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Abstracts / Plenary Sessions

CONTENTS

Monday, 9:15-10:00, Computational Physics 1

Sauro Succi, *IAC-CNR (Italy)*
Lattice Boltzmann simulations of complex flows across scales: turbulence, soft-glasses and quark-gluon plasmas

In the last two decades, the Lattice Boltzmann (LB) method has attracted major interest as a very versatile and efficient computational scheme for the numerical simulation of complex fluid problems across a broad range of scales, from fluid turbulence, to soft-glasses, all the way down to relativistic quark-gluon plasmas. In this talk, after introducing the basic ideas behind the LB method, we shall illustrate recent applications to large-scale turbulence, soft-glass rheology and shock-wave propagation in quark gluon plasmas. Finally, future challenges ahead will also be briefly touched upon.

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Monday, 10:30-12:00, Computational Physics 2

Yuko Okamoto, *Nagoya University (Japan)*
Enhanced configurational sampling methods for spin systems and biomolecular systems

Conventional Monte Calro and molecular dynamics simulations of spin and biological systems are greatly hampered by the multiple-minima problem, where the simulations tend to get trapped in some of a huge number of local-minimum-energy states which are separated by high energy barriers. In order to overcome this difficulty, we have been advocating the uses of generalized-ensemble algorithms which are based on non-Boltzmann weight factors. With these algorithms we can explore a wide range of the configurational space. The advantage of generalized-ensemble algorithms such as multicanonical algorithm, simulated tempering, and replica-exchange method lies in the fact that from only one simulation run, one can obtain various thermodynamic quantities as functions of temperature, pressure, and other parameters of the system. In this talk, I will present the results of our recent applications of generalized-ensemble algorithms to spin and biomolecular systems. Examples of the systems are Ising model, Potts model, protein, protein-ligand complex, etc.

Nandini Trivedi, *Ohio State University (USA)*
Topology and Correlations driving new materials, phases and phenomena

Quantum materials today can be classified as a function of the strength of Coulomb interactions U and spin orbit coupling λ, in units of the bandwidth W. At large U lie the 3d transition metal oxides that show phenomena such as colossal magneto- resistance and high Tc superconductivity. In the opposite quadrant we encounter topological band insulators with large λ but in weakly correlated s- and p- band materials. I will discuss the next frontier of 4d and 5d oxide materials in the central region of such a phase diagram and show how novel phases and phenomena arise from the close interplay of all three scales-- λ, U and W. I will critically review the combination of computational methods that are necessary to address the richness of the 4d and 5d materials. The role of advanced spectroscopies such as angle resolved photoemission, inelastic neutron scattering, THz spectroscopy, and resonant x-ray scattering using circularly polarized photons, to identify different response functions of complex oxides will also be discussed.

Tuesday, 8:30-10:00, Enabling Technologies for Computational Science 1

John Danskin, *NVIDIA*
The Physics of Computation and GPU Architecture

In 1974, Dennard et al argued that power dissipation of integrated circuits would be independent of circuit density, and that furthermore, same-circuit gate delays would scale with transistor feature size. Moore's law implied that circuit density would double every two years. Together, these implied that computational power per square inch and computational power per watt should double every 18 months. The rate of feature scaling, and feature dependent scaling of capacitance, resistance, and voltage have all fallen off of Dennard's projections. Despite this, by using massively parallel computation, GPUs have mostly been able to stay on the Moore's law overall performance curve. I'll explain how we've done this, what this means for programming models, and make some projections for the future of computing.

Karl Schulz, *Intel*
Enabling Technology Trends in High Performance Computing

This talk will highlight enabling technology trends in high performance computing, including hardware and software perspectives for current and future generation systems on the path to exascale. As we know, the total power budget that can realistically be deployed for future exascale systems requires energy-efficient innovations to be made across all facets of supercomputing design ranging from on-node (e.g. CPU, memory) enhancements, rack design and thermal cooling improvements, and enhanced high-speed communication layers to support high-bandwidth, low-latency message transfers efficiently. Indeed, performance per watt arguments at the node level have already lead to substantial gains in today's coprocessor/accelerator technologies. In this talk, we will highlight some of Intel's approach for

addressing these challenges, and the software and hardware implications for future generation systems and what it means for computational scientists.

Tuesday, 10:30-12:00, Enabling Technologies for Computational Science 2

Thomas Sterling, *CREST, Indiana University (USA)*
Computational Physics at Extreme Scale

The future of high performance computing is jeopardized by the end of Dennard scaling and the approaching end of Moore's Law, eliminating the two principal sources of exponential performance gain that has dominated the field for more than two decades. Future science applications demand increased fidelity, physics phenomenology, multi-scale formulation, efficiency, and scalability. It is further recognized that these must be achieved within a context that makes system use easier and therefore more productive than even today's systems while delivering two to three orders of magnitude performance advantage. The ParalleX execution model suggests an alternative paradigm for the representation and management of extreme scale physics applications that dramatically improves efficiency, scalability, and productivity through the exploitation of dynamic adaptive methods within the context of global address space. The HPX runtime system is an experimental resource management and task scheduling system which, when combined with the low level programming interface, XPI, offers an alternative strategy that promises new opportunities in science exploration and discovery through computation. ParalleX integrates advanced concepts including lightweight multi-threading, message-driven computation, multi-nodal processes, dynamic introspection, and heterogeneous resource control into a single computational framework to address the challenges of starvation, latency, overhead, and contention. Additional emerging capabilities provide promising paths to addressing the challenges of power consumption and reliability. By offloading much of the resource management decision from the user to the runtime system, ParalleX offers a means of simplifying methods for programming. This presentation will discuss the ParalleX model and its proof-of-concept implementations of HPX and XPI. A number of physics codes under development will be examined using these advanced concepts including wavelets and finite element codes for shockwave physics with reactive materials, adaptive mesh refinement (AMR) for multimaterial modeling, Fast Multipole Method codes for molecular dynamics, cosmology simulations, and computational electromagnetics, Barnes-Hut N-body codes for cosmological structure simulations and galaxy evolution, and LULESH for shock hydrodynamics.

James Sexton, *IBM*
A Vision for Data Centric Systems

Data Centric Systems (DCS) focus on the problem of data location, and the principle that moving computing to the data will lead to more cost effective, efficient, and easier to program systems than prior generation systems. DCS hardware, which is heterogeneous by nature, will provide leadership capabilities for Big Data, complex analytics, modeling/simulation and cognitive computing. DCS software will allow this hardware to be used efficiently. Fully exploiting these heterogeneous high performance

capabilities will require additional innovation in programming models. A central motivator for DCS is to ensure the attributes of the architecture and implementation lead to commercially viable Exascale systems. This means that investments in programming models, languages and software development will be preserved for the future and that new optimized code will be positioned to take advantage of Exascale features. We will explain our vision for Data Centric Computing, covering hardware, software and programming models.

Wednesday, 8:30-10:00, Computational Physics 3

Helmut Katzgraber, *Texas A&M University (USA)*
Four decades of frustration in spin-glass physics: Advances and applications

Spin glasses are archetypal model systems used to investigate the effects of frustration and disorder. Concepts from the study of spin glasses have been applied to fields as diverse as structural biology, geology, computer science and financial analysis. Thus, understanding these systems on a fundamental level is of paramount importance. Despite ongoing research spanning several decades, there remain many fundamental open questions, such as the existence of a spin-glass state in a field or the low-temperature structure of phase space for short-range systems. In recent years, however, the advent of fast and cost-effective computers, as well as the use of efficient algorithms has enabled researchers to probe these paradigmatic systems deep into the spin-glass phase. In parallel, research has also shifted towards applications of the spin-glass machinery to a plethora of research fields and, in particular, to the understanding of problems in quantum information theory and quantum computing. In this talk, I will illustrate why these frustrated systems are not so frustrating after all. First, an overview of spin glasses will be given, followed by recent developments on the low-temperature behavior of spin glasses. Furthermore, the use of spin glasses in quantum computing applications is illustrated with the central role they play in benchmarking quantum annealing machines, such that the D-Wave Two.

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A. Peter Young, *University of California, Santa Cruz (USA)*
Numerical Studies of the Quantum Adiabatic Algorithm

One of the major ongoing debates on the future of quantum annealers pertains to their robustness against the decohering effects of finite temperature and interactions with the environment. We argue that even in an ideal setting of very low temperatures and in the absence of a decohering environment, quantum annealers may find it challenging to solve optimization problems significantly faster than state-of-the-art heuristic classical algorithms. Here, we study the performance of the quantum adiabatic algorithm (QAA) on a variety of constraint satisfaction problems and a spin glass problem by studying the size dependence of the minimum energy gap during the evolution of the QAA. We do so by employing Quantum Monte Carlo schemes as these allow us to study these problems at much larger

scales than exact methods would allow. We find that in all cases a quantum phase transition occurs and the minimum gap decreases exponentially with system size, leading to an exponentially large running time for the QAA. Based on these and other results, we discuss potential modifications to the QAA that may improve the scaling of the minimum gap, leading to faster quantum adiabatic algorithms.

Wednesday, 10:30-12:00, Computational Physics 4

Ursula Rothlisberger, *Ecole Polytechnique Federale de Lausanne (Switzerland)*
Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Simulations of Biological Systems: From Understanding to Control

During the last years, we have developed nonadiabatic excited state dynamics methods based on Trajectory Surface Hopping/Linear Response Time-Dependent Density Functional Theory (TSH/LR-TDDFT) [1] and real time propagation TDDFT (PT-TDDFT) based Ehrenfest dynamics [2] and have combined them with mixed quantum mechanical/ molecular mechanical (QM/MM) simulations to study nonadiabatic processes in complex environments. We have also implemented the presence of external electromagnetic fields [3] in combination with local control theory for an on-the-fly pulse shaping to control population transfer between electronic states [4]. We have used these QM/MM simulations in ground and excited states to study photoactive proteins [5-7] and photoinduced protein and DNA damage.

In this talk, I will present our results on the structural, dynamical and optical properties of the visual pigment rhodopsin along the photocycle [5-7]. We performed a systematic study of the size and sampling dependence of the optical properties and assessed the performance of a variety of different electronic structure methods in describing the photoabsorption spectra [7]. By applying feature selection and causality inference algorithms, we were able to identify the main factors that influence the color tuning in this system [5]. We have applied similar techniques to identify photoprotection mechanisms in proteins by studying the photodynamics of the highly abundant cation-π motif, Lys+ - Trp.

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Brian Granger, *California Polytechnic State University (USA)*
Open source tools for exploratory and reproducible computational physics

Computing, and thus software, is one of the foundations of modern physics research and education. It is used for simulation, data analysis, statistical modeling, symbolic manipulation, experimental control, etc. The software we use for these activities has a profound affect on human behavior, attitudes and thought patterns. In this talk I will describe open source software tools and development patterns that are having an impact, through their attributes, on the practice of computational physics research and education.

Distributed version control systems, such as git, have attributes that enhance collaboration, reproducibility and open peer review. In the context of open source software, git/GitHub have enabled teams to scale their development activities efficiently in a way that encourages broad and open collaboration. Using the ecosystem of open source Python projects as an example, I will describe the best practices that have emerged for collaboration, peer review and testing. In particular, I will contrast these practices with those of traditional scientific research.

IPython is an open source source interactive computing environment for Python and other languages. Its attributes encourage exploration, reproducibility and reuse. Its main application, the IPython Notebook, enables users to create documents that combine live code with narrative text, LaTeX equations, images, video. These notebook documents provide a complete, reproducible record of a computation that can be converted to various formats (HTML, LaTeX, slideshows, Markdown, etc.) and shared with others. IPython enables scientists to create computational narratives that can be used in a wide range of settings in a reproducible manner.

To conclude I will give examples of researchers who have used these tools to conduct exploratory computational research and education in a manner that is open and reproducible.

Thursday, 10:30-12:00, Computational Physics 5

Steven Louie, *University of California, Berkeley; Lawrence Berkeley National Lab (USA)*
GW-based Methods for ab initio Studies of Electronic Excited-State Phenomena in Condensed Matter

In this talk, we discuss recent progress in the use of the GW approach and its extensions to compute electronic excitations and related spectroscopic properties of materials and nanostructures. This interacting-electron Green's approach incorporates many-electron interaction effects through the screened Coulomb interaction W. Inclusion of electron-hole interactions (excitonic effects) within the general framework moreover allows accurate ab initio study of optical responses and phenomena such as photo-induced structural changes. These many-electron effects are particularly important in reduced-dimensional systems and nanostructures, where symmetry, dimensionality and many-body interactions can lead to unusual manifestation of concepts/phenomena that may not be so prominent or have not

been seen in bulk materials. Several phenomena are discussed, exploring their physical origin and comparing theoretical predictions with experimental data.

Steven White, *University of California, Irvine (USA)*
Solving frustrated magnetic systems with the density matrix renormalization group

The density matrix renormalization group (DMRG) has become the standard approach for simulating strongly correlated electron systems in one dimension. Recent progress has allowed DMRG to be used for two dimensional systems, most notably in finding that the kagome lattice Heisenberg model has a spin liquid ground state. Recently, the matrix product wavefunctions produced by DMRG have been shown to be the simplest example of a wide class of tensor network states, all exploiting the low entanglement of ground states. These connections to quantum information have led to a large variety of new algorithms. I will give an overview of some of the recent developments, both in our conceptual understanding of the algorithms and in their application to frustrated 2D spin systems.

Thursday, 13:30-15:00, Computational Physics 6

Luigi Del Debbio, *University of Edinburgh (UK)*
Recent progress in simulations of gauge theories on the lattice: QCD at the physical point and new strongly-interacting dynamics beyond the Standard Model

Algorithmic progresses over the last ten years have made it possible to simulate quantum field theories on the lattice taking fully into account the contributions stemming from the fermion determinant. As a consequence lattice gauge theories have become a prime tool to study not only QCD at the physical point, but also strongly-interacting theories beyond QCD. The latter theories could play an important role for models of dynamical electroweak symmetry breaking (DEWSB). In this talk, I will briefly summarize the work on new algorithms, and the impact on the performance of Monte Carlo simulations. I will then explain what are the relevant questions for DEWSB, and discuss how these questions could be answered by numerical studies.

Romeel Davé, *University of the Western Cape (South Africa)*
Simulations of Galaxy Formation

Galaxies are the way by which we mark out the evolution of our Universe. Whether we use them to measure dark energy, study how stars form, explore the final frontier of reionization, or study them for their own sake, the problem of galaxy formation is a rich and long-standing area of astrophysics that remains remarkably poorly understood. This talk will give a brief introduction to the study of how galaxies form and evolve, discuss some of the key physical ingredients such as supernova-driven winds and black holes, highlight some successes and failures of current models, and in particular describe how powerful supercomputers are paving the way towards an improved understanding of how galaxies are born, live, and die within a cosmic ecosystem. By critically comparing such simulations with state of the

art observations using the world's most advanced telescopes, we are moving closer than ever towards understanding the origin of galaxies such as our own Milky Way, and completing our cosmic story from the Big Bang until today.