melts of short polymer chains |
| 8 | Sarra Douah , <i>Université des Sciences et de la Technologie d'Oran (Algeria)</i> , Partition function zeros for semi-flexible homopolymers |
| 9 | Shuhei Kawamoto , <i>Temple University (USA)</i> , Free energy analysis of membrane fusion |
| 10 | Abdiravuf Dzhurakhalov , <i>University of Antwerp (Belgium)</i> , Monte Carlo parameterization in the VirtualLeaf framework |
| 11 | Rui Travasso , <i>University of Coimbra (Portugal)</i> , Validity of the contact order-rate correlation in the folding of small, single domain proteins: A Monte Carlo simulation |
| 12 | Busara Pattanasiri , <i>University of Georgia (USA)</i> , Effect of surface attractive strength on structural transitions of a confined HP lattice protein |
| 13 | N. Atamas , <i>National Kyiv Taras Shevchenko University (Ukraine)</i> , Study of ionic liquids+aromatic mono-substituted benzene strongly diluted solutions by molecular dynamics at $t = 400\text{K}$ |
| 14 | Amir Azadi , <i>University of Massachusetts Amherst (USA)</i> , Emergent structure of multi-dislocation ground states in curved crystals |
| 15 | Kang Liu , <i>Boston University (USA)</i> , Physiologic Networks: Topological and Functional Transitions |
| 16 | Ronny Bartsch , <i>Boston University (USA)</i> , Phase Synchronization and co-existing forms of non-linear coupling between physiologic systems |
| 17 | Kristina Streu , <i>Boston College (USA)</i> , Stability of stapled p53 peptides bound to MDM2 |
| 18 | Johannes Bock , <i>University Leipzig ITP (Germany)</i> , Semi-flexible polymers in disordered media |
| 19 | Alemayehu Mengesha Cherkos , <i>Instituto Superioro Tecnico (Portugal)</i> , Effect of viscosity on Propagation of MHD Waves in Astrophysical Plasma |
| 20 | Sumantra Sarkar , <i>Brandeis University (USA)</i> , Shear Induced Rigidity in Athermal Solids |
| 21 | Yoelvis Orozco-Gonzalez , <i>BGSU/USP (USA)</i> , Implementation of the free energy gradient to the geometry optimization of molecular systems in complex environments |
| 22 | Md Zulfikar Ali , <i>Clark University (USA)</i> , In silico evolution of biochemical networks |

| 3 Materials Science and Nanoscience (Small Ballroom) | |
|--|---|
| 1 | Victoria Mazalova , <i>Southern Federal University (Russia)</i> , The combined XANES and DFT approach for study of nanomaterials. |
| 2 | Edwin Mapasha , <i>University of Pretoria (South Africa)</i> , Van der Waals Density Functional Study Of Lithium on Bilayer Graphene |
| 3 | Sergei Zakharchenko , <i>Moscow Institute of Physics and Technology (Russia)</i> , Algorithm of Shaping Multiple-beam Bragg's Acousto-optic Diffraction Laser Field Into 1D and 2D Patterns |
| 4 | Seiki Saito , <i>Kushiro National College of Technology (Japan)</i> , Study on Hydrogen Plasma - Carbon Material Interaction by Molecular Simulation in Submicron Scale |
| 5 | Yang Han , <i>Nanjing University (China)</i> , Electronic and Magnetic Properties of One and Two Dimensional Monolayer MoS ₂ with Sulfur Line Defect |
| 6 | Esam Abdul-Hafidh , <i>Royal Commission (Saudi Arabia)</i> , Modulus of Spherical Palladium Nanoparticles by Chen-Mobius Lattice Inversion Method |
| 7 | Alexander Popov , <i>Lomonosov Moscow State University (Russia)</i> , Multiscale simulation of thermal disruption in resistance switching process in amorphous carbon |
| 8 | Yasunari Zempo , <i>Hosei University (Japan)</i> , Development of the SSPH Method for Real-Space Electronic Structure Calculation |
| 9 | Andrey Baranov , <i>Moscow Institute of Physics and Technology (Russia)</i> , Eigen Frequency Piezoelectric Resonance Modes in Terms of Longitudinal Temperature Gradient Stimulated by Second Harmonic Generation |
| 10 | Stylianios Karozis , <i>National Center for Scientific Research "Demokritos" (Greece)</i> , A non-stochastic computational approach for the determination of the surface area of microporous solids |
| 11 | Tom Underwood , <i>University of Edinburgh (UK)</i> , Which crystal structure? Lattice-switch Monte Carlo can tell you |
| 12 | Zenan Qi , <i>Boston University (USA)</i> , Highly Ductile Graphene Kirigami |
| 13 | George Lithoxoos , <i>National Center for Scientific Research "Demokritos" (Greece)</i> , Determination of partial charges in inorganic-organic clusters based on DFT calculations |
| 14 | Katsuhiko Higuchi , <i>Hiroshima University (Japan)</i> , Electronic structure calculations for materials immersed in a uniform magnetic field via the relativistic tight-binding approximation method |
| 15 | Grigory Kolesov , <i>Harvard University (USA)</i> , Methoxy photo-dissociation on TiO ₂ surface: ab initio excited-state dynamics |
| 16 | Nicolas Sawaya , <i>Harvard University (USA)</i> , Computational Design of Excitonic Structures with DNA: Beyond Förster Resonance Energy Transfer |
| 17 | Khellil Bouamama , <i>University Setif 1 (Algeria)</i> , Ab-initio calculation of the structural and elastic properties of ternary metal nitrides TaxMo _{1-x} N and TaxW _{1-x} N |
| 18 | Nikolaos Papadimitriou , <i>National Center for Scientific Research "Demokritos" (Greece)</i> , Evaluation of the Efficiency of Clathrate Hydrates in Storing Energy Gases |
| 19 | Asanka Weerasinghe , <i>University of Massachusetts Amherst (USA)</i> , Multiphonon Raman scattering in monolayer WSe ₂ |
| 20 | Seyedeh Nazanin Khatami , <i>University of Massachusetts Amherst (USA)</i> , Optimizing Si _{1-x} GexSi _{1-y} Gey Superlattices for Thermoelectric Efficiency by Minimizing thermal Conductivity |
| 21 | Sanjay Kumar Singh , <i>Jiwaji University (India)</i> , Investigation of high pressure phase transition and electronic properties of Lutetium Nitride |

| 3 | Materials Science and Nanoscience, continued |
|----|--|
| 22 | Genri Norman , <i>JlHT RAS (Russia)</i> , On the difference and similarity between plasma-plasma and liquid-liquid first-order phase transitions |
| 23 | Rabab Zahira , <i>University of Agriculture Faisalabad (Pakistan)</i> , Co-precipitation synthesis, physical and magnetic properties of manganese ferrite powder |
| 24 | Lin-Lin Wang , <i>Ames Laboratory (USA)</i> , High-throughput Screening of Doped MnBi for Better Permanent Magnets |
| 25 | Berk Onat , <i>Harvard University (USA)</i> , Artificial Neural Networks for Representation of Potential Energy Surface of Li-Si Alloys |
| 26 | Farzaneh Shayeganfar , <i>Ecole Polytechnique de Montreal (Canada)</i> , Electronic Properties of Self-Assembled Trimesic Acid on Graphene |
| 27 | Sholeh Alaei , <i>METU (Turkey)</i> , Study of Structural, Electronic and Magnetic Properties of (Fe ₂ O ₃) _n Clusters Using Density Functional Theory |
| 28 | Angelo Ziletti , <i>Boston University (USA)</i> , Exciton transport and charge separation in artificial light harvesting systems: merging quantum non-adiabatic dynamics with electronic structure theory |
| 29 | Ali Khaledi Nasab , <i>Ohio University (USA)</i> , Localization of Envelop Functions in InAs/GaAs Dome-Shaped Quantum Dots |
| 30 | Ali Khaledi Nasab , <i>Ohio University (USA)</i> , Shape-dependent Properties of InAs/GaAs Quantum Dots in Presence and Absences of Wetting Layer |
| 31 | Xukun Xiang , <i>Michigan State University (USA)</i> , Atomistic simulation of systems driven through phase transitions by hot electron distributions |
| 32 | Nick Materise , <i>Northeastern University (USA)</i> , Evaluation of Periodic Green's Functions on Graphics Processing Units |
| 33 | Aram Shirinyan , <i>Kiev University and National Academy of Science (Ukraine)</i> , The nanophase diagrams of thin films based on molecular static simulations and the size effect |
| 34 | Guiping Zhang , <i>Renmin University of China</i> , Effects of Strain on Electronic Transport Property of Graphene Nanoribbons between metallic contacts |

| 4 | Fluid Dynamics (Small Ballroom) |
|---|--|
| 1 | Yao Shi , <i>Northwestern Polytechnical University (China)</i> , Numerical Simulation of Cavitation Characteristics for Pump-jet Propeller |
| 2 | Guang Pan , <i>Northwestern Polytechnical University (China)</i> , Numerical Simulation of Drag and Flow Noise Property on Structure for Carrier of Multi-loads AUV |
| 3 | Aydogan Ozdamar , <i>Ege University (Turkey)</i> , Computational Investigation of Flow Control by Means of Tubercles on Darrieus Wind Turbine Blades |
| 4 | Lev Barash , <i>Landau Institute for Theoretical Physics (Russia)</i> , Dependence of the fluid convection in an evaporating sessile droplet on the properties of the substrate |
| 5 | Jinwang Tan , <i>Boston University (USA)</i> , Modeling the growth and morphology of dendrites in Lithium air batteries |
| 6 | Ilias Tolias , <i>National Center of Scientific Research (Greece)</i> , CFD simulation of hydrogen deflagration in a vented room |
| 7 | William Lane , <i>Boston University (USA)</i> , Efficient simulations of heated gas-particle flows with immersed horizontal cylinders |

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|---|---|
| 4 | Fluid Dynamics, continued |
| 8 | Shreyas Mandre , <i>Brown University (USA)</i> , A reduced model for vortex shedding from a body using matched asymptotics |

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| 5 | Quantum Many-Body Physics (Large Ballroom) |
| 1 | Ying Tang , <i>Boston University (USA)</i> , Monte Carlo studies of spinon deconfinement in two dimensions |
| 2 | Zhi Wang , <i>Sun Yat-sen University (China)</i> , Rectification effect in Majorana fermion SQUID |
| 3 | Adam Iaizzi , <i>Boston University (USA)</i> , 1D Valence Bond Solids in a Magnetic Field |
| 4 | Zhao Liu , <i>Princeton University (USA)</i> , Matrix-Product-State Algorithm for Finite Fractional Quantum Hall Systems |
| 5 | Nils Blümer , <i>Gutenberg University Mainz (Germany)</i> , Tunable nanomagnetism in moderately cold fermions on optical lattices |
| 6 | Nils Blümer , <i>Gutenberg University Mainz (Germany)</i> , Fate of the false Mott-Hubbard transition in two dimensions |
| 7 | Cheng-Wei Liu , <i>Boston University (USA)</i> , Imaginary-time quench quantum Monte Carlo algorithm and its applications to spin-glass transitions |
| 8 | Edgar Josué Landinez Borda , <i>Universidade Estadual de Campinas (Brazil)</i> , Mechanical Properties of Solid Helium 4 by Path-Integral Monte Carlo Calculations |
| 9 | William Putikka , <i>Ohio State University (USA)</i> , Entropy and Thermopower in the 2D t-J Model |
| 10 | Hidemaro Suwa , <i>University of Tokyo (Japan)</i> , Gap Estimation and Level Spectroscopy for Quantum Spin Systems by Monte Carlo Method |
| 11 | Masahiko Higuchi , <i>Hiroshima University (Japan)</i> , Validity of the kinetic energy functional based on the coupling-constant expression in the pair-density functional theory |
| 12 | Kyle Robertson , <i>University of Vermont (USA)</i> , Monte Carlo Simulation of Superfluid Helium-4 in Mesoporous Silica |
| 13 | Krissia de Zawadzki , <i>Universidade de São Paulo (Brazil)</i> , Alternative numerical renormalization-group method to compute magnetic relaxation rates in dilute magnetic alloys |
| 14 | Mohammad Soltanieh-ha , <i>Northeastern University (USA)</i> , Interplay of charge, spin and lattice degrees of freedom on the spectral properties of the one-dimensional Hubbard-Holstein model |
| 15 | Shainen Davidson , <i>Boston University (USA)</i> , SU(3) classical representation of quantum dynamics of interacting spins |
| 16 | Thomas Lang , <i>Boston University (USA)</i> , Dynamic scaling from non-equilibrium quenching of correlated Dirac fermions |
| 17 | Alberto Nocera , <i>Northeastern University (USA)</i> , Pairing and nanoscale phase separation in Bose-Fermi mixtures |
| 18 | Daoxin Yao , <i>Sun Yat-sen University (China)</i> , Quantum Monte Carlo study of Disordered Spin Systems |
| 19 | Chia-Min Chung , <i>National Tsin Hua University (Taiwan)</i> , Entanglement spectroscopy using quantum Monte Carlo |

| 5 | Quantum Many-Body Physics, continued |
|----|--|
| 20 | Hitesh Changlani , <i>University of Illinois at Urbana-Champaign (USA)</i> , Stochastically Projecting Tensor Networks |
| 21 | Michael Zeitlin; Antonina Fedorova , <i>IPME RAS (Russia)</i> , Quantum Mechanics: Beyond Gaussians |
| 22 | Phillip Weinberg , <i>Boston University (USA)</i> , Using Local Updates to Evaluate Real Time Dynamics of Manybody Lattice Models |
| 23 | Hui Shao , <i>Beijing Normal University (China)</i> , Topological properties of valence-bond-solid states of the JQ3 model |
| 24 | Lu Liu , <i>Beijing Normal University (China)</i> , The effects of bond-disorder in the two-dimensional JQ ₃ model |

| 8 | Astrophysics and Space Plasma Physics (Small Ballroom) |
|---|---|
| 1 | Ke-Jung Chen , <i>UCSC (USA)</i> , Supernovae at the Cosmic Dawn |
| 2 | Pramod Kumar Purohit , <i>National Institute of Technical Teachers' Training & Research (India)</i> , Evaluation of geomagnetic storms effects on the GPS derived total electron content (tec) |
| 3 | Pramod Kumar Purohit , <i>National Institute of Technical Teachers' Training & Research (India)</i> , The statistical investigation of amplitude Scintillations at Indian high latitude Station Maitri, Antarctica |
| 4 | Carlos Arturo Soto-Campos , <i>Autonomous University of Hidalgo State (Mexico)</i> , An alternative model to cold dark matter for galactic rotation curves |
| 5 | Juan Hinojosa , <i>Texas A&M University (USA)</i> , The Surface Gravitational Expression of an Upwelling Thermal Mantle Plume: A Computational Model |

| 9 | Computational Physics Education (Ziskind Lounge) |
|---|--|
| 1 | Felix Garcia-Clemente , <i>University of Murcia (Spain)</i> , EJS: A JavaScript library which makes computational-physics education simpler |
| 2 | Samuel Castle , <i>Davidson College (USA)</i> , A Parallel Computational Model of Orbiting N-Body Clusters |
| 3 | Jay Wang , <i>University of Massachusetts Dartmouth (USA)</i> , Computational physics with meshfree methods |
| 4 | Hartmut Ruhl , <i>LMU (Germany)</i> , An effective PIC-solver for radiation reaction of electrons and radiation |

| 10 | Novel Computing Paradigms (Small Ballroom) |
|----|--|
| 1 | Kewei Du , <i>Institute of Software</i> , Heterogeneous Beam Dynamic Simulations for Linear Accelerator |
| 2 | Yun-Da Hsieh , <i>National Taiwan University</i> , Implementation of the Universal Tensor Network Library on GPU using Cuda |
| 3 | Andrew Pochinsky , <i>MIT (USA)</i> , Data parallel scientific programming with Qlua |

| 11 | General Computational Physics (Small Ballroom) |
|----|---|
| 1 | Brian Burrows , <i>Staffordshire University (UK)</i> , Confined Systems |
| 2 | Mitsuki Toogoshi , <i>Hosei University (Japan)</i> , Maximum Entropy Method for Optical Spectrum Analysis of Real-Time TDDFT |
| 3 | Ronald White , <i>James Cook University (Australia)</i> , A method for the accelerated numerical solution of fractional diffusion equations |
| 4 | Ronald White , <i>James Cook University (Australia)</i> , The application of pseudo-spectral methods to low-energy positron transport gases |
| 5 | Arman Kussainov , <i>al-Farabi National University (Kazakhstan)</i> , Neutron monitor data analysis through quantum transformation operator's eigenvalue statistics |
| 6 | Sul-Ah Ahn , <i>KISTI (Korea)</i> , Research Activity in High Performance Computational Physics: Co-authorship Network Analysis |
| 7 | Henio Rego , <i>CPS/Boston University and IFMA (USA)</i> , When a Text is Translated Does the Complexity of Its Vocabulary Change? Translations and Target Readerships |

Exhibitors

The following publishers will present exhibits at CCP2014:

- AIP Publishing
- Cambridge University Press
- Elsevier
- IOP Publishing

The exhibits are located in [Ziskind Lounge](#) and will be open [Monday-Wednesday](#).



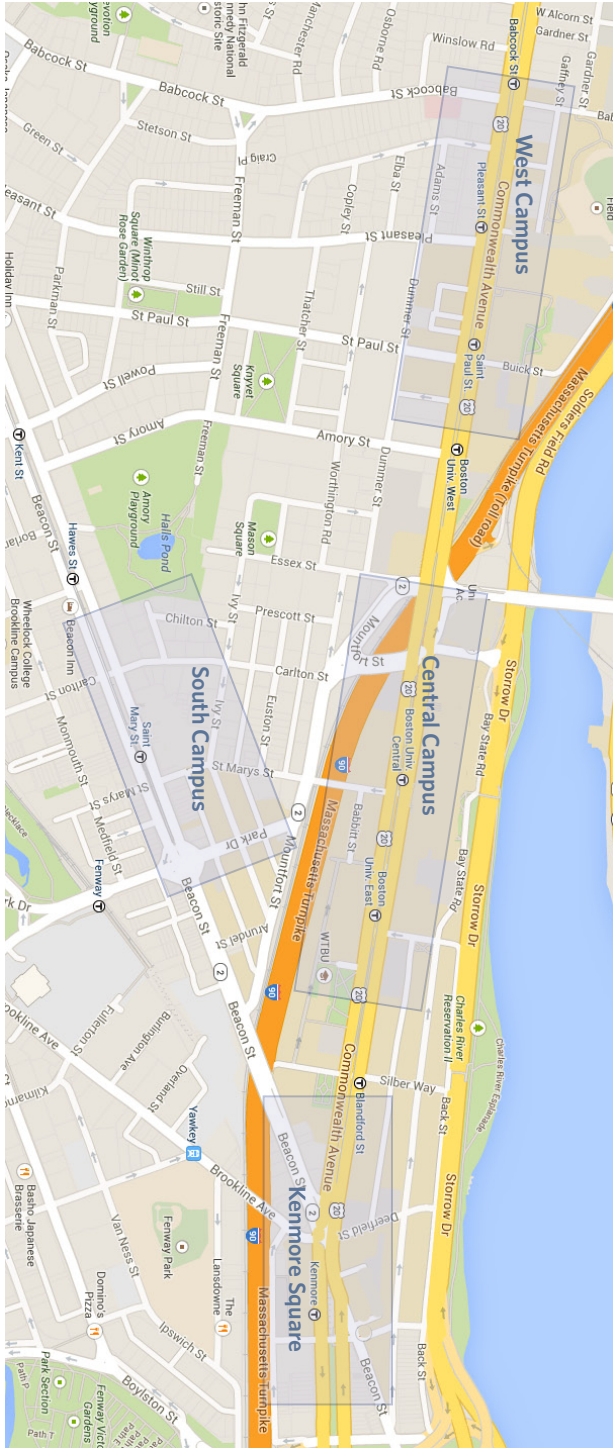
Food Court

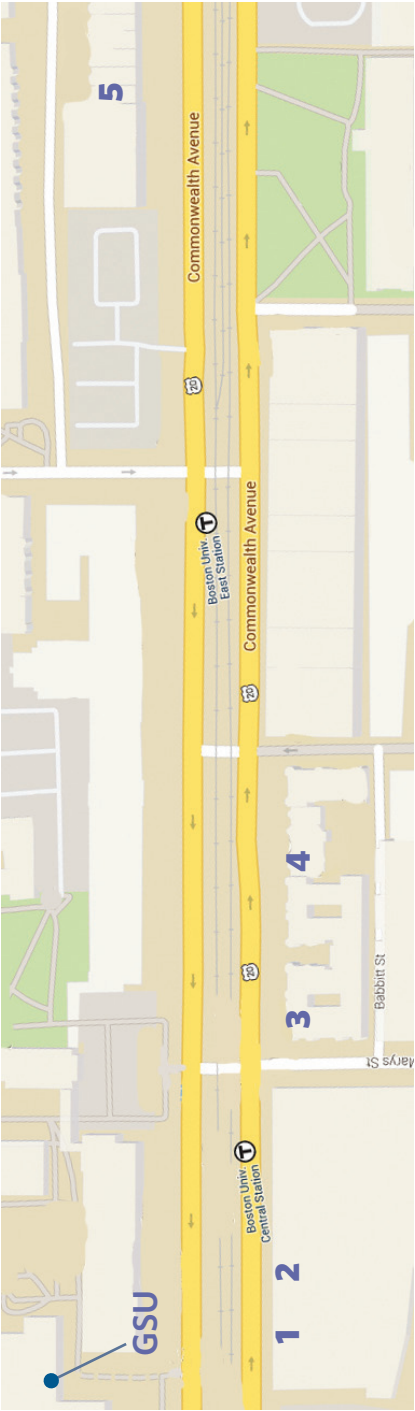
There is a food court with many options on the first floor of the GSU, down the stairs from the conference venue. Please note that many of these restaurants only accept cash.

Nearby Restaurants

There are also many restaurants on or near BU, which are listed on the following pages. The restaurants are arranged into 4 general areas: Central Campus, South Campus, West Campus and Kenmore Square; these areas are shown on the map on the opposite page. Listings include walking time from the GSU.

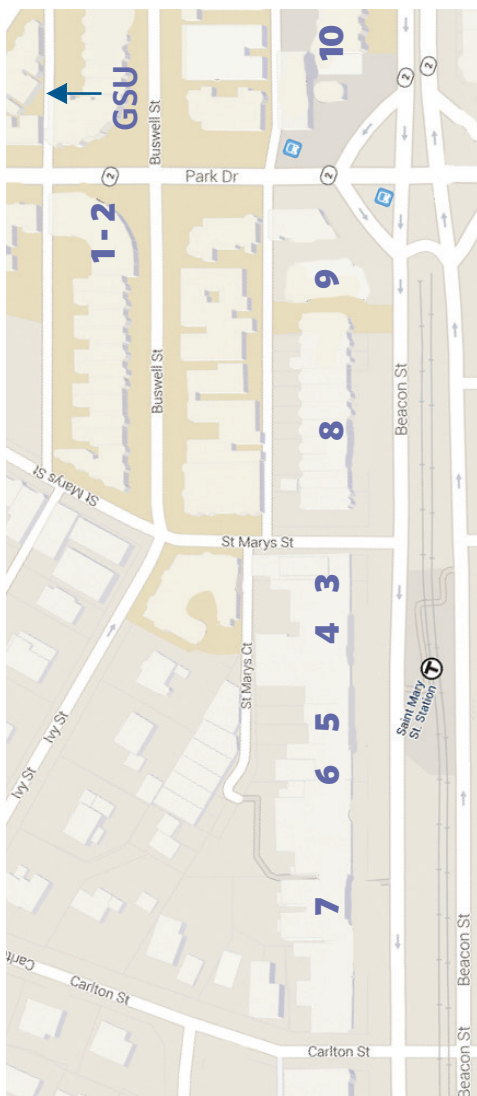
Restaurant Areas





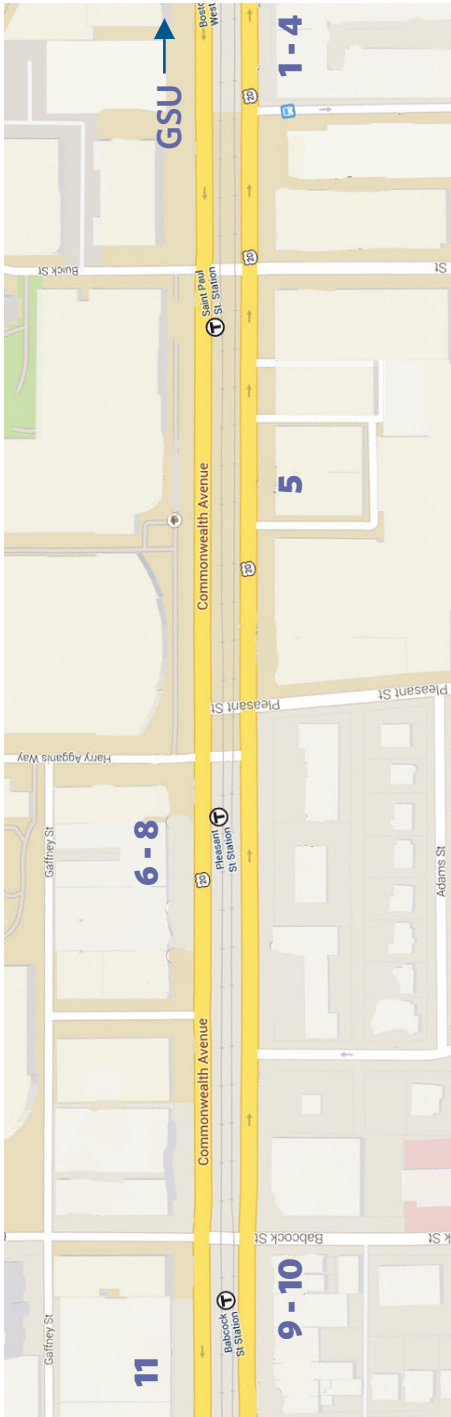
Central Campus

- 1 Nud Pob \$**
Thai
738 Commonwealth Ave (2 min)
- 2 Pavement Coffee House \$**
Coffee, sandwiches
736 Commonwealth Ave (2 min)
- 3 Beijing Café \$**
Chinese
728 Commonwealth Ave (3 min)
- 4 University Grill & Pizza \$**
American, pizza
712 Commonwealth Ave (4 min)
- 5 Noodle St \$**
Asian
627 Commonwealth Ave (7 min)



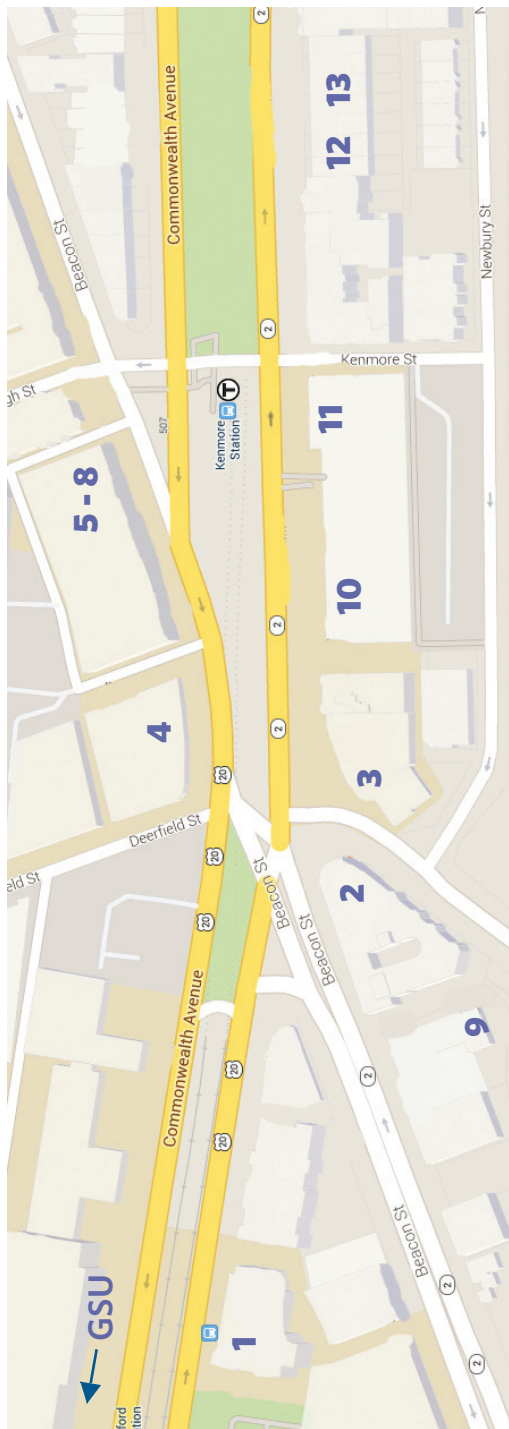
South Campus

- 1 **Mei Mei** \$
Asian
506 Park Dr (7 min)
- 2 **Crispy Crepes Café** \$
Mediterranean
512 Park Dr (7 min)
- 3 **Gyu-Kaku** \$\$
Japanese BBQ
1002 Beacon St (8 min)
- 4 **Sichuan Gourmet** \$
Chinese
1004 Beacon St (8 min)
- 5 **Japonaise Café** \$
Pastries, sandwiches
1020 Beacon St (9 min)
- 6 **Whole Foods Market** \$
Sandwiches, salad bar, prepared food
1026 Beacon St (9 min)
- 7 **Temptations Café** \$
Sandwiches, salads
1038 Beacon St (9 min)
- 8 **Sol Azteca** \$\$ (dinner only)
Mexican
914 Beacon St (9 min)
- 9 **The Elephant Walk** \$\$\$
French-Cambodian
900 Beacon St (9 min)
- 10 **Audubon Boston** \$\$
American
838 Beacon St (11 min)



West Campus

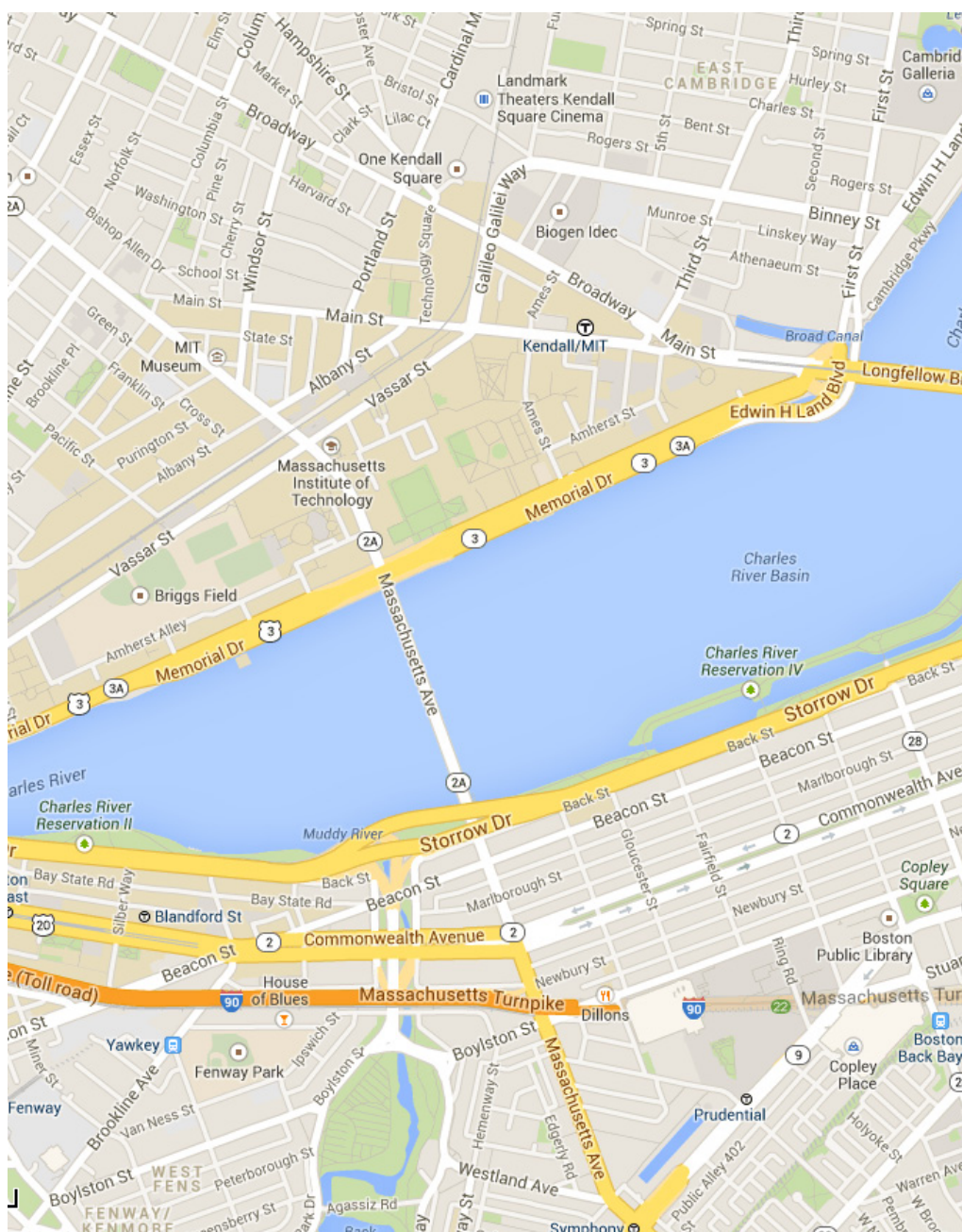
- 1 **Boston House of Pizza** \$\$
Pizza
173 Amory St (6 min)
- 2 **Chipotle** \$
Mexican
876 Commonwealth Ave (7 min)
- 3 **Otto** \$\$
Pizza
888 Commonwealth Ave (7 min)
- 4 **Panera** \$
Sandwiches, salads
888 Commonwealth Ave (7 min)
- 5 **Sunset Cantina** \$\$
Mexican
916 Commonwealth Ave (11 min)
- 6 **Raising Cane's** \$
Fast Food, chicken
949 Commonwealth Ave (11 min)
- 7 **Blue State Coffee** \$
Coffee, sandwiches
957 Commonwealth Ave (11 min)
- 8 **BurgerFi** \$
Burgers
961 Commonwealth Ave (11 min)
- 9 **T. Anthony's** \$
Pizza, Italian
1016 Commonwealth Ave (14 min)
- 10 **Angora Café** \$
Sandwiches, vegan
1024 Commonwealth Ave (14 min)
- 11 **Brown Sugar Café** \$\$
Thai
1033 Commonwealth Ave (15 min)



Kenmore Square

- 1 **Scoozi** \$\$
American, sandwiches, pizza
580 Commonwealth Ave (10 min)
- 2 **Pizzeria UNO** \$\$
American, Pizza
645 Beacon St (13 min)
- 3 **Qdoba** \$
Mexican
540 Commonwealth Ave (13 min)
- 4 **Bertucci's** \$\$
Italian
533 Commonwealth Ave (14 min)
- 5 **Bruegger's Bagels** \$
Bagels
644 Beacon St (14 min)
- 6 **Fin's** \$\$
Japanese, sushi
636 Beacon St (14 min)
- 7 **Thai Dish** \$
Thai
636 Beacon St (14 min)
- 8 **Uburger** \$
Burgers
636 Beacon St (14 min)
- 9 **Boston Beer Works** \$\$
American, pub
61 Brookline Ave (15 min)
- 10 **Eastern Standard** \$\$\$
American, French
528 Commonwealth Ave (15 min)
- 11 **Island Creek Oyster Bar** \$\$\$
American, seafood
500 Commonwealth Ave (15 min)
- 12 **Café 472** \$
Sandwiches, frozen yogurt
472 Commonwealth Ave (16 min)
- 13 **India Quality** \$\$
Indian
484 Commonwealth Ave (16 min)

Map of Boston



Map of Boston

