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Abstracts / Parallel Sessions

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PARALLEL SESSION ABSTRACTS

Monday, Parallel Sessions 1, 13:30-15:15

Materials Science and Nanoscience 1

Luca Ghiringhelli, *Fritz Haber Institute of the Max Planck Society (Germany)*
Big Data of Materials Science - Critical Role of the Descriptor
Co-Authors: Jan Vybiral; Sergey Levchenko; Claudia Draxl; Matthias Scheffler

Statistical learning of materials properties or functions so far starts with a largely silent, non-challenged step: the introduction of a descriptor. However, when the scientific connection between the descriptor and the actuating mechanisms is unclear, causality of the learned descriptor-property relation is uncertain. Thus, trustful prediction of new promising materials, identification of anomalies, and scientific advancement are doubtful.

For many, maybe most, material functions, the "cause → property/function" relation is complex and indirect. Let us label the "cause" by a multi-dimensional descriptor d, which is initially unknown. The property/function is a number P (e.g. the thermoelectric figure of merit of a material). Obviously, the nuclear numbers and stoichiometry uniquely identify the many-body Hamiltonian and its results. However, in order to establish a d → P mapping, the question is: What is the (microscopic) mechanism behind the desired quantity. In other words, what is the best descriptor d? At the same time, we like to request, that d should not require an involved computation. It should relate to simple material properties, or even properties of the involved atoms, e.g. energy levels and wave functions. Only then, the P(d) relation can serve the above-mentioned wanted purpose.

We analyze this issue and define requirements for a suited descriptor. For a classical example, the energy difference of zincblende/wurtzite and rocksalt semiconductors, we demonstrate how a meaningful descriptor can be found systematically.

Lin-Lin Wang, *Ames Laboratory (USA)*
Computational Modeling of Transition-Metal Alloyed Nanoparticles in Working Condition

Transition-metal alloyed nanoparticles (NPs) are key components in current and emerging energy technologies because they are found to improve catalytic activity and selectivity for many energy-conversion processes. However, the difficulty of characterizing and describing the structural and compositional changes in alloyed NPs under reactive conditions remains a significant challenge. To address this challenge, several examples will be presented to show the effects of adsorbate, support and alloying on the properties of alloyed NPs. Hydrogen-passivation was predicted to inhibit the shearing instability in small Pt NPs and stabilize the ordered bulk-like structure. Recently, this prediction on the effect of adsorbate on NP structure has been verified by experiments and the effect of different

supports has also been included. For the effect of alloying, two dominating factors and their interplay have been identified to determine the core-shell preference in alloyed NPs. Take a step further to address the challenge to describe the compositional profile of alloyed NPs under reactive condition, the cluster expansion (CE) method have been extended to treat both alloyed NPs and adsorbates on the same footing. The ability to evaluate the energetics over a huge number of configurations from the optimal CE Hamiltonian at the accuracy of the input first-principles calculations has been used to study the configurational thermodynamics of bimetallic NPs and adsorbates in detail. Ag-Au NPs has been found to prefer multi-shell configurations. The composition of Pd-Pt core-shell NPs can be tuned to give the optimal adsorption energy for hydrogen evolution reaction. The voltammetry for Pt(111)/H has been simulated to reveal the role of a small population of hydrogen adsorbed on non-fcc sites. With these examples, computational modeling is shown to provide an accurate description of the compositional profile for alloyed NPs and enable rational design of alloyed NP catalysts.

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Hossein Mosallaei, *Northeastern University (USA)*
Novel Materials Enabled with Core-Shell Dielectric-Plasmonic Particles

Materials are prime enabler of technology. Metamaterial has been a transformative field where by engineering elements in a building block unique phenomena could be achieved. In this presentation we will demonstrate by using only two types of materials, a positive dielectric and a negative plasmonic, how one can achieve a range of desired material parameters from 0 to infinity (positive and negative) combining them in core-shell fashion. We consider unique applications in the areas of lensing, guiding, and negative index materials (just to name few). Computation is very challenging as one will face a configuration of large area of complex elements where they are not periodic. Modal analysis will be implemented combined with translational theorems to express the electromagnetic fields and apply boundary conditions successfully. It will be illustrated how new materials can be constructed using the subwavelength nanoscale elements designed and engineered in graded-pattern across a structure, material design cell by cell.

Theodore Einstein, *Physics & CMTC, University of Maryland (USA)*
Characterizing Capture Zone Distributions (CZD) in Island Growth on Surfaces: Simulations Confront Experiments

In studies of epitaxial growth, analysis of the distribution of the areas of capture zones (i.e. proximity polygons or Voronoi tessellations with respect to island centers) is often the best way to extract the critical nucleus size i (the largest island size that can decay). For non-Poisson deposition (i.e. when island nucleation is not fully random), the normalized areas s of these Voronoi cells can be well described by the generalized Wigner distribution (GWD) $P_\beta(s) = a s^\beta \exp(-bs2)$ [1], particularly in the central region $0.5<s<2$ where the data is least noisy. Extensive Monte Carlo simulations [2] reveal inadequacies of our earlier mean field analysis and suggest $\beta = i+2$ for diffusion-limited aggregation. We summarize several recent applications to experimental systems (catalogued in a recent minireview [3]), highlighting insights gained from this perspective. Since simulations [2,4] generate orders of magnitude more data than experiments, they permit close examination of the tails of the distribution, which differ from the simple GWD form. We discuss some more sophisticated refinements [5] involving a fragmentation model. Scaling the data [4] is possible though not wholly desirable. Recent findings [6] indicate modifications appear for attachment-limited aggregation. Finally, we recount applications to social phenomena such the distribution of areas of arrondissements (districts, i.e. secondary administrative units) and of Metro stations in central Paris [5,7]. Work at UMD supported by NSF CHE 13-05892

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Vlad Sokhan, *National Physical Laboratory (UK)*
Electronically coarse-grained simulations in materials science

Improving the accuracy of the results and the quality of predictions is one of the major challenges in atomistic simulation of condensed matter. The solution is thought to lie in developing a multiscale approach that would seamlessly integrate quantum and classical dynamics and the early work in this field has been recognised by the 2013 Nobel Prize in Chemistry. The now standard methods are almost invariably using spatial decomposition into quantum and classical regions coupled together and describing phenomena on different scales.

In this talk I will present a powerful novel framework [1,2], in which the valence electrons of a molecule are replaced by a single quantum Drude oscillator that reproduces the electronic molecular responses to

all orders of polarization and dispersion terms, thus obviating the necessity of empirical van der Waals forces. Using this approach, we built a water model from molecular monomer and dimer properties [3] and show that this framework contains essential physics to accurately predict water's behaviour from ice phase to critical point [4]. The model can be further exploited to build a next generation non-reactive force field for materials simulation.

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Soft Matter and Biological Physics 1

Mark Robbins, *Johns Hopkins University (USA)*
Welding and healing of polymer interfaces: Strength from entanglements
Co-Authors: Ting Ge; Gary Grest; Dvora Perahia

Applying heat to polymer interfaces is a common means of welding polymer components or healing cracks in polymers. Once chains have diffused by their radius of gyration, the properties of the interface should be indistinguishable from those of the bulk. In practice, welds can achieve bulk strength at much shorter times. The mechanism of strength growth is difficult to determine with experiments, because they cannot directly access the evolution of molecular configurations and entanglements. Large-scale simulations are used to follow the dynamics of interdiffusion at welds and cracks and the associated changes in density and molecular conformations[1]. The evolution of entanglements is tracked using Primitive Path Analysis and shown to be directly related to the mechanical strength under shear and tensile loading. As in experiment, the maximum shear strength □max of a homop as a power of welding time t and then saturates at the bulk value. Simulations show that □max is proportional to the areal density of interfacial entanglements at short times and saturates when chains have formed 2-3 entanglements across the interface. Enthalpy limits interdiffusion across heteropolymer interfaces, and there is a corresponding reduction in interfacial entanglements and mechanical strength. A minimum loop length of order the entanglement length must diffuse across the interface to form entanglements. Crack healing is more complicated because of the presence of short segments produced during fracture. Segments that are too short to confer bulk strength, but longer than the entanglement length, remain near the interface for long time intervals. This leads to a plateau in strength that is below the bulk value. Crazes form under tensile loading. A low interfacial entanglement density can stabilize craze formation and significantly enhance the fracture energy, but the bulk fracture energy is recovered at about the same time as bulk shear strength. Supported by NSF Grant DMR-1006805, CMMI-0923018 and OCI-0963185.

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Marcus Mueller, *Georg-August-Universität, Institute for Theoretical Physics (Germany)*
Studying the kinetics of copolymer self-assembly

Copolymers are flexible macromolecules that are comprised of two (or more) blocks. The incompatibility between the constituents of different blocks gives rise to microphase separation on the length scale of 5 -70 nm. Much effort has been devoted to utilizing these soft materials as templates for nanostructures, e.g., for integrated circuits and memory devices, and fabricating defect-free structures or structures that differ from the thermodynamically stable morphologies in the bulk.

Computational modeling can contribute to optimizing material parameters such film thickness, interaction between copolymer blocks and substrate, geometry of confinement, and it provides fundamental insights into the physical mechanisms of directing the self-assembly, addressing both the equilibrium structure and thermodynamics and the kinetics of self-assembly.

I will discuss highly coarse-grained particle-based models that allow us to access the long time and large length scales associated with self-assembly [1,2], review computational methods [2,3] to determine the free energy of self-assembled structures [4,5] and to investigate the kinetic pathways of structure formation [6]. Opportunities for directing the kinetics of self-assembly by temporal changes of thermodynamic conditions will be discussed.

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Alexander Wagner, *North Dakota State University (USA)*
Towards a computational modeling of structure formation in colloidal drying

We present lattice Boltzmann models at different scales for the simulation of colloidal drying in the presence of polymers and structure formation in resulting phase-separation fronts. When a drop of colloid polymer mixture is exposed to an environment in which the solvent in which these particles are suspended evaporates an accumulation of non-volotile material at the rim of the drop is observed (coffee ring effect). When the solvent concentration is reduced beyond a certain threshold, the colloid polymer mixture undergoes phase separation. The structures formed by this phase-separation is

observed to depend on the processing conditions. In this presentation we will briefly present the experimental observations and our numerical approach to address the observed phenomena.

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Chandan Dasgupta, *Indian Institute of Science*
Complex Rheology of Nematogenic Fluids: Connection to Elastic Turbulence
Co-Authors: Rituparno Mandal; Buddhapriya Chakrabarti; Debarshini Chakraborti

The rheological behavior of complex fluids under shear exhibits many interesting features arising from the strong coupling between mesoscopic structure and flow. Complex temporal response indicating the occurrence of deterministic chaos has been observed in experiments on sheared wormlike micelles [1]. The chaotic behavior in this system, known as "rheochaos", occurs at very small values of the Reynolds number and arises from nonlinearities in the rheological constitutive equations. Similarly, sheared polymeric liquids show irregular flow behavior with fluid motion excited over a large range of spatial and temporal scales [2]. This behavior, akin to turbulent phenomena in Newtonian fluids, is termed "elastic turbulence". Both these phenomena show very similar statistical properties, e.g. power law decay in the power spectral density of fluctuating quantities such as shear rate/shear stress, depending on the controlling protocol.

To develop a theoretical understanding of these phenomena,we have studied numerically the full non-linear hydrodynamic equations [3,4] of a sheared nematic fluid (coupled nonlinear partial differential equations for the hydrodynamic velocity and order parameter fields) under shear-stress and strain-rate controlled situations, incorporating spatial heterogeneity in the velocity gradient direction. In a suitable parameter range, we find [5] irregular, dynamic shear-banding and establish by decisive numerical tests that the chaos we observe in the model is spatiotemporal in nature. In the chaotic regime, the power spectra of the order parameter stress and the total injected power show power-law behavior and the total injected power shows a non-gaussian, skewed probability distribution, which bear striking resemblance to elastic turbulence phenomena observed in polymer solutions, suggesting an intriguing connection between our model system and systems which are studied in experiments on elastic turbulence. The scaling behavior is found to be independent of the choice of strain-rate or shear-stress control method.

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Lampros Mountrakis, *University of Amsterdam (Netherlands)*
Looking into the transport of blood cells in flows without walls
Co-Authors: Eric Lorenz; Orestis Malaspinas; Bastien Chopard; Alfons G. Hoekstra

Blood is a dense suspension of deformable red blood cells (RBCs), which give rise to its complex behaviour in terms of both rheology and cell transport. In the context of thrombus formation in intracranial aneurysms [1], we are interested in the transport of platelets, a process dominated by the motion of RBCs. To inherently capture important phenomena, blood is modelled through its main constituents, plasma, RBCs and platelets with a validated two-dimensional model [2,3]. Results from this microscopical approach aid in the development of a validated coarse grained macroscopic model, governed by non-Newtonian Navier-Stokes and advection-diffusion equations depending on shear-rate and haematocrit.

To understand the impact of shear-rate and hematocrit gradients on transport, we employ and compare two virtual rheometers: the Lees-Edwards boundary conditions system (LEbc) [4] and the reverse-Poiseuille flow (RPF) [5], which are unbounded versions of Couette and channel flow respectively. These systems have the significant advantage of excluding wall effects difficult to quantify in dense suspensions, such as the wall-induced hydrodynamic lift [6] and, in channel-flows, the segregation of RBCs and platelets due to the formation of a red blood cell-free layer (CFL).

Our results show that RPF lacks a CFL, and despite that, the shear-induced migration of RBCs towards lower-shear rate regions is still present. Platelets exhibit an increased concentration in lower haematocrit areas, yet it is considerably less compared to pure channel flow. These basic mechanisms of transport appear to be independent of walls, still the presence of a wall seems critical for their amplification. Preliminary results for RPF suggest a diffusivity scaling with haematocrit and shear rate, similar to what is found for LEbc, but a lower bound on the system diffusivity is observed. This effect can be associated with the non-negligible size of RBCs compared to local gradients of haemoatocrit and shear rate.

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Fluid Dynamics 1

Monika Nitsche, *University of New Mexico (USA)*
Vortex Shedding and Low Order Models
Co-Author: Ling Xu

Vortex shedding is of fundamental interest in fluid dynamics, with many applications in physics, engineering, and biology, with relevance for example in biolocomotion. Numerical studies of separated flows using the full governing equations are numerically expensive, and in practice, low order approximations such as point vortex or vortex sheet models are often used instead. These models are based on simple algorithms used to satisfy the Kutta condition at sharp edges. The goal of the work I will present is to use highly resolved direct numerical simulations of flow normal to a finite flat plate to better understand detailed aspects of the flow and to obtain benchmark results to evaluate lower order models. Some of the details of the flow evolution revealed by the simulations include the presence and duration of an initial Rayleigh stage. This stage is characterized by a boundary layer of vorticity of almost constant thickness that surrounds the tip of the plate. After this initial period, vorticity concentrates near the tip forming a starting vortex that grows and eventually separates from the boundary vorticity. Using the simulations, we obtain values for the shed circulation, vortex trajectory and vortex sizes as a function of time and Reynolds number. We then compare the viscous results for accelerated flow past a flat plate with results obtained using the vortex sheet model, and determine the extent to which the model reproduces the flow.

George Karniadakis, *Brown University (USA)*
Microscopic theory of Brownian motion: Effects of memory and confinement
Co-Author: Changho Kim

We consider Brownian motion in the near-Brownian- limit. We adopt the generalized Langevin equation approach and investigate the memory function of the Brownian particle. As the mass ¡em¿M¡/em¿ of the Brownian particle increase, the memory function converges to the limit mem- ory function, the time integral of which gives the friction coefficient. The limit memory function can be obtained from the following two types of infinite-mass dynamics. From the frozen dynamics, where the Brownian particle is held fixed, the plateau problem is investigated, whereas the constant-velocity dynamics, where the Brownian particle moves at an infinitesimal velocity, the macroscopic definition of the friction coefficient is investigated. For finite but sufficiently large M, we analyze asymptotic behaviors of the memory function and obtain the asymptotic expansions of the velocity/force autocorrelation functions with respect to M. Using these results, we analyze numerical methods which evaluate the friction coefficient from the long-time behaviors of the time correlation functions.

In order to demonstrate our results, we apply them to the Rayleigh gas model, where a Brownian particle is suspended in an ideal gas. A systematic MD simulation study is performed with well-controlled statistical errors. MD simulation results are compared with analytic expressions for the limit

memory function, which we obtain from the two types of the infinite-mass dynamics. All theoretical predictions are confirmed and the finite-volume and finite-mass effects are separately investigated.

In addition, we demonstrate that our generalized Langevin equation approach can be applied to confined Brownian motion. A Rayleigh gas confined by two walls is investigated and a power-law decaying tail occurring in the memory function is analyzed. The effects of confinement and coupling with stochastic thermal character of the walls are discussed.

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Alex Hansen, *Norwegian University of Science and Technology*
A Monte Carlo Algorithm for Immiscible Two-Phase Flow in Porous Media
Co-Authors: Morten Vassvik; Isha Savani; Santanu Sinha

For more than three decades, the instabilities caused by one fluid invading the pore space of another in a porous medium have been studied resulting in a rich phase diagram depending on the wetting properties of the fluids with respect to the pore walls, their viscosities and the speed at which the invasion happens. The situation when two immiscible fluids flow simultaneously in the porous medium has been much less studied. At very slow flow rates, typically one of the fluids will be held in place by capillary forces whereas the other one percolates and is then free to flow. At higher flow rates, both fluids will flow and the interfaces between them change continuously. This simultaneous flow will reach a steady state where the macroscopic quantities characterizing the flow will have well-defined average values that remain unchanged or change slowly compared to the time scale associated with the flow at the pore level.

In Hansen and Ramstad (2009), it was proposed that a statistical mechanics describing steady-state flow of immiscible fluids in porous media could be built based on knowledge of the congurational probability, where configurations are defined by the distribution of interfaces between the two fluids in the porous medium. It was speculated that a Monte Carlo algorithm based on the configurational probability could be constructed which would be much more efficient numerically than time integration of the position of the interfaces. Based on Sinha et al. (2013), we derive the configurational probability for two-phase flow in porous media. We find that it is inversely proportional to the inverse total flow rate in the porous medium. We construct a Monte Carlo algorithm based on this probability and compare it to time integration of the same system. We find the Monte Carlo method to be significantly more efficient than time integration.

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Junxue Ren, *Wright State University (USA)*
PIC Algorithm with Multiple Poisson Equation Solves during One time Step
Co-Authors: Trenton Godar; Junxue Ren; James Menart

Reducing computational time with a PIC (particle-in-cell) algorithm is important because there are many physical situations that need to be modeled at the particle level that require large computational times. The goal of this work is to investigate the effect of using multiple Poisson equation solves within one time step of a PIC simulation. The hope of this investigation was the overall computational time for a given simulation would be reduced because larger time steps could be utilized.

In this work, a three-dimensional PIC code that tracks electrons and ions throughout a Cartesian computational domain is used. Full coupling between the particle positions and the electric field calculation is maintained. The difference in this PIC algorithm compared to other PIC algorithms is that Poisson's equation may be solved multiple times during one time step. It can be solved multiple times during the electron push only, multiple times during the ion push only, or multiple times during both the electron and ion push. The number of times Poisson's equation is solved during a time step is controlled by the user.

In this work results of the effects of altering the number of times Poisson's equation is solved during one time step are presented. These results are presented for a very simple plasma in a box situation. The effects of solving during just the electron push, just during the ion push, or during both pushes are presented; the results of altering the number of times Poisson's equation is solved during a single time step are presented; and the results of altering the time step size are presented. Initial results indicate that using multiple Poisson solves during one time step provides some ability to use larger time steps in PIC simulations, but the increase in time step size are not significant. It is felt that further investigation may be able to make this time step enhancement larger.

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Nils Moschuering, *LMU Munich (Germany)*
Adaptive-Particle-Refinement for PIC Simulations
Co-Author: Hartmut Ruhl

Particle-in-cell (PIC) codes commonly employ a finite-element method in order to solve Vlasov's equation and a finite-difference-time-domain method to solve Maxwell's equations. The number of quasi-elements used in the finite element solver is significant for the reliability of the obtained results and a defining property when evaluating the computational demands of a given simulation. Thus its dynamic adaption is regarded to be very useful. Important principles to consider during adaption are mainly given by: mass/charge conservation, momentum conservation, energy conservation, conservation of grid moments and conservation of the distribution function in momentum and configuration space.

Two main techniques have been developed ([1], [3] and with a different approach [2], [4]) which can be applied to a variety of numerical methods. Continuing from these results we present a new, fully relativistic, fully three-dimensional Adaptive-Particle-Refinement (APR) algorithm specialized for Cloud-in-Cell(CIC)-PIC which conserves the total momentum, total energy and total charge. No unphysical divergence in the electromagnetic fields is introduced and the momentum distribution is preserved up to a very fine degree (by choosing previous momenta). Our quasi-particle merging and splitting process incorporates extra measures to ensure a minimum number of different weight species in the simulation. Possible applications include:
1. Controlling the signal-to-noise ratio for various derived quantities.
2. Growing charge densities (e.g. in discharges or pair-production) can lead to a steep increase in quasi-particles and thus computational demand. Quasi-particle merging can counteract this.
3. For Monte-Carlo-Collisional (MCC) simulations it is imperative to have quasi-particles with comparable or equal weight in order to achieve statistical significance.
4. It represents an important step in order to implement Adaptive-Mesh-Refinement-PIC (AMR-PIC).

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Quantum Many-Body Physics 1

Ribhu Kaul, *University of Kentucky (USA)*
Deconfined quantum criticality in SU(N) magnets

Close to the absolute zero of temperature, when pushed to the edge between two phases of matter, simple lattice Hamiltonians of spins can display the incredibly rich phenomena of "quantum criticality". Quantum critical ground states are described by the most complex wavefunctions known to physicists, yet they can be categorized by "universality classes" that are independent of the details of the Hamiltonians that realize them. In this seminar I will show how such quantum critical spin systems can arise in real-world materials, and explain our successes in developing quantum many-body simulations of a new universality class of deconfined quantum critical points.

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Boris Svistunov, *University of Massachusetts, Amherst (USA)*
Diagrammatic Monte Carlo for Fermionic and Fermionized Systems

Under certain (controlled) conditions, Feynman diagrammatic series for fermionic systems features the phenomenon of sign blessing: The series converges despite factorial growth of the number of diagrams with diagram order. Diagrammatic Monte Carlo technique allows us to sample millions of Feynman diagrams. With the universal fermionization trick, we can fermionize essentially any (bosonic, spin, mixed, etc.) lattice system. The combination of fermionization and diagrammatic Monte Carlo yields a universal first-principle approach to strongly correlated lattice systems, provided the sign blessing is a generic fermionic phenomenon. We will present results for resonant fermions, fermionized spins-1/2 on triangular lattice, and repulsive Hubbard model.

George Batrouni, *Institut Non-Linéaire de Nice, University of Nice (France)*
Competition between the Haldane insulator, superfluid and supersolid phases in the one-dimensional Bosonic Hubbard Model
Co-Authors: Valery Rousseau; Benoît Gremaud; Richard Scalettar

The Haldane Insulator (HI) is a gapped phase characterized by an exotic non-local string order parameter. The parameter regimes at which it might exist, and how it competes with alternate types of order, such as supersolid (SS) order, are still incompletely understood. Using the Stochastic Green Function quantum Monte Carlo and the Density Matrix Renormalization Group, we study for a wide range of parameters the ground state phase diagram of the one-dimensional bosonic Hubbard model with contact and near neighbor repulsive interactions. Our main conclusions for this system are that the HI exists only at unit filling while the SS, the superfluid and charge density wave phases, exist for a very wide range of parameters (including commensurate fillings). The one body Green function displays

power law decay in the SS and SF phases. In addition, we show that at fixed integer density, the system exhibits phase separation.

Karine Piacentini Coelho da Costa, *University of Massachusetts, Amherst (USA)*
University of Sao Paulo (Brazil), Critical Exponents of the Superfluid-Bose-Glass Transition in Three Dimensions
Co-Authors: Nikolay Prokofev; Mikhail Kiselev; Zhiyuan Yao

The superfluid-insulator quantum phase transition that takes place in disordered bosonic system instigate many discussions and controversies since its first studies more than 20 years ago [1]. The understanding of this transition is relevant to various systems, to cite a few, 4He in porous media, thin superconducting films and cold atoms in disordered optical lattice [2,3]. Though many progress towards its thorough understanding were made, basics characterization of critical proprieties are still under debate. Specifically, recent experimental and numerical studies [3,4] of the critical-temperature exponent &phi in three-dimensional systems report strong violations of the key quantum critical relation, &phi=&nu z, where z and &nu are the dynamic and correlation length exponents, respectively, and question the conventional scaling laws for this quantum critical point.

We addressed this controversy numerically using the worm algorithm [5], a high performance Monte Carlo algorithm, both in its quantum and classical scheme. Our results demonstrate that previous work on the superfluid-to-normal fluid transition-temperature dependence on chemical potential (or magnetic field, in spin systems), Tc &prop (&mu-&muc)&phi, was misinterpreting transient behavior on approach to the fluctuation region with the genuine critical law. When the model parameters are modified to have a broad quantum critical region, simulations of both quantum and classical models reveal that the &phi=&nu z law [with &phi=2.7(2), z=3, and &nu = 0.88(5)] holds true, resolving the &phi-exponent "crisis".

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Yu-cheng Lin, *National Chengchi University (Taiwan)*
Neel to valence-bond-solid phase transitions in correlated valence-bond states

We study generalizations of the singlet-sector amplitude-product states in the valence-bond basis of S = 1/2 quantum spin systems. In the standard amplitude-product states, the weight of a tiling of the system into valence bonds (singlets of two spins) is a product of amplitudes depending on the length of

the bonds. While the standard amplitude-product states can describe a phase transition between an antiferromagnetic (Neel) state and a valence-bond solid (VBS) in one dimension, in two dimensions it cannot describe VBS order. We here introduce generalized amplitude-product states on the square lattice which include correlated weights for short-range bonds. With these correlated amplitude-product (CAP) wave functions, Neel state to columnar/plaquette VBS transitions are realized as a function of some parameter describing the bond correlations. We study such phase transitions of CAP wave functions on the square lattice. We find examples of direct first-order Neel-VBS transitions, as well as cases where there is an extended U(1) spin liquid phase intervening between the Neel and VBS states. In the latter case the transitions are continuous and we extract critical exponents and address the issue of a possible emergent U(1) symmetry in the near-critical VBS.

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Monday, Parallel Sessions 2, 15:45-17:30

Soft Matter and Biological Physics 2

Ivet Bahar, *University of Pittsburgh (USA),*
Structure-Encoded Dynamics of Proteins: Learning from Network Models and Experiments

Comparison of computational and experimental data in recent years highlights the significance of the intrinsic dynamics of proteins in facilitating, or enabling, biological functions. Intrinsic dynamics refer to the collective motions encoded in the native structure, predominantly defined by the network of inter residue interactions. Elastic network models (ENMs) coupled with normal mode analyses have proven in recent years to serve as useful computational tools for elucidating such structure-encoded propensities. In particular, the soft modes predicted by ENMs disclose cooperative mechanisms of reconfiguration, which relate to structural changes undergone during allosteric responses or molecular machinery. We present here in silico approaches based on ENMs of various levels of granularity, along with several examples of their use in unraveling biomolecular mechanisms of function, including their application to supramolecular systems dynamics. We also highlight the significance of complementing ENM-based studies by sequence-based correlation analyses and structure-based hybrid methods that bridge between atomic and coarse-grained scales.

Normand Mousseau, *Université de Montréal (Canada)*
Computational challenges for the study of amyloid processes

The dominant hypothesis in amyloid diseases considers small amyloid aggregates as one of most important toxic species. Because these structures are out-of-equilibrium, there atomistic properties are difficult to access experimentally. Computer simulations have therefore played an important role for their characterization over the last decade. Yet, full size amyloid aggregates are at the extreme limit of

what is accessible by computer today, forcing the use of a wide range of methods to accelerate sampling and simplify their description. In this talk, I will present some of the work we have done on amyloids, using simplified force fields such as the OPEP forcefield and simulations methods ranging from pure MD to the Activation-Relaxation Technique, including systems such as polyglutamine, α-synuclein, IAPP and various fragments of the A&beta protein. I will also discuss ongoing efforts for developing a new coarse-grained forcefield for amyloids. This work was done in collaboration with V. Binette, S. Côté, C. Eugène, R. Laghaei, and J. Nasica-Labouze as well as P. Derreumaux and P. Tuffery.

Ming-chya Wu, *National Central University (Taiwan)*
Correlated vibrations in ion-pair dynamics in mechanoactivation identifies functional domains of force-dependent titin kinase
Co-Authors: Kuan Wang; Jeffrey G. Forbes

Titin kinase is a mechanoenzyme, whose activity is activated by mechanical stretching and binding of calcium sensors. Stretching causes local and global conformational changes of secondary structures and complex movements of ion pairs and transient formations of salt bridges. This paper applies the adaptive time series analysis approach to study the mechanical responses of ion-pair movements to stretch unfolding through steered molecular dynamics (SMD) simulations, focusing on the ion-pair dynamics of mechanoactivation obtained from the SMD trajectories. Temporal correlation analysis of the ion-pair time series shows that the activation process involves changes of secondary structure. Spectral analysis defined several groups and subgroups of the ion pairs with vibrational damping/resonance in the scale of ~0.5Å, corresponding to vibrational modes of chemical bonds. Examination of these groups revealed the locations or neighboring structures of the autoinhibitory loop, ATP binding cleft, catalytic loop, and P+1 loop, all key functional domains of this kinase. We propose that the correlated vibrations of subgroups of ion pairs have significant correlations with functional domains, which can be used to identify, a priori, special functional and structural features of folded proteins.

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Wu M.-C., Forbes J. G. and Wang K., “Correlated vibrations in ion-pair dynamics in mechanoactivation identifies functional domains of force-dependent titin kinase”, Soft Matter Vol. 9, (2013), pp 9897-9906.

Christopher Roland, *North Carolina State University (USA)*
Investigating rare events with nonequilibrium work measurements: transition and reaction rates
Co-Authors: Celeste Sagui; Mahmoud Moradi

We present a formalism [1-2] for investigating transition pathways and transition probabilities for rare events in biomolecular systems. The formalism is based on combining Transition Path Theory (TPT) with the results of the nonequilibrium work relations, and shows that the equilibrium and nonequilibrium transition rates are in fact related. Aside from its fundamental importance, this allows for the calculation of relative equilibrium reaction rates with driven nonequilibrium simulations such as Steered Molecular Dynamics (SMD). The workings of the formalism are illustrated with a few examples including that of a circular random walk, a proline dimer, a proline trimer, and the alanine dipeptide.

References
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Statistical Physics 1: Networks

Mark Newman, *University of Michigan (USA)*
Large-scale structure in networks

Networks are of broad interest in physics, biology, engineering, and many other areas for the light they shed on the shape and function of complex systems. This talk will focus on the large-scale structure of networked systems -- what do they look like when you stand back and take in the whole network? This is a difficult question to answer because in most cases the networks we study are too large and complicated to allow us to actually make a picture of them. Two promising classes of methods for understanding structure are spectral methods and inference methods. This talk will demonstrate some applications of both and discuss some beautiful recent results that link the two together and reveal deep and unexpected truths about large-scale structure in networks.

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Hierarchical structure and the prediction of missing links in networks, Aaron Clauset, Cristopher Moore, and M. E. J. Newman, Nature 453, 98–101 (2008)
Mixture models and exploratory analysis in networks, M. E. J. Newman and E. A. Leicht, Proc. Natl. Acad. Sci. USA 104, 9564–9569 (2007)
Graph spectra and the detectability of community structure in networks, Raj Rao Nadakuditi and M. E. J. Newman, Phys. Rev. Lett. 108, 188701 (2012)

Lenka Zdeborova, *CEA Saclay and CNRS (France)*
Module detection in networks: phase transitions and optimal algorithms

A central problem in analyzing networks is partitioning them into modules or communities, clusters with a statistically homogeneous pattern of links to each other or to the rest of the network. A principled approach to address this problem is to fit the network on a stochastic block model, this task is, however, intractable exactly. In this talk we discuss application of belief propagation algorithm to module detection. In the first part we present an asymptotically exact analysis of the stochastic block model. We quantify properties of the detectability/undetectability phase transition and the easy/hard phase transition for the module detection problem. In the second part we introduce a new class of spectral algorithms based on a non-backtracking walk on the directed edges of the graph. We show that our

algorithm is optimal for graphs generated by the stochastic block model, detecting communities all the way down to the theoretical limit. We also show the spectrum of the non-backtracking operator for some real-world networks, illustrating its advantages over traditional spectral clustering.

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Aurelien Decelle, Florent Krzakala, Cristopher Moore, Lenka Zdeborová; Phys. Rev. Lett. 107, 065701 (2011).
Spectral redemption: clustering sparse networks;
Florent Krzakala, Cristopher Moore, Elchanan Mossel, Joe Neeman, Allan Sly, Lenka Zdeborová, Pan Zhang; Proceedings of the National Academy of Sciences 110, no. 52 (2013): 20935-20940

Florent Krzakala, *Ecole Normale Superieure (France)*
Belief-Propagation Guided Monte-Carlo Sampling

A Monte-Carlo algorithm for discrete statistical models that combines the full power of the Belief Propagation algorithm with the advantages of a detailed-balanced heat bath approach is presented. A sub-tree inside the factor graph is first extracted randomly; Belief Propagation is then used as a perfect sampler to generate a configuration on the tree given the boundary conditions and the procedure is iterated. This approach is best adapted for locally tree like graphs, it is therefore tested on the hard cases of spin-glass models for random graphs demonstrating its state-of-the art status in those cases. We will also shows how an approximate (yet very accurate) values of the free energy can be computed almost at no cost in many models using this approach.

References

http://arxiv.org/abs/1307.7846

Lev Shchur, *Landau Institute for Theoretical Physics (Russia)*
Relation of Parallel Discrete Event Simulations algorithms with the physical models

Parallel simulations are widely used nowadays, both in science and industry. It is clear that realistic models of scalable hardware and software should be dynamic, asynchronous, and quite inhomogeneous in time, and should use new methods of synchronization. One of the approaches based on the decomposing of simulation onto logical processes which synchronization can be performed using optimistic or conservative algorithm [1], or its combination in the manner it is realized in Parallel Discrete Event Simulations (PDES). There indications that ideas of PDES can be used in exaflops computer architecture.

In our presentation we demonstrate there some analogy of evolution of time horizon in PDES with some physical processes, f.e. with surface growth under molecular beam epitaxy [2,3], with directed percolation [4], etc. We review results in that area and present preliminary results on the PDES models on a number of networks, including small-world network.

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Bruce Boghosian, *Tufts University (USA)*
Asset exchange and the origin of Pareto's Law of wealth distribution

The so-called "Yard-Sale Model" of wealth distribution posits that wealth is transferred between economic agents as a result of transactions whose size is proportional to the wealth of the less wealthy agent. In recent work [1,2], we have shown that this model results in a Fokker-Planck equation governing the wealth distribution of the population. In the absence of any mechanism for wealth redistribution, solutions to this equation describe unbounded concentration of wealth. Using a mixture of analytical and numerical methods, we show that in the presence of a wealth redistribution mechanism, the steady-state solutions of this Fokker-Planck equation are very similar in form to Pareto's famous wealth distribution, including the cutoff at very low values of wealth, and the power law at very high values. Indeed, this appears to be the first microeconomic explanation of Pareto's century-old law of wealth distribution, a key observation of macroeconomics.

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Fluid Dynamics 2

Marc Gerritsma, *TU Delft (Netherlands)*
Structure preserving discretizations for computational physics

A physical model consists of conservation laws, equilibrium conditions, definitions and constitutive relations, [1]. The conservation laws, equilibrium conditions and definitions are so-called topological relations. More specifically, these topological relations are independent of metric. The topological relations are divided into two disjoint classes which we refer to as outer-oriented relations and inner-oriented relations. Physically the model is closed by adding the material dependent constitutive relations. Mathematically, the model is closed by adding the metric-dependent constitutive relations which connect the inner-oriented topological relations to the outer-oriented topological relations.

The accuracy of the physical model is determined by the accuracy of the constitutive relations.

Since the topological relations in a physical model are metric-free, we can represent them in a discrete setting without reference to mesh-dependent parameters. So these discrete topological relations hold on very coarse grids, but also on very fine grids in the limit when the mesh size goes to zero. Since these discrete relations hold universally they are called exact, [2]. The inner-oriented relations are represented on one mesh and the outer-oriented relations are represented on a dual mesh, [3]. The metric-dependent constitutive relations do depend on both meshes and their mesh parameters. It is in these metric-dependent relations where the numerical error resides. The more accurately we can represent the constitutive relations, the more accurate our numerical scheme will be.

So the constitutive relations play a special role in both physical and numerical modeling.

These ideas will illustrated through a reaction-diffusion model for a fully conservative least-squares formulation, see [4]. In this case the two constitutive relations are simple algebraic relations.

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Chun Liu, *Penn State University (USA)*
Energetic Variational Approaches in Complex Fluids

Complex fluids is ubiquitous in our daily life, from the food we eat, the things we use to the exact materials we are made of. It is also important in many industrial, physical and biological applications. Studying these materials requires a wide range of tools and techniques for different disciplinary, even within mathematics.

It is the competitions and couplings of different physics from multiple scales that give the complex fluids many interesting properties and applications. In this talk, I will demonstrate how to establish these coupling systems using energetic variational approaches.

These approaches are motivated by well-established works of Rayleigh, Landau and most of all, Onsager. In particular, we will emphasize the relations between those of kinematics and energetics. Such a framework not only are useful in the modeling, but also play important role in analysis as well as designing corresponding numerical algorithms.

Christopher Amey, *University of Massachusetts, Amherst (USA)*
Persistent Patterns and Mixed Phase Space Dynamics
Co-Authors: Andrew Poje; Bala Sundaram

Persistent patterns in periodically driven dynamics have been reported in a wide variety of contexts ranging from table-top and ocean-scale fluid mixing systems. We first illustrate a common framework for the emergence of these patterns by considering a simple measure of structure maintenance provided by the average radius of the scalar distribution in transform space. We then consider the important limit of small diffusion D by directly relating the spectral properties of the one period advection-diffusion operator to the phase-space geometry of the Lagrangian advecting field. We consider the Chirikov's standard map as variation of the map parameter allows for the creation of multi-scale mixed phase space structures where elliptic islands of various sizes and periodicities co-exist with extended regions of non-uniformly hyperbolic chaos. The relative algebraic simplicity of the map and the implementation of an efficient numerical scheme enables direct computation of a number of the most stable spectral modes of the advection-diffusion operator for D of O(10-9). Once the diffusive length scale falls below the size of any stable island structure, the spectral branch containing the dominant eigenmode behaves diffusively – i.e. the decay rate of the modes and the spectral gap between such modes scales with diffusion. Interspersed with modes localized on the full extent of the elliptical islands are other families of modes governed by local minima of the potential. In contrast to the diffusive, square-well modes, the decay rates of the super-localized, harmonic oscillator modes scale as D-1/2. Simple counting arguments, based on these known scaling relations and the purely Lagrangian geometry of the map, allow accurate prediction of the relative importance of the different spectral contributions for any finite value of D.

Blair Perot, *University of Massachusetts, Amherst (USA)*
Numerical Investigation of the Decay Rate of Isotropic Turbulence

All theories concerning the decay of isotropic turbulence agree that the turbulent kinetic energy has a power law dependence on time. However, there is still significant disagreement about what the value of the decay exponent should be. The primary theories, proposed by researchers such as von Karman, Saffman, Kolmogorov, and Batchelor, have the decay exponent at values of 1, 6/5, 10/7, 3/2, and 5/2. The debate over the decay exponent has remained unresolved for many decades because the decay exponent is an extremely sensitive quantity. Experiments have decay times which are too short to be able to accurately differentiate between the various theoretical possibilities, and all prior numerical simulations of decaying turbulence impose the decay rate a priori via the choice of initial conditions or initial turbulence forcing.

In this work, direct numerical simulation is used to achieve very long decay times, and the initial turbulence is generated by the Navier-Stokes equations themselves using the stirring action of the flow past 768 small randomly placed cubes. This is similar to the turbulence generation mechanism via wakes that is used in most wind tunnel experiments. Results over a range of turbulent Reynolds numbers (25 to 450) show agreement with the theoretical predictions of Saffman at both low and higher

Reynolds numbers. The transition from the Saffman high Re decay rate exponent (6/5) to the low Re decay exponent (3/2) is found to be abrupt. We hypothesize that most wall generated turbulence is likely to follow the Saffman decay theory.

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Duncan McGregor, *Oregon State University (USA)*
Modelling Arcs in Magnetohydrodynamic Generator Channels

Direct power extraction via magnetohydrodynamic (MHD) principles offers a potential step improvement in thermal efficiencies over energy systems utilizing traditional turbomachinery. This is principally due to the lack of moving parts in a MHD generator, as the temperature limits of the moving parts tend to limit cycle temperatures in traditional combustion driven systems.

It was established that a major weakness toward commercialization of MHD power generation was the durability of the current collectors on the walls of the generator (electrodes). The electrodes must withstand harsh conditions, and the most damaging and perhaps most difficult to predict phenomenon experienced in the generator was arcing. For the expected temperature range of these generators, the current passing through ceramic electrodes can be expected to transition from a diffuse state to a highly dense arc. From a design perspective, there is a desire to be able to measure and then prevent these damaging arcs.

In the arc state we expect the current densities in the channel to be many orders of magnitude larger than in the diffuse state. Given these large differences in current density, the induced magnetic fields are measurably different close to the arc. The idea of reconstructing current densities from external magnetic flux density measurements has been successfully applied to fuel cells and vacuum arc remelters.

We model the induced fields in an MHD generator channel, terms usually neglected in low magnetic magnetic Reynold's number flows, using a natural fixed point iteration. Further we present a sensitivity analysis of induced fields to current density profiles in a 3D, simplified model.

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Novel Computing Paradigms 1

Thomas Cheatham, *University of Utah (USA)*
Molecular dynamics simulation of nucleic acids: Convergence, reproducibility, assessment/validation, and data dissemination enabled by GPUs on XSEDE and Blue Waters

Advances in simulation methods, continued optimizations of atomistic force fields, and increases in available computational power have coupled together over the past few decades to transform our understanding of biomolecular structure, dynamics, interactions and function. Such methods can aid in the design of new drugs, monitor how RNA and protein molecules fold, and aid in the interpretation of experimental data. Development of advanced “ensemble-based” sampling methodologies in the AMBER suite of programs, such as multidimensional replica-exchange molecular dynamics methods, running on large CPU and GPU resources has pushed the capabilities further. We are now able to reproducibly converge (in independent runs) the conformational ensembles of RNA tetranucleotides [1-2] and even RNA tetraloops. This provides a means to assess and validate the force fields and to test improvements or alterations to the force fields in a systematic manner. Using large ensembles of independent simulations poses significant data management and analysis issues which we continue address with further developments in the CPPTRAJ program optimization and parallelization [3]. To make better use of the data we are also exploring means to automatically mine and display the data, and also better means to search and disseminate the data (iBIOMES) [4]. All of these issues, developments and current barriers will be discussed in the context of large-scale use of XSEDE and Blue Waters computational resources.

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Ying-jer Kao, *National Taiwan University*
Uni10: the Universal Tensor Network Library

Tensors provide a natural and compact representation for multidimensional data, and algorithms based on tensor networks have recently found their applications in quantum physics, quantum information science, quantum chemistry, image/pattern recognition and data science. However, programming tensor network algorithms is tedious and error prone due to the complexity in keeping track of multiple tensor indices. There are also further complications in bookkeeping the indices as many scientific applications require these tensors to obey certain symmetries. For a given tensor network, storing the connectivity of the network and detemining the optimal contraction sequence are also crucial for further analysis.

To address these issues, we develop a C++ framework geared toward the application in tensor network algorithms called Uni10, the Universal Tensor Network Library[1]. It provides basic symmetric tensor storage and operations with features such as Einstein summation convention and easy-to-use interface, storage for graphical representations of networks, and an engine to construct and analyze the contraction tree for a given network. A heuristic algorithm is implemented to search for an optimal binary contraction order based on the computational and memory constraints. I will also discuss our implementation of Uni10 on GPU.

References
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Joshua Anderson, *University of Michigan (USA)*
Monte Carlo and Molecular Dynamics simulations of soft matter in the GPU era
Co-Authors: M. Eric Irrgang; Jens Glaser; Sharon Glotzer

Monte Carlo and Molecular Dynamics simulations are powerful tools to study soft matter systems. GPUs are massively parallel compute processors that deliver an order of magnitude faster performance than a multi-core CPU and enable researchers to run larger or longer simulations than previously possible. We present an overview on HOOMD-blue, our open-source GPU accelerated particle simulation toolkit, and several examples of its use in soft matter research. HOOMD-blue v1.0 supports MD using a variety of potentials, standard integration routines, strong scaling to thousands of GPUs, and a scriptable python-driven interface. We have also developed parallel algorithms for hard particle Monte Carlo simulations, which we are currently working on adding to HOOMD-blue.

Jens Glaser, *University of Michigan (USA)*
Strong Scaling of a Molecular Dynamics code on 1000's of GPUs

We discuss the challenge and bottlenecks in scaling a GPU molecular dynamics code, HOOMD-blue 1.0, up to 1000's of GPUs. We show performance data on the Titan supercomputer, and compare to the

LAMMPS molecular dynamics software. HOOMD-blue's scaling capabilities are particularly well suited for large-scale simulation of polymer systems or particle fluids. We demonstrate how the recently developed GPUDirect RDMA protocol can be used to enhance the scaling of HOOMD-blue on GPU-aware MPI implementations, and show benchmarks on the second-ranked Green500 system.

References
http://codeblue.umich.edu/hoomd-blue

Hyun Lim, *South Dakota State University (USA)*
A Parallel Implementation of the Time-Decomposition Approach for the time-dependent Dirac Equation
Co-Authors: Arthur Kurlej; Robert Vaselaar; Jung-Han Kimn; Isaac Lyngass

In this talk, we present parallel implementation of the Dirac equation in 1(space)+1(time) dimension using space-time finite element discretization. We show that the space-time finite element method for the time-based Dirac equation converges to analytic solutions without artificial stabilization or after-simulation tuning even in the low-mass regime. Due to the large size of the problem, using a parallelizable preconditioner is vital for successful numerical simulation. Therefore we also present an additive Schwarz preconditioner based on a time decomposition method and KSP (Krylov Subspace) solver previously proposed for the wave equation. We expect that this result will be useful in calculating the behavior of high energy fermions, even at very low masses, such as neutrinos.

Tuesday, Parallel Sessions 1, 13:30-15:15

Soft Matter and Biological Physics 3

Marina Guenza, *University of Oregon (USA)*
A coarse-graining method that preserves the free energy, structural correlations, and thermodynamic state of polymer melts from the atomistic to the mesoscale

Based on the solution of the Ornstein-Zernike Equation, we present our analytical coarse-grained model that is structural and thermodynamic consistent across multiple length scales.[1] The model in this way is fully predictive, when the potential is used as an input in mesoscale molecular dynamic simulations of polymer melts.

The model is analytical and depends on molecular and thermodynamic parameters of the system under study, as well as on the direct correlation function in the k -->0 limit, c0.[2] This single non-trivial quantity parameterizes the coarse-grained potential. The value of c0 can be obtained numerically from the PRISM integral equation, or directly from the experimental compressibility of the system.
DIrect comparison with united atom simulations of both the analytical equations and mesoscale simulations shows quantitative consistency of structural and thermodynamic properties independent of the chosen level of representation.[3]

In the mesoscale description, the potential energy of the soft-particle interaction becomes a free energy in the coarse-grained coordinates which preserves the excess free energy from an ideal gas across all levels of description. The total free energy of the coarse-grained system is reduced by only the configurational entropy associated with the removal of degrees of freedom from an ideal chain. The structural consistency between the united-atom and mesoscale descriptions means the relative entropy between descriptions has been minimized without any variational optimization parameters. The approach is general and applicable to any polymeric system in different thermodynamic conditions.

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Celeste Sagui, *North Carolina State University (USA)*
Free energy methods for biomolecular simulations
Co-Authors: Mahmoud Moradi; Volodymyr Babin; Christopher Roland

In the past few years, several methods targeting the computation of the Landau free energy using non-equilibrium dynamics have become popular. These methods introduce a time-dependent potential to bias the original potential energy. In the long time limit, the biasing force is expected to compensate for the free energy gradient, so that the biasing potential eventually reproduces the free energy surface. In this talk we review these methods as well as extensions that enhance sampling of phase space (such as multiple walkers and replica exchange). In particular, we discuss the Adaptively Biased Molecular Dynamics (ABMD) method that was developed in our group and implemented in the AMBER 10-14 codes. We illustrate its capabilities by applying it to challenging systems that undergo a transition in handedness: polyproline peptides that include transitions between the PPII and PPI forms, transitions between B-DNA and Z-DNA, polyglutamine-polyproline systems (in the context of polyglutamine diseases).

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Thomas Salez, *(CNRS / ESPCI)*
A direct quantitative measure of surface mobility in a glassy polymer
Co-Authors: Yu Chai; Joshua McGraw; Michael Benzaquen; Kari Dalnoki-Veress; Elie Raphael; James Forrest

The simple geometry of a polymer film on a substrate with a step at the free surface is unfavourable due to the excess interface induced by the step, thus allowing for a new nanoprobe of the melt state rheology. After describing the experimental technique [1], we demonstrate how the theoretical tools [2,3] enable to directly probe the surface evolution of thin polymer films below the glass transition temperature Tg [4]. While above Tg the entire volume between the substrate and the free surface participates to the flow, below Tg only a near surface region responds to the excess interfacial energy. In the latter case, the developed thin film theory for flow limited to the free surface region is in excellent agreement with experimental data. Strikingly, the system transitions from whole film flow to surface localised flow over a narrow temperature region near the bulk glass transition temperature. The measurements and model presented provide a quantitative measure of surface mobility in a sample geometry where the confinement of polymer chains and substrate effects are negligible. Therefore, this study may contribute to solve further the ongoing controversy around glass transition in polymer films.

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Xizhong An, *Northeastern University (China)*
MPFEM modeling and mechanism analysis on the compaction of binary granular system
Co-Authors: Fen Huang; Yuxi Zhang

A multi-particle FEM (MPFEM) which incorporates the characteristics of DEM and traditional FEM, was utilized to study the packing densification behavior of various 2D binary amorphous and crystalline initial structures (generated by DEM modeling) subjected to single action die compaction. The densification dynamics, the macro- and micro-structures of the final compacts for each case were characterized and analyzed. The results show that:(1) At the initial stage of compaction, the equivalent von Mises stress of large and small particles reaches the yield strength at different deformation amount;(2) For ordered initial packings, no obvious sliding and rolling can be observed during compaction. Compared with the compacts formed by the packing of mono-sized particles, the relative densities of compacts formed by binary initial ordered packings were improved greatly, but their increasing speed with the compaction pressure is slow. Different initial ordered packing structures indicate different densification behavior; (3) For amorphous initial packing, with the movement of upper punch, the force chain along the compaction direction appears. And with the further increase of pressure, the particle deformation increases, and the force chain propagates with a higher density and in hierarchy. The accompanying sliding and rolling during early compaction makes the transient evolution of force network in density and transmission directions; (4) The compaction curves for amorphous initial packings are comparable

even the composition of large and small particles in the binary mixtures is different, which implies that the composition does not create significant effects on the compaction process. While different compaction curves and corresponding micro-properties can be identified when the initial packing structure is different, however, nearly fully dense final packings with the same relative densities can be formed under similar compaction pressure.

Guangjie Shi, *University of Georgia (USA)*
Protein Folding of the HOP Model: A Parallel Wang-Landau Study
Co-Authors: Thomas Wust; Ying Wai Li; David P. Landau

The hydrophobic-polar (HP) model [1] has served as a coarse-grained lattice protein folding model ("an Ising model" for protein folding) attracting scientists from various disciplines because of its simplicity yet challenging computational complexity. Wang-Landau sampling [2,3] combined with pull and bond-rebridging moves has shown to provide a powerful computational means to shed new light on many difficult problems based on the HP model, e.g. protein surface adsorption [4] or the effects of sequence mutations [5]. However, simplification into only H and P monomers may yield too large ground state degeneracies which stands in contrast to the generally unique ground states of natural proteins. We propose a simple modification, by introducing a new type of "neutral" monomer, O, i.e. neither hydrophobic nor polar, thus rendering the model more realistic without increasing the difficulties of sampling tremendously. With the newly developed parallel Wang-Landau sampling (replica exchange Wang-Landau) scheme [6] and the same set of trial moves, we investigated several widely studied HP proteins and their HOP counterparts. Three different proteins: crambin, cytochrome c and ribonuclease A, with lengths of 46, 103 and 124 monomers, respectively, are converted into HP [7] as well as HOP sequences. Dramatic differences in ground state and thermodynamic properties have been observed, e.g. the estimation of ground state degeneracy for the 46mer are 460,000 and 20 for the HP and HOP models, respectively, and the latter shows more significant structural transition signals (specific heat, tortuosity, etc.) in the low temperature region.

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Statistical Physics 2: Jamming, Hard Spheres

Werner Krauth, *ENS Paris (France)*
Rejection-free, Irreversible, and Infinitesimal Monte Carlo Algorithms and Melting in two dimensions

I show how the lifting principle and a new pairwise decomposition of the Metropolis filter allows one to design a class of powerful rejection-free Markov-chain Monte Carlo algorithms that break detailed balance yet satisfy global balance. These algorithms generalize the recent hard-sphere event-chain Monte Carlo method. As an application, I present recent progress in our understanding of the phase diagram for two-dimensional soft disks, particles interacting with a repulsive power-law pair interaction. These results complement, and confirm, earlier results for hard-disk melting, and lead to a general understanding of melting in two dimensions.

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Salvatore Torquato, *Princeton University (USA)*
New Algorithm to Generate Jammed Sphere Packings

I describe a new algorithm to generate a diverse class of jammed disordered and ordered sphere packings with very high fidelity across Euclidean space dimensions. The task is posed as an optimization problem that is solved using linear programming techniques [1]. I will discuss how the algorithm leads to efficient generation of the densest sphere packings in high dimensions [2], a problem of importance in digital communications, and its ability to produce maximally random jammed sphere packings that are exactly isostatic in two and three dimensions with novel characteristics that have heretofore not been observed [3].

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Masaharu Isobe, *Nagoya Institute of Technology (Japan)*
Nucleation of Hard Spheres in local Monte Carlo, Event-Chain Monte Carlo, and Molecular Dynamics

Co-Author: Werner Krauth

Nucleation, crystallization and melting phenomena between phases are one of the most attractive topics in the history of computer simulation. Since the microscopic mechanism such as particle collective motion is important to understand the macroscopic phase transition, many numerical simulations have investigated after the solid-fluid phase transition in hard sphere system was discovered by conventional Monte Carlo(MC) and Molecular Dynamics(MD)in 1957[1,2].

In the hard sphere system, due to serious numerical difficulties such as long time equilibration and finite size effects, it is necessary to improve not only computer facilities itself but efficient algorithm for obtaining the equilibrium. Recently, the fast algorithm based on MC without rejection in the hard disk/sphere systems was proposed by Bernard, Krauth and Wilson [3], called "Event-Chain MC". Event-Chain MC is much faster (in CPU time)than conventional MC and efficient Event-Driven MD [4] in the calculation of global orientational order parameter in 2D hard disk system [5].

In this paper, we clarify the usefulness of Event-Chain MC based on CPU time by directly comparing with effient Event-Driven MD quantitatively in 2D Binary mixture and 3D nucleation/melting process in the hard sphere system. We found that both methods generates completely same final equilibrium states and confirmed that Event-Chain MC have an advantage for equilibration especially when we compute the system in dense and large particle number.

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Chandan Dasgupta, *Indian Institute of Science*

Short-time relaxation in glass-forming liquids from dynamics in a meta-basin of the potential energy landscape

Co-Author: Pranab Jyoti Bhuyan

The relation between the dynamics of glass-forming liquids [1] and properties of the potential energy landscape visited by the system during its time-evolution has been a subject of extensive investigations [2]. However, a clear interpretation of the short-time β relaxation of glass-forming liquids in terms of dynamics in the potential energy landscape is not yet available. We have studied the relation between dynamics in a meta-basin [3] of the potential energy landscape and β relaxation in a binary Lennard-Jones mixture. Meta-basins are determined from the series of inherent structures obtained by minimizing the potential energy, starting from configurations obtained from a constant-temperature molecular dynamics (MD) simulation. The eigenvalues and eigenvectors of the Hessian matrices of the

inherent structures in a meta-basin are then used to calculate various dynamical quantities in the harmonic approximation. We find that the results of the harmonic calculation begin to deviate from MD results at time scales substantially shorter than the β-relaxation time corresponding to the plateau in the mean-square displacement versus time plot. The agreement between the results of our analysis of the dynamics in a meta-basin and those of MD simulations is found to extend to longer times when anharmonic effects are included in the analysis in an approximate way [4]. In particular, calculations in which anharmonic effects are included correctly reproduce the dependence of the β-relaxation time on temperature and system size at temperatures near the ideal glass transition temperature Tc of mode-coupling theory [5]. These results establish that the dynamics of glass-forming liquids in the β-relaxation regime at temperatures near Tc can be understood from fluctuations inside individual meta-basins visited by the system during its time evolution. However, the inclusion of anharmonic effects are essential for a quantitative description of β relaxation in this temperature range.

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Ronald Dickman, *Universidade Federal de Minas Gerais (Brazil)*
Inconsistencies in steady state thermodynamics
Co-Author: Ricardo Motai

Among the many open questions in nonequilibrium physics, a central issue is whether thermodynamics can be extended to systems far from equilibrium. A specific extension of this nature is steady state thermodynamics (SST), which was proposed some fifteen years ago [1]. Using driven stochastic lattice gases, we ask whether consistent definitions of an effective chemical potential &mu and an effective temperature Te are possible. These intensive parameters are determined via coexistence, i.e., zero flux of particles and energy between the driven system and a reservoir. In the lattice gas with nearest-neighbor exclusion, temperature is not relevant, and we find that the effective chemical potential, a function of particle density and drive strength, satisfies the zeroth law, and correctly predicts the densities of coexisting systems under weak exchange. In the Katz-Lebowitz-Spohn driven lattice gas both &mu and Te need to be defined. We show that in this case the zeroth law is violated for Metropolis exchange rates, and determine the size of the violations numerically. The zeroth law appears to be violated for generic exchange rates. Remarkably, the system-reservoir exchange scheme proposed by Sasa and Tasaki [2] is free of inconsistencies [3]. This is because the rate depends only on the change in the state of the donor system, and is independent of that of the acceptor. We find, nevertheless, that this extension of thermodynamics has very limited predictive power: numerical experiments on driven lattice gases with a nonuniform drive show that in general, SST does not predict the coexisting densities correctly.

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General Computational Physics 1

Panos Argyrakis, *University of Thessaloniki (Greece)*
Network of the FP7 collaboration projects
Co-Author: Maria Tsouchnika

The Framework Programmes were developed as a strategy of the European Commission to enhance research and technology advances in its member countries. In past work, several research groups attempted to assess the FP5 and FP6 effectiveness, using largely statistical methods, and network analysis. Here, we study the data of FP7 following the network approach. The nodes of the network represent the institutions and the edges the collaboration between two institutions. All previous publications focused exclusively on the set of accepted proposals, which were implemented as projects, out of the set of all submitted proposals. The set of rejected proposals, however, may involve potentially valuable information complementary to that of the accepted ones. Therefore, it would be interesting to examine the network of collaborations formed by the rejected proposals, too, and subsequently compare it to that formed by the accepted ones. Any differences, or lack thereof, between these two networks, could be useful in further assessing the effectiveness of the FP Programmes. In order to get a more comprehensive picture of the network, we aggregate the data into three geographic scales (city, region and country) and thus we get six more networks, two for each of the accepted and rejected case. We first determine the basic network properties in all four scales, and compare them to those of the accepted FP6 proposals network that were studied in previous studies. The comparison of the two snapshots of the same network provides useful information on how this network of collaborations evolved in time. Furthermore, focusing on the country scale, we use Minimum Spanning Trees and a variety of centrality indices at the country scale of the two networks to study the structural properties of these networks and compare them to find any possible differences. Specifically, we determine the countries that serve as the most influential and significant nodes, in each case. Our results show that there are some interesting differences between the two networks, especially at the country scale.

Larry Engelhardt, *Francis Marion University (USA)*
Quantum spin simulations made simple

We have developed software that makes it very simple for a non-expert to simulate quantum spin systems. It allows one to define a quantum Hamiltonian by drawing dots (for spins) and lines (for bonds), and the values of physical parameters are varied by clicking and dragging sliders. This software was developed by undergraduate physics students using Easy Java Simulations (EJS),[1] and it can be freely downloaded from the ComPADRE Digital Library.[2]

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Guiping Zhang, *Renmin University of China*
Effects of contact and strain on electronic transport properties of graphene: exact and renormalized transfer matrix method

The effects of metallic contacts on electronic transport of graphene had not been completely estimated however widely discussed[1-3], hence we propose two powerful methods, i.e., exact [4] and renormalized transfer matrix method [5,6]. On one hand, results from exact transfer-matrix methods are valid for all sheet widths and lengths. In the limit of the large width-to-length ratio relevant to recent experiments, we find a Dirac-point conductivity of 2e2/√3h and a sub-Poissonian Fano factor of 2 − 3√3/π=0.346 for armchair graphene; for the zigzag geometry they are respectively 0 and 14. Our results reflect essential effects from both the topology of graphene and the electronic structure of the leads [4,6], giving a complete microscopic understanding of the unique intrinsic transport in graphene.

On the other hand, renormalized transfer matrix method (RTMM)5 utilizes U times of multiplication of traditional transfer matrix (U linear to the length) to eliminate numerical instability. Then Gauss elimination method combined with optimization greatly reduces the computational complexity from O(U3) to O(U). RTMM is powerful to investigate transport in large scale system (up to 106 carbon atoms) with irregular structure, disorder and impurity [7], and under magnetic field.

Consistent with observations, the conductance through graphene nanoribbons (GNRs) monotonically decreases, when the stress is parallel to the transverse direction [8]. As the stress is perpendicular to the transverse direction, the conductance increases till the gap opens in armchair GNRs (AGNRs), while monotonically increases in ZGNRs. The transmission peak of neutral and strained AGNRs is determined by the edge state of strained ZGNRs. The topology of the structure in GNRs determines that bonds parallel to and perpendicular to the transverse direction are positively and negatively correlated with electronic transport through GNRs between quantum wire contacts respectively.

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Zine El Abidne Chaoui, *University of Setif (Algeria)*
An optimized analytic model for charged particle transport in water

Cross sections of charged paricles interactions are needed in many area of physics. Knowledge of accurate elatic differential angular distributions and mean free paths of electrons with water molecule is of great importance in medical and radiation physics. These two quantities are often used as a data base in general purpose Monte Codes to model the transport of particles.The present work provides an accurate description of the elastic scattering process. In a first step, electron cross section with water molecule in a wide electron energy range from tens eV to few MeV are calculated using quantum mechanical tools. Starting from a static plus an exchange potential representing the electron-molecule interaction and by partial waves analysis, accurate elastic differential cross sections are obtained. Consequently a data base of angular distribution tables of elastic collision of electrons with water molecule can be generated. However, use of these tables during the transport process in Monte Carlo codes is time consuming. For this reason use of an analytic model is suited.As a second step, we present a new analytic model to describe the elastic interaction of electron with water molecule in a wide energy range. The suggested analytic model can be considered as a good approximation of the quatum mechanical model using partial wave analysis. It is mainly based on an optimization of the first and second transport elastic cross sections calculated from partial wave analysis. As a summury, the data base of electron elastic interaction with water molecule needed for Monte Carlo simulations is replaced by a simple expression to generate any angular distribution in one step. The obtained model can be easily implemented in Monte Carlo codes for charged particle transport.

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Nikita Kirnosov, *University of Arizona (USA)*
Non-BO calculations of rovibrational states of systems with Coulomb interactions using explicitly correlated all-particle Gaussian functions
Co-Author: Ludwik Adamowicz

Recent high accuracy non-BO calculations of small diatomic molecules employing explicitly correlated Gaussian basis set have revealed some interesting non-adiabatic effects. The approach

can be extended to study more exotic (including muonic) systems which challenge researchers to use more efficient software and hardware paradigms.
Some of the possible approaches are discussed and results presented.

Mitsuyoshi Tomiya, *Seikei University (Japan)*
Scar State on Time-evolving Wavepacket
Co-Authors: Kentaro Kawamura; Hiroyoshi Tsuyuki; Shoichi Sakamoto; Eric Heller

Recently it is found that accumulation of a time-evolving wavepacket in chaotic billiards makes scar-like localization [1,2], It emerges along classical unstable periodic orbits, when the wavepackets are launched along the orbits. Sufficiently long time after launching, the wavepacket spread all over the billiards and does not seemingly express any particular texture besides randomly granular pattern, though, the time-average of the absolute square of the wavepacket, which we shall call the accumulation, reveals the localization. The enhancement is apparently resembles the well-known scar states of stationary waves on chaotic billiards [3,4,5,6]. Therefore we may call it the “dynamical scar” in order to distinguish it to the original scar.

Expanding the accumulation by the eigenstates of the system, it can be easily shown that the states whose coefficients are larger often have the scar. The histogram of the square of the coefficients have the similar pattern to the weighted spectrum, which is also Fourier transform of the autocorrelation function [7]. However the coefficient histogram rattles much more violently than the weighted spectrum. In chaotic billiards relatively smaller amount of selected eigenstates which usually have the scar have dominant contribution to the histogram. And simultaneously it also lets the "dynamical scars" emerge. Actually, averaging over a proper energy range to smooth out its spiky behavior, the averaged histogram is almost the same as the weighted spectrum.

Furthermore, applying the semi-classical approximation, the weighted spectrum function plays crucial role to evaluate the wave function. For instance, the semi-classically evaluated accumulation on the periodic orbits matches remarkably with the numerically calculated one on the orbits.

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Joan Adler, *Technion (Israel)*
Efficient simulated annealing of segmented telescopes by invoking their analogy with SOS models
Co-Authors: Lee Yaacobi; Irina Paykin; Erez Ribak

Since single mirror telescopes are heavy and difficult to manufacture and install, segmented, multiple mirror systems have become popular. Such systems are analogous to surfaces of Solid-on Solid (SOS) models, with similar Hamiltonians, although the SOS system energy has to be minimiized and the image quality maximized. Both systems have multiple valleys (peaks) in their phase space. Experience with finding groundstates of the SOS models inspired the application of simulated annealing to telescope phasing to obtain optimal images. Older studies at the Technion will be reviewed and details of the algorithms used in our newest studies of both computer and analog systems will be described. Movies of image phasing will be presented.

Quantum Many-Body Physics 2

Federico Becca, *National Council for Research (CNR) and SISSA (Italy)*
Variational wave functions for strongly-correlated models

Variational wave functions represent a very powerful tool to study many-body systems, the Bardeen-Cooper-Schrieffer and Laughlin states being two important examples. In this talk, I will show that extremely accurate wave functions can be constructed to describe the low-energy physics of magnetic systems in presence of frustrating interactions. This is a particularly interesting situation, since new exotic phases of matter may appear, such as spin liquids featuring topological order and elementary excitations with fractional quantum numbers. I will show that resonating-valence bond (RVB) states, constructed by using slave-particles approaches, strongly suggest that spin-liquid phases may be stabilized in the highly-frustrated regime of spin-1/2 Heisenberg models on Kagome and square lattices.

Furthermore, I will show how it is possible to study time-dependent problems (e.g., the real-time evolution of a generic initial state, the so-called quantum quenches) by using variational wave functions. The case of the Bose-Hubbard model is considered in one and two spatial dimensions, with particular emphasis on light-cone effects in the spreading of correlations. The accuracy of the variational method is benchmarked with state-of-the-art time-dependent density-matrix renormalization group calculations.

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Philippe Corboz, *Institute for Theoretical Physics, University of Amsterdam (Netherlands)*
Recent progress in simulating strongly correlated systems with tensor network methods
Co-Authors: Frederic Mila; Matthias Troyer; T.M. Rice

Tensor networks are a class of variational wave functions enabling an efficient representation of quantum many-body states, where the accuracy can be systematically controlled by the so-called bond dimension. A well known example are matrix product states (MPS), the underlying tensor network of the famous density matrix renormalization group (DMRG) method, which has become the state-of-the-art tool to study (quasi-) one dimensional systems. Progress in quantum information theory, in particular a better understanding of entanglement in quantum many-body systems, has led to the development of tensor networks for two-dimensional systems, including e.g. projected entangled-pair states (PEPS) or the 2D multi-scale entanglement renormalization ansatz (MERA). These methods have been generalized to fermionic systems, and provide one of the most promising routes for the simulation of strongly correlated systems in two dimensions, in particular models where Quantum Monte Carlo fails due to the negative sign problem.

In this talk I report on recent progress in simulating fermionic and frustrated systems with infinite PEPS (iPEPS) which is a tensor network ansatz for 2D wavefunctions in the thermodynamic limit. For the t-J model this method reveals an extremely close competition between a uniform d-wave superconducting state and different types of stripe states, with lower variational energies than in previous state-of-the-art studies for large 2D systems [1]. For the Shastry-Sutherland model in a magnetic field iPEPS predicts a new type of state [2] which helps to understand the intriguing magnetization process observed in SrCu2(BO3)2. Finally, I will discuss prospects and future directions in the field of tensor networks.

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Roger Melko, *University of Waterloo (Canada)*
Quantum Kagome Ice
Co-Authors: Juan Carrasquilla; Zhihao Hao

Among the new phases of matter sought in the 21st century, two-dimensional quantum spin liquids (QSL) are particularly coveted due to their promise of revolutionizing not only materials science and technology, but also our fundamental understanding of the structure of condensed-matter theory. Despite their importance, concrete knowledge of the microscopic mechanisms that cause magnetic moments to remain disordered to very low temperatures in a QSL remain obscure. Here, we study a theoretical model for a broad class of frustrated magnetic rare-earth pyrochlore materials, the so-called quantum spin ices. When subject to an external field along the [111] crystallographic direction, the resulting Hamiltonian, which is free from the "sign problem", retains a mix of geometric frustration and quantum fluctuations between spins in decoupled two-dimensional kagome planes. Using large-scale quantum Monte Carlo simulations, we demonstrate that the phase diagram of this kagome spin model

contains a region with no magnetic long-range order, and a gap to excitations, which could possibly be an elusive Z2 QSL. This suggests a systematic experimental procedure for searching for two-dimensional QSLs within the broader class of three-dimensional pyrochlore quantum spin ice materials.

Wenan Guo, *Beijing Normal University (China)*
Novel quantum glass of bosons in a random potential in two dimensions
Co-Authors: YanCheng Wang; Anders Sandvik

We use quantum Monte Carlo simulations of the two-dimensional Bose-Hubbard model to study the quantum glass emerging from the superfluid and Mott-insulator states in the presence of random potentials. Rare large superfluid domains in a Mott background make the glass gapless although it is insulating. Contrary to the commonly accepted paradigm, we show here that the compressibility κ of the glass at filling $\rho=1$ in the region between the Mott and superfluid phases follows the form $\kappa \sim {\rm exp}(-b/T^\alpha)$ with $\alpha <1$. This is explained by a percolation scenario for critical clusters. We also find a dynamic exponent $z < 2$ at the glass-superfluid transition, which indicates that the singular part of the compressibility is zero at the MG-SF critical point. At high disorder strengths, where a glass state reappears from the superfluid, we find a conventional compressible Bose glass.

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http://arxiv.org/abs/1110.3213v2

Thomas Lang, *Boston University (USA)*
Mott Transitions of Correlated Fermions from SU(2) to SU(N)

We discuss the instabilities upon the introduction of local Coulomb repulsion and explicit SU(N)-symmetric Heisenberg-like spin exchange to Dirac Fermi-surfaces, quadratic band touching point-like Fermi-surfaces and full Fermi-surfaces. The extension to higher symmetries allows us to study the melting of phases as a function of correlations as well as symmetry. We explore the quantum phases emerging in the SU(N)-symmetric Hubbard and Heisenberg models on the honeycomb lattice, Bernal-stacked honeycomb bilayer and the square lattice at half-filling by means of projective (zero temperature) quantum Monte Carlo simulations from SU(2) to the large-N limit for even values of N. We find SU(N)-spin symmetry broken phases at small values of N and weak coupling, and staggered flux phases, resonating valence bond plaquettes as well as columnar valence bond crystals in the limits of large-N and strong interactions.

Lattice Field Theory 1

Taku Izubuchi, *RIKEN BNL Research Center (USA)*
Lattice QCD calculations for particle physics

To test our current understanding of the fundamental law of particle physics, accurate theoretical calculations and precise experimental results are needed to meaningfully confront each other. The anomalous magnetic moment of muon, (g-2)_mu, provides one of the most stringent tests of this kind. Current and future experimental accuracies, 0.54 ppm and 0.14 ppm, respectively, require theoretical calculations of QCD contributions. I will review recent progress of Lattice QCD calculations of (g-2)_mu, including recent algorithmic developments on statistical and systematic error reductions.

Aida El-Khadra, *University of Illinois (USA)*
Lattice QCD and Quark Flavor Physics

The strong interaction is a force which binds quarks, antiquarks and gluons together into protons, neutrons and other similar particles. This force is also responsible for binding protons and neutrons into nuclei. The theory which describes the strong interaction is Quantum Chromodynamics (QCD). It is part of the so-called standard model of particle physics, which successfully describes almost all our experimental observations in particle physics. However, a quantitative understanding of bound state properties from QCD requires nonperturbative methods. Lattice QCD is such a method. It is systematically improvable and controllable. Lattice QCD calculations use monte carlo methods, that require large scale numerical simulations, and hence significant computational resources. The scope of the simulations affects the precision of the calculations.
The lack of precision in understanding hadrons from the fundamental theory is one of the outstanding problems of particle physics. This problem also affects the experimental effort at the intensity frontier, in particular, on quark flavor physics. The goal of the intensity frontier effort is to search for new physics via confronting theory with precision experimental measurements. Since QCD effects are a dominant contribution to the standard model expectation for many of these processes, precise lattice QCD calculations are an essential ingredient in this effort.

In this talk I review the status of lattice-QCD calculations relevant to quark flavor physics. I describe recent developments that are moving these calculations towards their precision goals and their impact on the landscape of lattice flavor physics calculations.

Steven Gottlieb, *Indiana University (USA)*
Electromagnetic effects of the light hadron spectrum

For some time, the MILC Collaboration has been studying electromagnetic effects on light mesons. These calculations use fully dynamical QCD, but only quenched photons. That is, the sea quarks are electrically neutral, while the valence quarks carry charge. The photons are quenched and use the non-compact formalism. We have new results with lattice spacing as small as 0.045 fm. In addition, we have

been looking at baryon operators in well-defined taste multiplets defined by J. Bailey. We consider how well chiral perturbation theory describes some of these results and the implications for light quark masses.

Oliver Witzel, *Boston University (USA)*
Lattice-QCD determination of B-meson decay constants and semileptonic form factors

We calculate the leptonic decay constants fB and fBs and semileptonic form factors for B->pi l nu and Bs->K l nu in lattice QCD using domain-wall light quarks and nonperturbatively tuned relativistic b-quarks. We present results with a complete systematic error budget based on simulations with two lattice spacings a~0.11 and 0.08 fm and five sea-quark ensembles with pion masses as light as 290 MeV. Combining our results for B->pi l nu form factors with experimental data from BaBar and Belle we extract the CKM matrix element |V_{ub}|.

Stefan Krieg, *Forschungszentrum Juelich (Germany)*
From quarks to hadrons and back: spectral and bulk properties of strongly interacting matter from Lattice QCD
Co-authors: Claudia Ratti, Christopher Schroeder, Kalman Szabo, Balint Toth

Computing, from first principles, the hadron masses to percent accuracy [1], is only possible through simulations of Lattice Quantum Chromodynamics (QCD). With the advent of the present class of Pflop Machines and novel simulation algorithms, we now can proceed to compute per-mille effects in the particle spectrum, i.e. the proton-neutron mass difference. This difference is due to a subtle cancellation of already small effects (due to the mass difference of the up- and down-quarks and the presence of electromagnetic interactions). I will report on a Project [2,3] to compute this and other mass differences using simulations of Lattice QCD and Quantum Electrodynamics and discuss the new simulations methods and highly efficient code employed.

In the case of the proton and the neutron, quarks and gluons are confined to the hadron. If we, however, increase the temperature of the system sufficiently, both particles will 'melt' and quarks and gluons behave as free particles ('quark-gluon-plasma'). This transition is described by the Equation of State (EoS) of QCD [4]. I will discuss an ongoing project (e.g. [5]) aimed at calculating the EoS including the effects of a dynamical charm quark, which is relevant for temperatures larger than 300-400 MeV.

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Tuesday, Parallel Sessions 2, 15:45-17:30

Materials Science and Nanoscience 2

Hsin Lin, *Graphene Research Centre and Department of Physics, National University of Singapore*
Topological Crystalline Insulators: A New Phase of Quantum Matter
Co-Authors: Yung Jui Wang; Wei-Feng Tsai; Cheng-Yi Huang; Arun Bansil

The recently discovered topological crystalline insulators harbor multiple Dirac surface states protected by a discrete set of crystalline space group symmetries and show immense promise for novel quantum applications. In this talk, I will present a first principles investigation as well as a model Hamiltonian of the nontrivial surface states and their spin and orbital texture in the topological crystalline insulator SnTe and related compounds. The (001) surface states exhibit two distinct energy regions of the Fermi surface topology separated by a Van-Hove singularity at the Lifshitz transition point. The surface state band structure around X(pi,0)-point consists of two “parent” Dirac cones centered at X and vertically offset in energy. When they intersect, the hybridization between the electron-branch of the lower parent Dirac cone and the hole-branch of the upper parent Dirac cone opens a gap at all points except along the mirror line, leading to the formation of a pair of lower-energy “child” Dirac points shifted away in momentum space from the time-reversal-invariant point X. Interestingly, the two parent Dirac cones must have different orbital character since they were found to be associated with orbitals with opposite sign of mirror eigenvalues in order to deliver the correct spin texture and band dispersion. Such nontrivial spin and orbital texture of the Dirac cones, which are of immense importance in determining a variety of materials’ properties, have been confirmed recently by spin- and angle-resolved photoemission and Fourier-transform scanning tunneling spectroscopy. In particular, the intensity and energy dependences of interference patterns show distinct characteristics which can directly be attributed to orbital effects. I will also discuss the breaking of crystal symmetry and mass acquisition of Dirac fermions.

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Zenan Qi, *Boston University (USA)*
Strain Engineering of Graphene Hexagon and Nanobubbles
Co-Authors: Dario Bahamon; Alex Kitt; Harold Park; Vitor Pereira; David Campbell; Antonio Castro Neto

We studied mechanical and electronic properties of graphene by strain engineering nano-structures in two-dimensional and three-dimensional deformations. By using a combined atomistic simulation approach with molecular mechanics, molecular dynamics, tight binding and Landauer-Buttiker formalism, we explored possible deformation patterns to induce tunable pseudomagnetic field (PMF) distributions and studied the Landau levels arising from the PMFs. We found that a graphene Y-junction structure can generate a pseudomagnetic quantum dot and selectively guide the electrons' trajectories with strained leads. We showed that valley degeneracy is broken when both strain-induced PMFs and external real magnetic fields are present. Further, graphene nano-bubbles can also be controlled as functional blocks by manipulation of geometries, pressure, size and substrate. The simulation results illustrate the promising potential of graphene for the design of electronic NEMS/MEMS devices by strain engineering.

References
Authors acknowledge supports of NRF-CRP award, NSF and Banco Santander

Vladimir Stegailov, *JIHT RAS (Russia)*
Graphite melting: atomistic kinetics resolves long-standing controversy
Co-Author: Nikita Orekhov

Graphite is the most refractory single element solid. Despite its abundance and importance the graphite melting temperature Tm remains a subject of controversy. The variation of the experimentally measured Tm values is more than 1000K [1,2]. The Tm values tend to group in the low temperature and high temperature sets [3]. The pressure dependence of the graphite melting curve provided an additional puzzle. According to experimental measurements this dependence has a maximum around 5-6 GPa. The interpretation of the maximum is connected with the possible liquid-liquid phase transition (LLPT) in liquid carbon similarly to other substances.

Liquid carbon was studied in the pioneering works at the dawn of the ab initio molecular dynamics (MD) [4] that provided a certain evidence on the coordination changes in liquid carbon at 100GPa and hence supported the LLPT hypothesis. Subsequently equations of state for carbon that reproduce the LLPT in the graphite melting pressure range were developed [5]. Atomistic simulation methods became mature enough to handle the graphite melting problem as soon as the sophisticated interatomic potentials for carbon had been created (AIREBO [6] and LCBOP [7]). However despite considerable effort no confirmation of the LLPT in liquid carbon was found [8]. The pressure dependencies of the graphite melting temperature calculated for the LCBOP type models display no evidence of the maximum [9].

In our MD calculations we consider heterogeneous melting at the solid-liquid phase boundary and homogeneous nucleation of melt in graphite at high degrees of superheating. The results of MD calculations provide a model that explains the controversies connected with graphite melting. The preliminary results have been published in [10].

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Jenni Portman, *Michigan State University (USA)*

Evidence of stacking disorder induced gap opening in the ground state of 1T-TaS2

Co-Authors: Dat Thanh Do; Bhanu Mahanti; Phillip M. Duxbury

1T-TaS2 is a transition-metal layered compound that shows unique electronic properties, resulting from a variety of temperature dependent phases with different structures. ForT<190K, this material displays a commensurate charge density wave (C-CDW) phase characterized by insulating behavior corresponding to the opening of a gap at the Fermi energy. To better understand the C-CDW phase and explain its quantum mechanical origin, we perform density functional theory calculations of the electronic band structure of 1T-TaS2 and quantify the effect that spin orbit coupling and Hubbard repulsion have on the ground state. Our results show that neither of these interactions is sufficient to reproduce the insulating gap seen in experiment, an observation which is confirmed by our calculation of the phonon band structure and absorption spectrum. Next we consider the effect of different stacking configurations of the TaS2 layers and find evidence of gap opening for bilayers in the presence of disordered stacking, while monolayer configurations remain metallic regardless of whether stacking disorder is included or not. We fit the resulting non dispersive energy levels with a tight binding model to quantify the interlayer coupling strengths.

Hiroaki Nakamura, *National Institute for Fusion Science (Japan)*
A Binary-Collision-Approximation Simulation Study on the Dependence of Noble Gas Absorption upon Crystal Orientation of Tungsten
Co-Authors: Seiki Saito; Atsushi M. Ito; Arimichi Takayama; Yasuhiro Oda

To find plasma facing materials (PFM), which must endure a plasma irradiation, is one of the important issues in order to realize the nuclear fusion reactor. Tungsten material is one of the candidates of PFMs. However, bubble or nano-structure formation in tungsten is observed under the irradiation of helium onto the tungsten surfaces. This structure appears not only in tungsten but also in other materials, e.g., iron. The nano-structure weakens mechanical strength and increases the tritium retention. Therefore it is better to avoid the nano-structure formation in PFM. To achieve this aim, it is necessary to reveal the mechanism of the nanostructure formation in PFM under helium gas irradiation [1]. Intuitively, the nano-structure formation is regarded as the phenomenon composed of the invasion of helium gas into PFM, the diffusion of helium in PFM and the transformation of PFM material. In this paper, we pick up the first process of the fuzz structure formation, that is, the invasion process. We calculate the absorptivity of noble gases into tungsten.

We use a binary corrison approximation (BCA) to solve scattering phenomena between tungsten atoms and injected atoms, i.e., noble gas atomes. The BCA simulation is performed by ACA‡T (atomic collision in any structured target) code[2,3]. In BCA simulation, multi-body interactions in a material approximate to consecutive two-body interactions between a projectile atom and the nearest neighbor atom. Using this code, we calculate the absorptivity as well as the penetration depth and sputtering yield which are basic information to reveal the nano-structure formation[4]. We found that these physical quantities depend on the crystal orientation of the target tungste. In this paper, we show that the dependence of these quantities quantitatively.

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Abdiravuf Dzhurakhalov, *University of Antwerp (Belgium)*
Computer simulation of the interaction of ringlike carbon clusters with nanographene
Co-Authors: Vasiliy Stelmakh; Ishmumin Yadgarov

The ideal structure of graphene can be disrupted by various ways, such as by the producing the vacancies and by the replacement of carbon atoms with other atoms, in particular, with nitrogen or silicon atoms [1]. In our work, the structural changes of a rectangular nanographene ribbon consisting of 272 atoms as a result of its interaction with ringlike carbon clusters have been studied.

Using the second-generation of Brenner interatomic potential [2], the interaction of the ringlike C7, C12 and C13 carbon clusters with nanographene has been simulated on the basis of Monte Carlo energy minimization method. The interaction of C7 cluster results slightly in the change of both cluster structure and the structure of nanographene. Meantime the interaction of C12 and C13 clusters cause the destruction of the local nanographene structure and the formation of ripple nanographene sheet. Besides, the shape of these clusters also changes significantly.

The cohesive energy of the nanographene and binding energies of carbon clusters have been calculated and compared before and after interactions. Thus, the interaction of nanographene with clusters may lead to a significant defect formation of the nanographene and to the change of the shape and cohesive energies of clusters and graphene. As the defects and structural changes in graphene result in the change of its properties, the interaction of carbon or other clusters can be used as nanoengineering technique for the modification of graphene sheets.

The results of computer simulations, the various structural changes and modifications of nanographene ribbon caused by the interaction of ringlike clusters are presented and discussed.

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Statistical Physics 3: Spin Models

Youjin Deng, *University of Science & Technology of China*
Universal amplitudes in the canonical ensemble
Co-Authors: Hao Hu; Henk Blote

Universal amplitudes play an important role in the numerical study of critical phenomena. We study the finite-size scaling of universal amplitudes in the q-state random-cluster model under the constraint that the total number of occupied bonds is fixed, so that the canonical ensemble applies. We observe that at criticality, new finite-size corrections with exponent ycan=-|2yt-d| are induced, where yt=1/&nu is the thermal renormalization exponent and d is the spatial dimension. Moreover, we find that universal values of dimensionless parameters like Binder ratios and wrapping probabilities are modified for systems with 2yt-d>0. For the bond percolation model where thermal fluctuations are absent, the correction exponent ycan still occurs, and universal amplitudes like the excess cluster number are not only modified but become non-universal. A full explanation should take into account fluctuation-suppression effects, in addition to the well-known Fisher renormalization mechanism.

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Pablo Serna, *University of Murcia (Spain)*
Loop models with crossings
Co-Authors: Adam Nahum; Andres M. Somoza; Miguel Ortuno

The universal behaviour of two-dimensional loop models can change dramatically when loops are allowed to cross. We present models with crossings studied by extensive Monte Carlo simulations. Our main focus (the `completely packed loop model with crossings' or CPLC) is a simple generalisation of well-known models which shows an interesting phase diagram with continuous phase transitions of a new kind. These separate the unusual `Goldstone' phase from phases with short loops. In addition to studying the new critical points, we characterise the universal properties of the Goldstone phase in detail, comparing renormalisation group (RG) calculations with numerical data on systems of linear size up to L=106 at loop fugacity n=1. Very large sizes are necessary because of the logarithmic form of correlation functions and other observables.In order to be able to access these big systems, we developed a parallelizable transfer-matrix-like technique and implemented it in CUDA language. We present in detail this technique and its application to the loop models.The CPLC is relevant to polymers on the verge of collapse, and a particular point in parameter space maps to self-avoiding trails at their &Theta-point. Finally, one of the phase transitions considered here is a close analogue of those in disordered electronic systems - specifically, Anderson metal-insulator transitions - and provides a simpler context in which to study the properties of these poorly-understood (central-charge-zero) critical points.

Robert Swendsen, *Carnegie Mellon University (USA)*
Solving the inverse Ising model with multi-spin interactions
Co-Author: Joseph Albert

Monte Carlo simulations of Ising models generate spin configurations with Boltzmann probabilities. An inverse problem starts with spin configurations and has the goal of finding the interaction parameters. The problem first arose in the determination of renormalized coupling constants from Monte Carlo renormalization group simulations, and a general solution was found using correlation function matching. Similar inverse problems have recently become of interest in fields like biology, sociology, and neuroscience. We've extended the earlier solution to solve such inverse problems for models including multi-spin interactions, but without translational invariance.

Wolfhard Janke, *University of Leipzig (Germany)*
Non-Standard Finite-Size Scaling at First-Order Phase Transition
Co-Authors: Marco Mueller; Desmond A. Johnston

We note that the standard inverse system volume scaling for finite-size corrections at a first-order phase transition (i.e., 1/L^3 for an L × L × L lattice in 3D) is transmuted to 1/L^2 scaling if there is an exponential low-temperature phase degeneracy. The gonihedric Ising model which has a four-spin interaction, plaquette Hamiltonian provides an exemplar of just such a system. We use multicanonical

Monte Carlo simulations of this model to generate high-precision data which provides strong confirmation of the non-standard finite-size scaling law. The dual to the gonihedric model, which is an anisotropically coupled Ashkin-Teller model, has a similar degeneracy and also displays the non-standard scaling. Further potential applications will be briefly discussed.

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Edyta Malolepsza, *Boston University (USA)*

Generalized ensemble method applied to study systems with strong first order transition

Co-Authors: Jaegil Kim; Tom Keyes

We would like to present results from applying generalized ensemble method to studies of systems with strong first order transition such as water and methane clathrate. We present statistical temperature, entropy and free energy functions calculated for the systems under different pressures, as well as changes in structures associated with the phase transition process.

In systems with strong first order transition entropy exhibits a convex dip across transition region. Consequently, the statistical temperature curve around the transition exhibits negative slope (called S loop or back-bending), and canonical probability density functions become bimodal with peaks localized outside of the S loop region. Inside the S loop region states are unstable in the canonical ensemble and as a result studying of equilibrium phase coexistence becomes impossible. To overcome this problem, a novel method was proposed by Kim, Keyes and Straub [1], where an optimally designed generalized ensemble sampling was combined with the replica exchange method. This new technique uses parametrized effective sampling weights that lead to unimodal energy distribution by transforming unstable states in canonical ensemble into stable ones. In the present study, the generalized ensemble method, originally developed to use with the Monte Carlo technique, was implemented to work with molecular dynamics in isobaric ensemble and coded into LAMMPS, a highly optimized open source molecular simulation package.

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Patrick Malsom, *University of Cincinnati (USA)*

The limitations of the Onsager-Machlup functional

Co-Author: Frank Pinski

The Onsager-Machlup (OM) functional has been used to define an effective "thermodynamic action" that describes the distribution of pathways as a molecule changes conformations. We use this action to explore rare events: molecular transitions substantially impeded by one or more energy barriers. Using an efficient technique, we sample the OM action and generate transition paths that are constrained to start and end in specified energy basins. We find that even for simple systems, such an ensemble is not

compatible with the thermodynamic (Boltzmann) distribution. To understand these results, we have used a Monte Carlo method to derive a functional similar to the OM functional. Using this new perspective, we identify the cause of the unphysical result and conclude that the OM functional alone is not sufficient to describe a thermodynamic ensemble of paths. In particular, we show that only a certain subset of Brownian paths are consistent with the correct thermal fluctuations.

Computational Physics Education 1

Ruth Chabay, *North Carolina State University (USA)*
Computation and Conceptual Understanding in Introductory Physics

The process of constructing and exploring computational models can offer significant support for the development of conceptual understanding of key ideas in physics. However, most students in the U.S. who take introductory physics courses in university have had no prior exposure to programming. By selecting a minimal set of computational concepts to teach, and by introducing these concepts in the context of physics activities, we have been able to engage beginning students in constructing and refining computational models of interesting physical systems. The use of VPython allows students to produce navigable real-time 3-D animations as a side effect of their physics calculations. Research on how students engage with such models has helped refine instructional strategies. Examples from mechanics and from an introductory level course on soft condensed matter will be discussed.

Francisco Esquembre, *Universidad de Murcia (Spain)*
Facilitating programming computational physics simulations for tablets
Co-Author: Félix Jesús Garcia-Clemente

Motivation is a powerful tool to help students learn. And being able to simulate Physics phenomena on tablets can be a great motivation for Computational Physics students. We introduce a major version of the successful Easy Java/Javascript Simulations (EjsS) modeling tool (http://www.um.es/fem/EjsWiki) that allows Physics teachers and students to create, share, and distribute Java and Javascript simulations with a minimal amount of training. Simulations created with EjsS can implement a great variety of computational algorithms, and visualize the result using attractive scientific graphics and interactive user interfaces. The software provides tools to solve ordinary and delay differential equations, with or without discontinuities (events). The Javascript support of EjsS allows students to create computational physics programs and simulations that run in smartphones and tablets. We have also created a Reader App for Android and iOS that allows a user to collect and organize a number of JavaScript simulations for use off-line. When on-line, the Reader App connects to the OSP Collection at the comPADRE digital library, to download additional ready-to-use, tablet-enabled simulations.

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http://www.um.es/fem/EjsWiki

Beate Schmittmann, *Iowa State University (USA)*
K-12 outreach and student recruitment with computational science

The Department of Computer Science at Iowa State University has developed a Computational Thinking Competition. It seeks to introduce K-12 students to problem solving with computational thinking in the context of their current coursework in Iowa schools. Student projects are in the form of computational models that help students to understand a problem, understand all of the requirements for a solution, be able to test their solution, and demonstrate the solution. Prior to the competition, students can sign up for a Computational Thinking Workshop so that they understand what computational thinking is and how they can apply it to a project, either for their regular schoolwork, or for the CTC. Other components of the program are K-12 Teacher Certification Classes and Family/Student Programming Nights.
I will describe the program, its outcomes, and discuss it portability to computational physics programs.

Jan Tobochnik, *Kalamazoo College (USA)*
The Computational Physics Section of the American Journal of Physics
Co-authors: Harvey Gould

One of the most challenging aspects of the undergraduate physics curriculum is providing interesting projects that give students meaningful research experience. Computationally-related projects provide a low cost entry into contemporary research, and many problems can be made accessible to undergraduates. Because of the paucity of accessible papers in the research literature, we have started the Computational Physics section of the American Journal of Physics. The section publishes papers that provide the background necessary to explore interesting suggested problems, which are accessible to advanced undergraduate and beginning graduate students. We will discuss the philosophy of the section and examples of papers that have been published. One of the goals of this presentation is to convince more computational physicists to submit manuscripts for the section.

Novel Computing Paradigms 2

Martin Berzins, *University of Utah (USA)*
Multiscale and Multiphysics Computations on Presnt and Future Architectures
Co-Authors: Alan Humphrey; Todd Harman

The challenge of undertaking solving large and complex multiscale and multiphysics calculations on present and future large scale computer architectures is addressed. The computational framework employed is the Utah Uintah software. This software employs a layered approach of an abstract graph-based formulation that generates tasks for a sophisticated runtime system that executes the tasks asynchronously and adaptively. The success of this approach is briefly described and a particular case study used to describe the solution of a challenging combustion problems. A key feature of this problem is the need to model radiative heat transfer by ray tracing. The implementation of this approach is described and its performance examined on both GPus and CPUs.

Erik Schnetter, *Perimeter Institute (Canada)*
Automated Code Generation for Solving PDEs on Modern HPC Architectures

Modern HPC applications employ increasingly advanced discretisation methods to study multi-physics problems. Modern HPC architectures consist of heterogeneous multi-core many-node systems with deep memory hierarchies. Developing applications that are able to explore cutting-edge physics on cutting-edge HPC systems has become a complex task that requires significant HPC knowledge and experience, where entirely too much hardware detail is exposed to the application developer.

We describe Chemora [1,2], a generic framework for solving systems of Partial Differential Equations (PDEs) that targets modern HPC architectures. Chemora is based on Cactus, which sees prominent usage in the computational relativistic astrophysics community, and uses automated code generation to create C++, CUDA, or OpenCL code. PDEs are expressed either in a high-level latex-like language or in Mathematica. Discretisation is defined separately from equations, and can include e.g. Finite Differences, Discontinuous Galerkin Finite Elements, Adaptive Mesh Refinement (AMR), or multi-block systems.

Using the Einstein equations as example, we show how Chemora can be used to implement complex systems of PDEs for CPUs and accelerators. Important high-level and low-level transformations and optimizations are applied automatically, leading to code with quite reasonable efficiency. The performance often surpasses manually written code, if only because automated code generation simplifies exploring the optimization parameter space of complex code bases.

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Xavier Saez, *Barcelona Supercomputing Center (Spain)*
First experience with Particle-in-cell Plasma Physics code on ARM-based HPC systems
Co-Authors: Alejandro Soba; Edilberto Sanchez; Mervi Mantsinen; José María Cela

During the last two decades, supercomputers have grown rapidly in performance at the cost of a similar growth in power consumption. However, nowadays the computer's performance is limited by power consumption and power density, so new developed platforms have to be based on the power efficiency. The Mont-Blanc project [1] appeared with the aim to design computer architectures capable of delivering an Exascale performance using 15 to 30 time less energy than present architectures. The

reduction of energy consumption will be achieved by using energy-efficient processors originally designed for mobile and embedded systems.

Particle-in-cell (PIC) is one of the most used methods in plasma physics simulations [2]. The individual particles are tracked in a continuous phase space, whereas densities and the current are computed concurrently on stationary mesh points. The quality of results achieved relies on tracking a very large number of particles. Therefore, PIC codes require intensive computation and need to be adapted to new platforms constantly.

EUTERPE is a gyrokinetic PIC code for global linear and non-linear simulations of fusion plasma instabilities in 3D geometries [3,4]. It is targeted towards traditional HPC clusters running MPI with a domain cloning method. In doing so, the number of processors can increase without hugely boosting the interprocessor communications [5].

In this work, we will explore the feasibility of porting a PIC code (EUTERPE) to an ARM [6] multi-core platform from the Mont-Blanc project. The used prototype is based on a system-on-chip Samsung Exynos 5 with an integrated GPU. It is the first that could be used for HPC, since it supports double precision and parallel programming languages.

In order to check the ported code for a realistic problem we will perform the Rosenbluth-Hinton test[7]. In 3D geometries this kind of simulation, even linear, is very time consuming[8]. For this test we use the maximum amount of cores on the prototype.

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Elise de Doncker, *Western Michigan University (USA)*

Scalable Software for Multivariate Integration on Hybrid Platforms

Co-Authors: John Kapenga; Fukuko Yuasa; Omofolakunmi Olagbemi

The paper describes the software infrastructure of the ParInt package for multivariate numerical integration, layered over a hybrid parallel environment with distributed memory computations (on MPI), and multi-threaded components running on the nodes and many-core accelerators.

ParInt supports the computation of multivariate integrals over hyper-rectangular and simplex regions. The algorithms and tools in the parallel integration engine include: (i) an adaptive region subdivision algorithm, equipped with a load balancing strategy to handle localized integrand difficulties such as peaks and singularities; (ii) a non-adaptive Quasi-Monte Carlo method based on Korobov lattice rules; (iii) Monte Carlo methods for high dimensions and/or erratic integrands; (iv) 1D QuadPack programs for repeated integration in successive coordinate directions; (v) a user interface based on the ParInt plugin compiler which pre-processes the user problem specification and integrand function to be linked with the ParInt executable.

Our objective has been to provide the end-user with state of the art problem solving power packaged as portable software. Repeated integration with 1D QuadPack routines has been proven extremely effective for applications to Feynman loop integrals with severe singularities in high-energy physics [1]. We will further give test results of the multivariate ParInt engine, with significant speedups for a set of multi-loop Feynman integrals.

Other applications include the computation of multivariate normal and Student-t distribution integrals, financial derivatives for mortgage backed security problems and option pricing, rank-based fitting in Bayesian statistics, medical physics (e.g., allowing an efficient computation of radiation dosage in oncology), and analysis of taste test trials in behavioral psychology. Even moderate size problems in these areas may tax simple multicore processors, and benefit from the cluster environment and many-core coprocessors.

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Yasunari Zempo, *Hosei University (Japan)*

Real-Time and Real-Space Program Tuned in K-Computer

Co-Authors: Masaya Ishida; Eiji Tomiyama; Hideki Yamamoto

Time-dependent density functional theory (TDDFT) is one of the most prominent and widely used methods for calculating excited states of medium-to-large molecules, and it is recognized as a powerful tool for studying electronic transitions of molecules [1]. In our calculations, the real-time and real-space technique is adopted in solving equation by the finite difference approach [2]. In particular, the real-space approach is suitable for large-scale parallel computing, and also allows the capture of a clear physical image. Within the framework of this approach, we can solve for the wavefunctions on the grid with a fixed domain, which encompasses the physical system of interest [3].

We have transported our code from Earth Simulator (ES) to K-Computer (KC). However, the expected performance was not realized, although it has been tuned in EC, and achieved remarkable linear scalability and significant parallelization efficiency. There are architectural differences between ES and KC: In ES each node has eight vector processors, and there is a high speed inter and intranode

communication; In KC, each nodes has eight cores per processor and each node connected by a special interconnect. Taking account of these differences, we have applied the following implementations and obtained the 37% better total performance.

First, we have stated with OpenMP and MPI hybrid parallelization, and optimal rank mapping, where the zyx-mapping is adopted in the 3D process. It is fairly effective to get rid of the unnecessary processes such as zero clear and data copy. In calculation loops, the improvement of thread efficiency provides an efficient OpenMP process. Introducing the MPI_test call, communication concealment in MPI processes works effectively in the code. It takes a role of a trigger for MPI_isend and MPI_irecv processes. The detail will be introduced in the presentation.

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Lattice Field Theory 2

John Negele, *Massachusetts Institute of Technology (USA)*
Understanding the Structure of Nucleons using Lattice QCD

I will describe for non-specialists the use of lattice QCD, numerical solution of QCD on a discrete space-time lattice, to calculate the properties of protons and neutrons, the basic building blocks of nearly all the matter in the observed universe, from first principles. I will then describe recent success[1], after decades of effort, in obtaining agreement with experiment for the charge radius, magnetization radius, magnetic moment, and fraction of momentum arising from quarks. I will also discuss calculation of electromagnetic form factors [2], exploration of the origin of the nucleon spin, prediction[3] of scalar and tensor charges needed in planning searches for physics beyond the Standard Model in cold neutron decay experiments, and future challenges

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[1] Nucleon Structure from Lattice QCD Using a Nearly Physical Pion Mass
J. R. Green, M. Engelhardt, S. Krieg, J. W. Negele, A. V. Pochinsky, S. N. Syritsyn
arXiv:1209.1687, 2012
[2] Nucleon Scalar and Tensor Charges from Lattice QCD with Light Wilson Quarks
J. R. Green, J. W. Negele, A. V. Pochinsky, S. N. Syritsyn, M. Engelhardt, S. Krieg
Phys Rev D.86.114509, 2012, arXiv:1206.4527
[3] Nucleon electromagnetic form factors from lattice QCD using a nearly physical pion mass
J. R. Green, J. W. Negele, A. V. Pochinsky, S. N. Syritsyn, M. Engelhardt, S. Krieg
arXiv:1404.4029, 2014

William Detmold, *MIT (USA)*
Dark Nuclei
Co-Authors: Andrew Pochinsky; Matthew McCullough

We consider two-colour QCD with two flavours of quarks as a possible theory of composite dark matter and use lattice field theory methods to investigate nuclear spectroscopy in the spin J=0 and J=1 multi-baryon sectors. We find compelling evidence that J=1 systems with baryon number B=2,3 (and their mixed meson-baryon counterparts) are bound states - the analogues of nuclei in this theory. We discuss aspects of the novel phenomenology of such a dark nuclear sector.

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Dark Nuclei I: Cosmology and Indirect Detection
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Dark Nuclei II: Nuclear Spectroscopy in Two-Colour QCD
By William Detmold, Matthew McCullough, Andrew Pochinsky.
arXiv:1406.4116 [hep-lat].

Sergey Syritsyn, *RIKEN BNL Research Center (USA)*
Nucleon Structure on a Lattice at the Physical Point
Co-Authors: Tom Blum; Shigemi Ohta; Andrew Pochinsky; Michael Engelhardt; Jeremy Green; Taku Izubuchi; Chulwoo Jung; Stefan Krieg; Meifeng Lin; Stefan Meinel; John Negele

Lattice QCD has recently achieved the point where realistic calculations of proton and neutron structure are possible. Such calculations are currently underway and their results will shed light on a number of outstanding puzzles about nucleon structure, among which are the origin of the proton spin and the more recent enigmatic discrepancy in the proton radius measurements. In addition, studying structure of the proton and the neutron is necessary to interpret experiments looking for physics beyond the currently accepted Standard Model of particle physics, which fails to explain the predominance of matter over antimatter in the Universe and the nature of the Dark Matter. Inherent numerical complexity of lattice QCD requires a combination of various stochastic noise reduction techniques. I will present initial results from one of the most sophisticated lattice nucleon structure studies so far, which incorporates chirally symmetric "Mobius Domain Wall" discretization of fermions directly at the physical point and discuss the outlook for the impact of these results on experimental programs.

Venkitesh Ayyar, *Duke University (USA)*
Semimetal-Insulator transition without a fermion bilinear condensate

Semimetal-Insulator transition arises when massless Dirac fermions become massive due to interactions through the mechanism of spontaneous symmetry breaking. In most cases this occurs when some fermion bilinear order parameter becomes non-zero in the insulator phase. Here, we explore the possibility of Dirac fermions acquiring a mass through interactions, but without such an order

parameter. We consider a staggered lattice fermion system on a cubical space-time lattice and introduce an on-site four-fermion interaction with coupling constant U . Using the symmetries of the system on the lattice, we can argue for the existence of massless fermions at small U . For very large values of U , we can argue that the fermions must become massive but without the formation of any fermion bilinear condensate. Monte Carlo results suggest that this simple picture extends to intermediate couplings where there seems to be a second order phase transition. We use finite size scaling techniques to extract the critical exponents at this transition.

Wednesday, Parallel Sessions 1, 13:30-15:15

Materials Science and Nanoscience 3

Caterina Cocchi, *Humboldt-Universität zu Berlin (Germany)*
From Molecules to Organic Crystals: Optical Excitations from First Principles
Co-Author: Claudia Draxl

Time-dependent (TD) density functional theory (DFT) is doing remarkably well in capturing the strongly bound excitons of isolated systems, even with the most simple exchange-correlation kernels, like the TD local density approximation (LDA). Though, due to a spurious long-range behavior, TD-LDA is known to fail in describing bound excitons in solids. Aiming at understanding when and why TD-DFT can be relied on, we compare this methodology with many-body perturbation theory (MBPT). To do so, we apply the most accurate approach to describe optical excitations, including the GW method and the Bethe-Salpeter equation. We systematically go from isolated molecules to their crystalline phase and perform an in-depth analysis of their absorption spectra, showing what governs the excitations when going from the molecule to the solid. In our study, we consider different systems, starting from small carbon-based molecules (e.g. methane) up to molecular materials such as oligothiophenes and azobenzenes, which are relevant for optoelectronic applications. Moreover, we analyze the influence of intermolecular orientation and interaction on the excitonic effects in these systems [1]. All the calculations are performed with the all-electron code "exciting" (http://exciting-code.org), where all the quantities entering the TD-DFT and MBPT formalisms are treated on the same footing [2].

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Rodion Belosludov, *IMR, Tohoku University (Japan)*
Computation Modelling of Thermodynamic Properties of Nanoporous Materials toward Gas Storage and Separation
Co-Authors: Oleg Subbotin; Vladimir Belosludov; Yoshiyuki Kawazoe

Theoretical model for calculating the thermodynamic properties of nano-porous materials with weak guest-host interactions was proposed for gas storage/separation applications. The proposed model accounted for multiple cage occupancy, host lattice relaxation, and the description of the quantum nature of guest behavior [1]. Using this approach, the phase diagrams of the pure and clathrate hydrates [2-3] were constructed and they are in agreement with available experimental data. In order to evaluate the parameters of weak interactions, a time-dependent density-functional formalism and local density technique entirely in real space have been implemented for calculations of vdW dispersion coefficients for atoms/molecules within the all-electron mixed-basis approach. The combination of both methods enables one to calculate thermodynamic properties of nano-porous materials without resorting to any empirical parameter fittings [4]. Using the combined approach it may not only confirm the existing experimental data but also predict the unknown region of thermodynamic stability of various nano-porous compounds with weak guest-host interactions. Recently, thermodynamic stability of ozone hydrates has been studied in a wide range of temperatures and pressures. It has been found that the stabilization of ozone in clathrate hydrates is useful for enrichment and long time storage of ozone without usage of carbon chlorines or fluorides. The formation of binary CH4-CO2 hydrate has been investigated at different gas phase compositions, pressures and temperatures using original thermodynamic approach. Equilibrium compositions of the formed hydrates have been determined as a function of the gas phase composition. The obtained results agree with the available experimental data. It was also demonstrated that carbon dioxide can replace methane in the hydrate phase at temperatures and pressures typical for the permafrost regions or below the seafloor.

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Stephanie Valleau, *Harvard University (USA)*
Electromagnetic study of the chlorosome antenna complex of Chlorobaculum tepidum
Co-Authors: Semion Saikin; Davood Ansari-Oghol-Beig; Masoud Rostami; Hossein Mossallaei; Alan Aspuru-Guzik

Green sulfur bacteria are an iconic example of nature’s adaptation: thriving in environments of extremely low photon density, the bacterium ranks itself among the most efficient natural light-harvesting organisms. The photosynthetic antenna complex of this bacterium is a self-assembled nanostructure, ≈60 × 150 nm, made of bacteriochlorophyll molecules. In this talk, I will discuss our recent study of the system from a computational nanoscience perspective by using electrodynamic

modeling [1]. Three different nanostructures, built from two molecular packing moieties, are considered: a structure built of concentric cylinders of aggregated bacteriochlorophyll d monomers, a single cylinder of bacteriochlorophyll c monomers, and a model for the entire chlorosome. The model is employed to extract optical spectra, concentration and depolarization of electromagnetic fields within the chlorosome, and fluxes of energy transfer for the structures. The second model nanostructure shows the largest field enhancement. Further, field enhancement is found to be more sensitive to dynamic noise rather than structural disorder. Field depolarization, however, is similar for all structures. This indicates that the directionality of transfer is robust to structural variations, while on the other hand, the intensity of transfer can be tuned by structural variations.

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Huan Tran, *University of Connecticut (USA)*

Designing Organotin Polymers For Energy Storage Applications

Co-Authors: Vinit Sharma; Rampi Ramprasad; Arun Mannodi-Kanakkithodi

Density functional theory (DFT) calculations suggest that polymers having tin atoms in their backbones may have high dielectric constants [1,2]. A class of organotin polymers, called tin esters, were then synthesized, realizing this prediction [3,4]. Motivated by this result, we developed a high-throughput screening scheme to quickly predict the desired performances for an energy storing dielectric, i.e high band gaps and dielectric constants. Our scheme is based on three essential components. The first component is a database of crystalline organotin compounds/polymers, built up from the low-energy structures which are either predicted by the minima-hopping method [5,6] or taken from the Crystallography Open Database [7]. The properties of these compounds, i.e., energies, band gaps, and dielectric constants, were calculated at the DFT level. Second, a fingerprint is carefully developed to capture the bonding environment of the examined crystalline compounds. Final, Kernel Ridge Regression model is used to quickly predict the desired properties of a compound/polymer solely from its fingerprint, given that the model is trained with the database of related materials. We describe the scheme and show that it works very well for organotin polymers as well as other related crystalline compounds.

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Sahar Sharifzadeh, *Boston University (USA)*
Understanding the Photophysical Properties of Organic Polycrystalline Films
Co-Authors: Leeor Kronik; Jeffrey Neaton; Cathy Wong; Hao Wu; Naomi Ginsberg

Organic semiconductors are a highly tunable class of optically active materials that are promising as next-generation photovoltaics. Utilizing these materials for efficient solar energy conversion relies on an understanding their excited-state electronic structure, i.e. how light absorption, charge transfer, and charge transport relate to the properties of their molecular components and are influenced by solid-state morphology. While many organic materials have varying degrees of disorder, crystalline films with long-range order provide an opportunity to understand many fundamental physical properties relevant to solar energy conversion. Here, we combine theory and experiment to investigate the nature of low-energy excitons within 6,13-bis(triisopropylsilylethynyl)-pentacene (TIPS-Pen) polycrystalline thin films. First-principles many-body perturbation theory and optical absorption spectroscopy on ordered domains reveal multiple low-energy absorption peaks that are composed of delocalized excitonic states. Moreover, comparison of predicted and measured angle-resolved absorption spectra reveals the exact inter-grain orientation within measured films. We discuss the implications of this study for understanding exciton dynamics as measured by spatially-resolved transient absorption spectroscopy. This work was supported by the Department of Energy and computational resources were provided by the National Energy Research Scientific Computing (NERSC) Center.

Ilnur Saitov, *Joint Institute for High Temperatures (Russia)*
First principle calculation of shocked xenon reflectivity
Co-authors: Vladimir Stegailov, Genri Norman

The reflectivity of shocked xenon was measured in the unique experiments of Mintsev and Zaporoghets in 1989 for wavelength &lambda = 1064nm [1] and further for 694nm and 532nm [2]. There is no theoretical explanation of these results in frames of the standard methods of nonideal plasma theory. In [3] it was shown that the Drude model, with collisional frequency in Born approximation, gives reflectivities that are 2.5 – 3 times larger than the experimental values at low densities. The results of other approaches to the collision frequency calculation also can not provide better explanation of steep slope of reflectivity drop with decreasing of density. In [3] the assumption of significant width to the shock front gives a good agreement with the experimental data. However, there are no experimental evidences of this effect. The reflectivities of shoked xenon, calculated by Desjarlais [4], were obtained in frames of the approach of density functional theory. Kubo-Greenwood formalism was used for calculation of the optical properties. In comparison with [3] in [4] shock has an ideal step profile. The approach, used in this work, is approximately the same with method in [4]. In the density functional theory framework the values of reflectivity coefficient from shocked xenon plasma are calculated. Their dependencies on the incident radiation frequency and the plasma density are considered. The Fresnel formula is used. In contrast to [4] the expression for the longitudinal component of the dielectric tensor

in the long wavelength limit is used for calculation of the imaginary part of the dielectric function [5]. The real part of the dielectric function is determined by means of the Kramers-Kronig transformation. The agreement of obtained results in this work with experimental data [1, 2] is better than in [4]. An approach for calculation of the plasma frequency in the shocked xenon is proposed.

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Statistical Physics 4: Spin Models

Koji Hukushima, *University of Tokyo (Japan)*
Equilibrium-state simulations of some (spin) glass models in finite dimensions

Mean-field theory of spin glasses has provided a number of novel concepts for understanding of a phase transition in disordered glassy systems. In particular, replica-symmetry breaking (RSB) plays an essential role in describing complex free-energy structure. It turns out that the pattern of RSB is clarified into two distinct classes, full RSB and one-step RSB. Despite extensive studies including large-scale numerical simulations, no conclusion has been reached about the issue whether the RSB concepts survive in short-ranged spin-glass models in finite dimensions. In recent years, some mean-field spin-glass models with the one-step RSB have attracted much attention of many researchers. These models are regarded as a prototype of a phenomenological picture of structural glass transition, called random first-order transition (RFOT), which is characterized by a thermodynamic transition with a discontinuous order parameter without latent heat. The advisability of the RSB picture in finite dimensional spin glass models comes to an issue again in the context of the structural glass transition. In this talk, we present some results of large-scale Monte Carlo simulations based on extended ensemble method for lattice glass model and Potts-glass model in finite dimensions. Our findings for the latter are fully compatible with those expected from the RFOT picture based on the one-step RSB.

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An extended ensemble Monte Carlo study of a lattice glass model,
K. Hukushima, S.Sasa, J. of Phys.: Conf. Ser., 233, 012004 (2010).

Wenlong Wang, *University of Massachusetts, Amherst (USA)*
Population annealing Monte Carlo: An effective simulation for spin glasses
Co-Authors: Jonathan Machta; Helmut Katzgraber; Burcu Yucesoy

Systems with rough free energy landscapes such as spin glasses are difficult to simulate using conventional Monte Carlo methods. Population annealing is a Monte Carlo method for sampling the equilibrium states of systems with rough free energy landscapes. I will introduce the algorithm and then present simulation results for the three-dimensional Edwards-Anderson model. I will discuss the strengths and weaknesses of population annealing compared to parallel tempering (the standard method for simulating spin glasses) and also compare population annealing to simulated annealing for finding ground states.

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Tasrief Surungan, *Hasanuddin University (Indonesia)*

Spin glass behavior of the antiferromagnetic Heisenberg model on scale free network

The study of spin glasses (SG's) has been an active research field for the last three decades. The importance of the systems lies in the fact that they have some significance not only for other parts of physics, but also for such fields as computer science, mathematics and biology, including many technological applications. They are a class of random magnets with rich physical properties, such as infinite number of ground states, memory effect and aging phenomena. Random frustration is considered to be the key ingredient for the existence of SG behavior. It is realized by the presence of both ferromagnetic (FM) and antiferromagnetic (AF) interactions in regular lattices. We previously observed spin glass behaviour of the antiferromagnetic Ising model on scale free network (SFN)[1]. It is a new type of spin glass systems, different from the canonical ones which requires random distribution of ferromagnetic and antiferromagnetic interactions. Here we study spin glass behavior of Heisenberg spin models with AF interaction on SFN. The canonical spin glass Heisenberg model is not observed in the d-dimensional regular lattices for ($d \leq 3$)[2]. We can make an analogy for the connectivity density C of SFN with the dimensionality of the regular lattice. It should be plausible to find the critical value of C for the existence of SG behaviour, analogous to the lower critical dimension (d_l) for the canonical SG systems. We used Replica Exchange algorithm of Monte Carlo Method and calculated the SG order parameter. We observed low temperature SG behavior and estimated the critical temperature and exponents.

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Elmar Bittner, *ITP, Heidelberg University (Germany)*
MuCa vs WL: A tight race
Co-Author: Wolfhard Janke

We perform a competitive analysis to study the relative performance of the two best-known generalized-ensemble algorithms: the multicanonical Monte Carlo and the Wang-Landau method. To keep things as simple and clear as possible, we take the exactly solvable two-dimensional Ising model as test case and we show also some results for the three-dimensional Ising model.

Alexandra Valentim, *Universidade Federal do Paraná (Brazil)*
Exploring Replica-Exchange Wang-Landau sampling in higher-dimensional parameter space
Co-Authors: Shan-Ho Tsai; Ying Wai Li; Carlos Eduardo Fiore Dos Santos; Markus Eisenbach; David P. Landau

The Wang-Landau (WL) Monte Carlo method [1] has the property of generating a flat histogram in some random walk space, where the parameters for the random walk and the flatness criterion can be chosen according to the system of interest. Due to these characteristics and to the simplicity of the algorithm, the WL approach has been applied to different kinds of systems [2-5], including those with rough free energy landscapes and strong first-order phase transitions. Recently a parallel approach based on this method, namely, Replica-Exchange Wang-Landau (REWL) sampling [6] was proposed and has been shown to scale well up to several thousands of computing processors in different applications. This generic scheme combines the advantages of WL sampling, replica exchange and true parallelism. The WL method has also been successfully used in simulations that require a random walk in a higher-dimensional parameter space [3,4], but the viability of the REWL has not been explored yet. The simulations in the higher-dimensional parameter space are more challenging because phase space can display empty regions with no realizable configurations, and the convergence of the algorithm will depend strongly on how the ranges of parameters are split. We started to look at this direction by implementing the REWL method for the 2D Ising model using a random walk in energy and magnetization space, and compare the splitting of the phase space using segments with different geometries. Previous work [4], in which a similar scheme of parallel simulation was implemented without allowing replica exchange between overlapping subwindows and with a different way to combine the density of states pieces, led to discontinuities in the final density of states over the entire range of parameters. From our results, it appears that the REWL algorithm is able to overcome this difficulty, and we expect that an adaptive subwindows approach will help to better sample the edges of the configuration space.

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Raul Toral, *Institute for Cross-Disciplinary Physics and Complex Systems (Spain)*
Weighted-ensemble Brownian dynamics simulation: Sampling of rare events in non-equilibrium systems
Co-Authors: Justus Kromer; Lutz Schimansky-Geier

Rare events are ubiquitous in many biological, chemical and physical processes. Whereas the density of states is known in systems at thermal equilibrium, interesting phenomena often occur in non-equilibrium systems. Computer simulations are widely used to estimate the density of states or transition rates between them. As Brownian dynamic simulation provides computational costs that are inversely proportional to the state's probability, one needs to use specialized methods to sample adequately states with low probability or low transition rates. We have developed an algorithm based on the previously developed weighted-ensemble (WE) Brownian dynamics simulations that allows one to calculate the stationary probability as well as transition rates between particular states. The space of interest is divided into several regions and the probability for finding the system in them is calculated by generating equally weighted walkers in each region. By moving to the underlying dynamics, the walkers transport probability between the regions. Our algorithm, based on WE Brownian dynamic simulations, uses a uniform distribution of walkers within each region. It outperforms Brownian dynamics simulation by several orders of magnitude and its efficiency is comparable to weighted-ensemble Brownian dynamic simulations in all studied systems and lead to impressive results in regions of low probability and small rates. As a check of the efficiency of the method, we have computed numerically the stationary probability distribution for the classic double well potential and verified Kramer's law for the probability current. In both cases we obtain an astounding precision as we are able to sample states whose probability is of the order of 10^{-300} and compute currents of the same order. We apply this technique to cases for which no exact results are known as the bistable potential under the presence of colored noise and the stochastic FitzHugh-Nagumo system in the excitable regime.

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Astrophysics 1: Cosmology and Galaxy Formation

Mike Boylan-Kolchin, *University of Maryland (USA)*
The Local Universe as a Dark Matter Laboratory

The standard cosmological model, which posits that the energy content of the Universe is dominated by two mysterious components (dark matter and dark energy), has been very successful on large cosmological scales. On galactic and sub-galactic scales, however, a number of potential issues have arisen; these issues may point to new fundamental physics or to previously unappreciated processes in galaxy formation. I will review how we are using the Local Group of galaxies to probe the nature of dark matter, highlighting the essential role that numerical simulations are playing in current studies. I will also describe the computational challenge of modeling various different models of dark matter, along

with the potentially revolutionary implications for the standard model of particle physics if clear signals of non-standard dark matter physics can be found.

Claude-andre Faucher-Giguere, *Northwestern/CIERA (USA)*
The Universe on a computer: Cosmological simulations of galaxy formation

Cosmological simulations start from Big Bang initial conditions and simulate a representative volume of the Universe to the present time. They follow the dynamics of dark matter, stars, and gas and have been very successful at explaining the large-scale structure that we measure in the distributions of galaxies and intergalactic gas across cosmic time. Due to finite resolution and an incomplete set of physical processes, these simulations have however struggled to produce realistic galaxies on small scales. I will discuss our group's efforts to dramatically improve the predictive power of cosmological simulations by explicitly resolving the internal structure of simulated galaxies and the "feedback" processes from stars and black holes that affect the formation and evolution of galaxies (the FIRE project). I will highlight some of the computational limitations of our current work, and emphasize how progress has not only been enabled by improved computational tools but also by a better understanding of the most important physics.

Claudio Gheller, *CSCS (Switzerland)*
Numerical cosmology on the GPU with Enzo and Ramses
Co-Authors: Romain Teyssier; Franco Vazza; Markus Wetzstein; Peng Wang

The availability of general purpose GPUs has made possible their effective usage for scientific computing. Many codes can now run on GPUs with remarkable performance. In astrophysics, Enzo[1] and Ramses[2] are prime examples of such applications. Both are Adaptive Mesh Refinement (AMR) multi-species codes, designed to describe the evolution of cosmological structures, galaxies, gas clouds etc. The AMR approach provides high spatial resolution only where this is actually required, thus ensuring minimal memory usage and computational effort. Different AMR techniques have been adopted by the two codes, namely Structured AMR by Enzo and Fully Threaded Tree by Ramses. They pose different major challenges for parallel implementation. The two codes have been ported to GPUs adopting different strategies (driven by the AMR approach) and programming models, Enzo exploiting CUDA and Ramses using OpenACC. The different solutions used for the GPU refactoring will be described and the most relevant solutions for each implementation discussed. A number of benchmarks comparing the GPU and the CPU versions of the codes will be presented, highlighting the enhancements obtained with the refactoring and pointing out the main factors currently limiting further performance improvements.

Enzo's GPU implementation is currently used in a project within the CHRONOS programme[3], supporting high-end computational physics applications running on the Piz Daint HPC system at ETH CSCS. Such system provides 7.8 PFlops peak performance by means of more than 5000 GPU equipped computational nodes. The project aims at studying the origin and evolution of the magnetic field within large-scale structures and the possibility of detecting effects related to the early seeding of the cosmic

magnetic field at the scale of cosmic filaments and in the outskirts of galaxy clusters by means of a number of high resolution magneto-hydrodynamic simulations. The preliminary results of the project will be discussed.

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Robert Hohlfeld, *Boston University (USA)*
Instability of Counterrotating Flow in an Astrophysical Disk
Co-Author: Richard Lovelace

We use an N-body simulation, constructed using GADGET-2, to investigate an accretion flow onto an astrophysical disk that is in the opposite sense to the disk's rotation. In order to separate dynamics intrinsic to the counter-rotating flow from the impact of the flow onto the disk, we consider an initial condition in which the counter-rotating flow is in an annular region immediately exterior the main portion of the astrophysical disk. Such counterrotating flows are seen in systems such as NGC 4826 (known as the "Evil Eye Galaxy"). Interaction between the rotating and counterrotating components is due to two-stream instability in the boundary region. A multi-armed spiral density wave is excited in the astrophysical disk and a density distribution with high azimuthal mode number is excited in the counterrotating flow. Density fluctuations in the counterrotating flow aggregate into larger clumps and some of the material in the counterrotating flow is scattered to large radii. Accretion flow processes such as this are increasingly seen to be of importance in the evolution of multi-component galactic disks.

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Ke-jung Chen, *University of California, Santa Cruz (USA)*
Cosmic Impact of the First Binaries

We present the cosmological simulations of impact of the first binaries. Recent studies of the first star formation suggest that those stars tend to form into binaries or multiple stellar systems instead of single stars, so the first stars could be less massive than we originally thought. It implies the first stars would die as score collapse supernovae instead of pair-instability supernovae, both of them are very different in nucleosynthesis yields and explosion energies. We use the well-tested massively- parallel combined

N-body and smoothed-particle hydrodynamics code Gadget-2, modified to include detailed cooling, chemistry, and radiative transfer of primordial gas to study the impact of the first binaries. We take realistic Pop III stellar models and their nucleosynthesis products as initial inputs for our cosmological simulations and trace the transport of supernova metals that can significantly affect the chemical enrichment in the primordial intergalactic medium. In this talk, we discuss the impact of the first binaries to the early Universe and their observational signatures for the forthcoming James Webb Space Telescope.

Quantum Many-Body Physics 3

Tao Xiang, *Institute of Physic*s, Chinese Academy of Sciences (China)
Renormalization of quantum many-body systems by the projected entangled simplex states
Co-Authors: Zhiyuan Xie; Jing Chen; Jifeng Yu; Xin Kong; Bruce Normand

We propose a new class of tensor networkstates, named as projected entangled simplex states (PESS), for studying ground state properties of quantum lattice models. It extends the pair correlation in the projected entangled pair states (PEPS) to a simplex. The PESS is an exact repre-sentation of the so-called simplex solid states and an efficient trial wavefunction that satisfies the area law of entanglement entropy. We introduce a simple update renormalization method for evaluating the PESS wavefunction based on the higher order singular value decom-position of tensors under the framework of imaginary time evolution. By applying it to the spin-1/2 Heisenberg model on the Kagome lattice, we obtain an accurate result for the ground state energy, which agrees with other numerical calculations and sets a new upper bound for the ground state energy.

Corinna Kollath, *University of Bonn (Germany)*
Spreading of correlations in strongly correlated (dissipative) quantum gases

Atomic gases cooled to Nanokelvin temperatures are a new exciting tool to study a broad range of quantum phenomena. In particular, an outstanding and rapid control over the fundamental parameters, such as interaction strength, spin composition, and dimensionality allows to realize and observe many different situations far from equilibrium. One of the fundamental questions is the spreading of correlations under the change of a parameter of the system as e.g. the interaction strength. In one-dimensional systems often the correlations are carried by quasi-particle excitations which propagate almost ballistically through the system. We will present results of such a propagation after an abrupt parameter change in comparison with experimental results. We extend the investigation to a slow change of a parameter where the spreading dynamics takes a generalized 'light-cone' form. Further, I will contrast the spreading in an isolated system to the spreading in systems subjected to dissipative couplings. One focus will be the question of how in a repulsively interacting fermionic gas, coherence between pairs of fermions can emerge by local coupling to an incoherent environment. The numerical results are obtained with the time-dependent density matrix renormalization group (or matrix product state) methods and the application to dissipative systems will be outlined.

Chisa Hotta, *University of Tokyo (Japan)*
Grand canonical analysis in one and two dimension: A route to measuring bulk properties in an applied field
Co-Authors: Satoshi Nishimoto; Naokazu Shibata

"Grand canonical numerical analysis" is a technique we recently developed for quantum many-body systems to efficiently obtain the bulk physical quantities without employing a finite size scaling[1,2]. Its procedure is simple enough; preparing an open system typically of length L>10, and by systematically scaling down the Hamiltonian from center toward both ends, one could endow the role of small particle bath to the edge sites with a negligibly small energy scale. In the lowest energy solution of this deformed Hamiltonian, the particles on the cluster are self-organized to tune the particle number near the system center to their thermodynamic limit by using the “edges” as a buffer.

We show several examples of one- and two-dimensional quantum spin systems where the bulk magnetization curve is obtained within the accuracy of 10-3$-10-4. In the case of two-dimension, we also comment on the importance of keeping the aspect ratio of the systems closer to unity in order to properly reproduce the true two-dimensional quantities[3].

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Adrian Del Maestro, *University of Vermont (USA)*
A quantum Monte Carlo method to compute entanglement entropies of interacting bosons in the spatial continuum

We present a scalable algorithm for computing Rényi entanglement entropies in systems of itinerant bosons in the spatial continuum via quantum Monte Carlo. This method is applicable to the study of spatial mode entanglement, particle partitioned entanglement, and the entanglement of particles under a spatial partitioning. We demonstrate its utility by studying a non-trivial interacting Bose gas in one spatial dimension where we uncover a logarithmic scaling of the entanglement entropy in the number of particles and confirm bounds on it related to the experimentally measurable condensate fraction. For the first time, this method opens up the numerical study of quantum correlations in experimentally relevant quantum fluids such as helium-4 and cold atomic gases.

Edwin Stoudenmire, *Perimeter Institute (Canada)*
Corner Contributions to Entanglement Entropy in Critical Systems
Co-Authors: Roger Melko; Ann Kallin; R.R.P. Singh; Paul Fendley

Because of their scale invariant nature, critical systems in two dimensions can harbor universal terms in their entanglement entropy depending on the geometry of the cut between the entangled subsystems.

For certain special systems, the coefficient of a term associated with a sharp corner geometry has been found to roughly count the number of bosonic fields, similar to the central charge of a 1+1 conformal field theory. While this corner term is difficult to compute directly with most numerical approaches, the numerical linked cluster method can access it naturally. By using the density matrix renormalization group as the cluster solver, we are able to go to higher orders than previously possible, and find strong evidence supporting the analogy between the corner coefficient and the 1+1d central charge.

Wednesday, Parallel Sessions 2, 15:45-17:30

Materials Science and Nanoscience 4

Volodymyr Turkowski, *University of Central Florida (USA)*
Development and application of DFT+DMFT and TDDFT+DMFT techniques for nanosystems
Co-Author: Talat S. Rahman

We have developed computational approaches to examine ground state properties, excitations and nonequilibrium response of strongly correlated nanostructures. The algorithm is based on merging Dynamical Mean-Field Theory (DMFT) with both Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TDDFT). The DMFT approach has already been established as a reliable tool to study correlation effects in terms of effective model Hamiltonians (Hubbard-type). It has also been successfully combined with DFT for calculations of the static properties of strongly correlated extended systems. The main element of the success of the theory is based on its ability to describe effects of dynamical fluctuations, missed in DFT+U and other approaches. These effects are, however, crucial for cases in which the local Coulomb repulsion energy U and the kinetic energy of the electrons are comparable, as found most often in correlated materials. Our recent extension of DFT+DMFT to nanosystems [1] demonstrates the feasibility of the method and shows that magnetic properties of 10-100-atom transition-metal structures can be obtained with computational cost comparable to that of standard DFT calculations. We have further generalized the approach to time-dependent cases by deriving the DMFT expression for the key element of the TDDFT theory - exchange-correlation kernel [2], and applied it to several bulk and nanoscale systems in which we expect electron correlations to play an important role: $YTiO_3$, Ce, Ce_2O_3 and VO_2. We demonstrate that contrary to standard TDDFT, our approach is capable of describing correctly the excitation spectrum as well as nontrivial nonequilibrium response of correlated systems. Technical simplicity and physical transparency of our proposed methods allow their extension to systems containing few hundred atoms in complex environment. The details of the techniques and their application to nanoscale systems will be discussed in the context of available experimental and other theoretical results.

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Kenichi Asano, *Osaka University (Japan)*
Trions and Biexcitons in Semiconducting Single-Wall Carbon Nanotubes

In low-dimensional semiconducting systems, the exciton binding energies are significantly enhanced by the confining effect. Typical examples are found in ideal one-dimensional semiconductors, the single-wall carbon nanotubes (SSWCNs). In these systems, also trions and biexcitons are expected to have large binding energies. Although the enhanced stability of trions and biexcitons had been observed in previous theories, the difference between the SSWCNs and usual quantum wire systems on the semiconductor heterostructures had not been clarified. This was because the model used there was oversimplified and all the important features of the carbon nanotubes were missing, which are the strong nonparabolicity of energy bands, the form factors in the interaction potential, the interband screening effects, and the self-energy corrections.

Here, by including all of the above mentioned features of SSWCNs, we evaluate the binding energies and the wave functions of trions and biexcitons. It is found that the binding energies are suppressed by the interband screening and the form factor effects. Since this suppression works more effectively on the biexcitons than on the trions, the binding energies of the trions exceed those of the biexcitons, which is never seen in the usual quantum wire systems.

Previous theories adopted some variational wave functions or diffusion Monte Carlo methods. We instead applied the Lanczaos method to this problem for the first time; in taking into account the band nonparabolicity and the form factors in the interaction potential, an extra numerical difficulty arises, that the Hamiltonian should be represented in the momentum space. We present a technique dveloped here to store this complicate matrix in a limited memory size and to accelerate the matrix multiplication on the vector.

References
[1] Kouta Watanabe and Kenichi Asano, Physical Review B 83, 115406 (2011).
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Georgios Tritsaris, *Harvard University (USA)*
On the possibility of photocatalytic water splitting on rutile TiO2(110): a theoretical study
Co-authors: Dmitry Vinichenko, Grigory Kolesov, Efthimios Kaxiras

Solar-based hydrogen production by photocatalytic water splitting offers a route towards the delivery of clean fuel. Semiconductor metal oxides have been typically employed to mediate the photon-induced catalytic process but a comprehensive description of the elementary reaction pathways and charge-carrier dynamics is largely lacking even for the widely used TiO2. We performed Ehrenfest molecular dynamics within the framework of time-dependent density functional theory to assess the possibility of water oxidation by photogenerated hole on rutile TiO2. We find that molecular water adsorbed on a

clean TiO2(110) surface readily dissociates under extreme ultraviolet irradiation, and that dissociation on defect-containing surfaces could be thermally assisted under weaker excitation.

References
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David A. Strubbe, *Massachusetts Institute of Technology (USA)*
Photoisomerization dynamics of solar thermal fuels with TDDFT excited-state forces
Co-authors: Jeffrey C. Grossman

Solar thermal fuels (STFs) are an unconventional paradigm for solar energy conversion and storage which is attracting renewed attention. A material absorbs sunlight and stores the energy chemically via an induced structural change, which can later be reversed to release the energy as heat. Two important factors for STFs are the absorption cross-section and the quantum yield for photoisomerization. We employ massively parallel time-dependent density-functional theory (TDDFT) calculations with the Octopus real-space code [1] to obtain the optical absorption and follow the structural changes after absorption for candidate STF molecules such as azobenzene and norbornadiene/quadricylcane. We use our new excited-state forces formulation for TDDFT in the Casida or Tamm-Dancoff approaches, which is based on density-functional perturbation theory and does not require any additional sums over unoccupied states. Our results show the photoisomerization mechanism in these molecules, to aid in further improvement of STF materials by functionalization and attachment to templates [2,3].

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Iskakova Kulpash, *Kazakh National Pedagogical University (Kazakhstan)*
The modeling of the energy levels GaAs
Co-authors: Aisara Amanova, Rif Akhmaltdinov

In the simulation and calculation of the energy A3B5 compounds vary from the amount and spatial orientation. Depending on the number of cores in the cluster and their spatial arrangement of the energy changes periodically with different amplitudes. The arrangement of groups of atomic cores in different directions of space subjects to certain laws of a series. In various directions of the arrangement of the atomic cores appear parallel intersecting spaces. The real images of these spaces are antisymmetric to the spaces of atomic core. If the law of a number of numerical arrangements of the atomic cores is characterized by integer coordinates, the components of the atomic arrangement of the planes are described by fractional coordinates. In figure 1 is shown the spatial arrangement of GaAs with 918 atomic core. The violation of uniformity arises after a group of 918 atoms.
In the simulation of the energy levels, taking into account the screening of individual atoms packed on these segments of the wave vectors observed uniform behavior of the wave vectors. The calculation

shows that if we consider separately space clusters of atomic cores and interatomic space, behavior of last of the wave vector will go on smooth periodic functions. We observed quasiperiodic change in the difference. At the border radius of coverage this periodicity is broken. At increasing the radius of coverage this periodicity is restored to the previous radius, but it is broken on the new range. Thus, boundary conditions lead to a violation of the periodicity. We simulated these regularities of the lattice. The figure 1 shows the four first neighbors of As in the lattice. The neighboring ions Ga (blue) form a tetrahedron with the center of As (red). The boundary atoms can approximately account for modeling the interface of the quantum dot with the matrix.

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Bin Hwang, *Michigan State University (USA)*

Effective transient states for nonequilibrium systems under ultrafast control pulses

Co-authors: Prof. Phillip Duxbury, Jenni Portman, Mr. Ersoy Edward

We investigate the transient states in nonequilibruim time-dependent systems. Intense ultrafast laser pulses allow the preparation of transient states of matter exhibiting strong non-equilibrium between electrons and lattice. By controling the laser pulse, we are able to change the transient states of these quantum systems. The optical and structural properties as well as the temporal evolution of such states provide insight into the mutual dependence of electronic and atomic structure. We approach the problem by showing examples from charge-density-wave systems and model two level systems. In both of these, nonequilibrium techniques can be used to qualitatively describe the common short-time experimental features. Through simulations based on non-equilibrium Green's function formalism and time dependent master equations approaches we show how to achieve effective transient states for nonequilibrium systems under ultrafast control pulses.

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Novel Computing Paradigms 3

Norbert Attig, *Julich Supercomputing Centre (Germany)*
The Path to Exascale: A European Perspective

Recent developments in supercomputing are reviewed covering both the latest hardware trends and the increasing difficulties faced by scientists in utilising these machines to perform large-scale numerical simulations. The role of one of the major European players in supercomputing, the Julich Supercomputing Centre (JSC) in Germany is described in this context. Since 1986 the primary mission of JSC has been the provision of supercomputing capacities of the highest performance class to the scientific and engineering research communities at national and European universities and research institutions [1].

With the increasing prevalence of architectures based on massively parallel and multi-core processor topologies, simulation scientists are now compelled to take scalability into account when developing new models or when porting long-established codes to new machines. To meet this challenge, JSC has pioneered the introduction of community-oriented support units for scientific computing, so called Simulation Laboratories. Progress in establishing these units and first success stories are reported on [2].

Besides its efforts in strengthening the computational sciences, JSC is actively investigating future architectures and their application, primarily in cooperation with hardware vendors. Since 2010, JSC has established joint Exascale Laboratories with IBM, Intel, and NVIDIA, to give such collaborations a more formal framework with binding resource commitments, multi-year work plans, and agreements on intellectual property rights. First-hand experiences with this new kind of collaboration and some highlights are presented [3].

Finally, an outlook is given of the most challenging requirements of applications in the near future and how applications should evolve over the next few years to profit most from Exascale developments.

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[3] http://www.fz-juelich.de/ias/jsc/EN/Research/HPCTechnology/ExaScaleLabs/_node.html

Lars Korsterke, *Texas Advanced Computing Center (USA)*
Heterogeneous computing. What is it and do we need it?

Heterogeneous computing promises more compute power while consuming less energy. However employing GPUs and Xeon Phi's come with a hefty price tag. Only software that is highly adapted to these new architectures will gain any performance increase. In my talk I will address these questions:
* What is heterogeneous computing?
* How can it help producing better results faster?

* Is it worthwhile exploring for the broader audience?
And finally I will try to shed some light on the question whether the future will really be heterogeneous or not.

Feng Chen, *Brown University (USA)*
GPU Spectral Method and Stable Parareal Method for Large-scale Computational Science

Large-scale problems in scientific simulation and data analysis lead to high computational costs in both spatial and temporal dimensions. There is an increasing demand of new mathematical algorithms scalable on modern supercomputing architectures for this growing complexity. However, the global nature in space and the sequential nature in time pose a great challenge for the parallelization of related algorithms. In this presentation, we first discuss recent efforts to develop GPU-suited spectral methods for advanced applications in computational physics. We introduce a decoupling strategy that maps spectral methods to the Nvidia CUDA programming model. We then introduce the parallel-in-time approach to break the sequential bottleneck of the time direction. Motivated by the instability of the original parareal method for wave problems, we propose an adjoint parareal method and a reduced basis parareal method. We outline the theoretical ideas behind these new parareal methods and discuss their robustness and efficiency.

Throughout the presentation we shall illustrate the performance with computational examples in order to highlight the major advantages of the proposed approach. In the end of the talk, we shall mention future work and challenges associated with large-scale scientific computing. Part of the work is done in collaboration with Jan Hesthaven (EPFL & Brown), Yvon Maday (Paris IV & Brown), and Jie Shen (Purdue).

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Patrick Dreher, *North Carolina State University (USA)*
Proof of Concept Implementation of a Cloud Computing Infrastructure within a Supercomputer Architecture
Co-authors: Mladen Vouk, Georgy Mathew, William Scullin

Traditional high performance computing is capable of focusing tremendous amounts of sustained state-of-the-art computational resources onto physics applications over extended periods of time using batch style operating environments. In addition to this mode of HPC, there is an increasing demand for more complex workflows that involve large fluctuations in the levels of HPC physics computations required at

various times during the calculations. Some of the workflow components may also require richer environments of operating system features and schedulers than normally found in a batch oriented HPC environment. In this paper a proof of concept design is described that rearranges access to the nodes on both an IBM BG/P using the Kittyhawk utility and on IBM BG/Q platform using a FusedOS. Both platforms use the Virtual Computing Laboratory as the cloud computing system that is embedded within the supercomputer. This design and implementation allows a cloud to be configured so that it can capitalize on the specialized infrastructure capabilities of a supercomputer without resorting to virtualization while simultaneously also providing the flexibility in the software stack, schedulers, workflows and on-demand HPC supercomputer resources levels normally only found in a cloud architecture. These types of user reconfigurable environments have been created on the IBM Blue Gene/P and Blue Gene/Q supercomputers at the Department of Energy's Argonne Leadership Computing Facility (ALCF). Beyond the novelty of constructing such a system, these new prototype HPC cloud computing systems allow for the possibility of experimentation with new schedulers and operating systems within a working HPC environment that may be different from the native OS and schedulers on the HPC supercomputer itself. These customized HPC Cloud Computing designs may have applicability across a wide range of HPC computational physics domains, applications and cloud bursting needs and requirements.

Charles Still, *Lawrence Livermore National Laboratory (USA)*
Estimating the Impact of Future Advanced Architectures on ASC Multiphysics Codes
Co-Authors: Christopher J. Clouse, Ian Karlin, J. Robert Neely, Brain S. Pudliner, Michael R. Zika

There have been three distinct eras in High Performance Computing, the mainframe era, the vector era, and the distributed memory era. Each period brought lessons that are largely relevant today as we consider future architecture technology. While the emerging era builds on the previous ones, it is strikingly different from them in the computational characteristics imposed on physics algorithms. Specifically, the drive for more energy efficiency, which ultimately can lead to extreme scale computing, ushers in a paradigm shift: algorithm (and code) performance is no longer dominated by the rate at which floating point operations can be performed (FLOPS). Instead, computations are limited by factors such as memory motion, locality and overall concurrency.

There exist very large multiphysics codes modeling many areas of science and engineering, such as Inertial Confinement Fusion, High---Energy Density physics, and structural engineering. A multiphysics code can integrate more than a dozen tightly coupled physical models operating at disparate spatial and temporal scales, carefully balanced to ensure accuracy, and comprising more than one---million lines of source code. These codes have very long development cycles, and correspondingly long life---spans, and are particularly challenged by the looming paradigm shift.
In this presentation, we discuss some of the emerging advanced architectures, their characteristics, the impact on several physics models, and conclude with an example from Arbitrary Lagrangian Eulerian (ALE) Hydrodynamics using the proxy application LULESH.

Quantum Computing 1

David Clader, *Johns Hopkins University (USA)*
Preconditioned quantum linear system algorithm
Co-Author: Bryan Jacobs, Chad Sprouse

We describe a quantum algorithm that generalizes the quantum linear system algorithm [Harrow et al., Phys. Rev. Lett. 103, 150502 (2009)] to arbitrary problem specifications. We develop a state preparation routine that can initialize generic states, show how simple ancilla measurements can be used to calculate many quantities of interest, and integrate a quantum-compatible preconditioner that greatly expands the number of problems that can achieve exponential speedup over classical linear systems solvers. To demonstrate the algorithm's applicability, we show how it can be used to compute the electromagnetic scattering cross section of an arbitrary target exponentially faster than the best classical algorithm.

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Bryan Clark, *University of Illinois at Urbana Champaign (USA)*
The cost of simulating quantum mechanics on a quantum computer
Co-author: Dave Wecker, Bela Bauer, Matthew Hastings, Prof. Matthias Troyer

One of the most commonly suggested applications for a quantum computer is simulating quantum systems. Although clearly promising in the limit of large quantum computers, we explore whether quantum simulations are a practical application area for small quantum computers. We show that, at least for the application of quantum chemistry, the standard algorithms in the worst case require significantly more resources then can be envisioned in the near-term. We discuss the potential way forward including recent suggestions for how to improve this situation and whether the worst case scenarios apply.

Boixo Sergio, *Google (USA)*
Experiments with the DWave prototype
Co-author: Troels Roennow, Mark Dykman, Masoud Mohseni, Mohammad Amin, Alireza Shabani, Hartmut Neven, Zhihui Wang, Joshua Job, Sergei Isakov, David Wecker, John Martinis, Daniel Lidar, Matthias Troyer, Vadim Smeltanskiy

Quantum annealing is an optimization method designed to take advantage of quantum phenomena, such as quantum superposition, tunneling and quantum fluctuations. Diabatic transactions between energy levels, and thermal excitations and relaxation, can play an important role in quantum annealing (as opposed to adiabatic quantum computation). DWave has implemented a physical quantum annealing prototype with up to 512 qubits. The decoherence time scale in this device is much shorter

than the annealing time. I will review recent work done in this prototype. On the one hand, we find evidence of entanglement within eight superconducting flux qubits. On the other hand, we find no evidence of a quantum speedup for the case of random Ising glasses when the entire data set is considered, and obtain inconclusive results when comparing subsets of problems on an instance-by-instance basis. I will present preliminary new results and theory comparing noisy quantum annealing, the DWave prototype, and several numerical models.

Jonathan Moussa, *Sandia National Labs (USA)*
Maximum entropy quantum simulation

A common goal of quantum simulation and quantum computation is the controlled unitary evolution of a quantum state with errors that are known and small. However, it is often the case that control is limited and errors are unknown and possibly large. We consider the case where a large ensemble of identical systems is available and measurements on one subset of systems are used to inform the control of another subset to apply limited error correction. This is based on monitoring a set of expectation values and enforcing the instantaneously exact evolution of predictable values while applying maximum entropy reconstruction to unpredictable values. The reconstruction is efficiently approximated by maximizing an entropy estimator based on known expectation values. This is a dynamic generalization of existing static methods for free energy calculations based on optimization constrained by consistency of expectation values. We study new entropy estimators and apply maximum entropy evolution to quantum simulation of spin chains and quantum computation of the Grover search algorithm.

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Debasish Banerjee, *ITP, Uni Bern (Switzerland)*
Measurement driven quantum dynamics
Co-authors: Uwe-Jens Wiese, Fu-Jiun Jiang, Mark Kon

Real-time evolution of large-scale quantum systems remain a formidable challenge to address theoretically. Studies with numerical simulations are hindered by the sign problem. The effect of measurements on the quantum system will then be considered, and to what extent it helps to simplify the problem. As a concrete example, we consider a large quantum system with spins $\frac{1}{2}$ whose dynamics is driven entirely by measurements of the total spin of spin pairs. This gives rise to a dissipative coupling to the environment. When one averages over the measurement results, the corresponding real-time path integral does not suffer from a sign problem. Using an efficient cluster algorithm, we study the real-time evolution of a 2-d Heisenberg antiferromagnet, which is driven to a

disordered phase, either by sporadic measurements or by continuous monitoring described by Lindblad evolution.

Computational Physics Education 2

Spencer Wheaton, *University of Cape Town (South Africa)*
Infusing Computational Physics throughout the Undergraduate Curriculum

Computational physics is now widely viewed as an essential ingredient in most undergraduate physics curricula. The challenge, however, is to seamlessly integrate authentic computational activities into the programme. In this talk, I will review the approaches taken at the University of Cape Town, South Africa, where we have developed instructional materials that address the particular needs of our students (for example, many of our first year students have no previous experience with computers, let alone programming, and are not concurrently registered for a course in computer science). Although VPython is the preferred language at first year (driven largely by the choice of textbook), students are allowed to code in their preferred language in senior years. The laboratory component of our courses provides a natural context for most of these activities. In addition, an army of Lego Mindstorms robots is used to introduce students to the graphical programming language LabVIEW.

At the third year level, students use locally-developed simulations and guided-inquiry worksheets in lectures to explore the concepts of thermal and statistical mechanics. This topic provides an excellent opportunity to introduce students to basic Monte Carlo methods.

At the fourth year (Honours level), a series of simulations and worksheets has been developed that allow students to investigate more sophisticated computational physics techniques (e.g. sampling of arbitrary probability distributions, Monte Carlo integration methods etc.). In this way, students are able to appreciate the important concepts underlying these techniques before tackling the challenge of implementing their own computational codes.

Shobhana Narasimhan, *Jawaharlal Nehru Centre for Advanced Scientific Research (India)*
Teaching Density Functional Theory through Experiential Learning: Examples from the Developing World

Today, quantum mechanical density functional theory is often the method of choice for performing accurate calculations on atomic, molecular and condensed matter systems. Such calculations provide data that can be used to interpret experiments, gain insight into structure-property relationships, and design novel materials. With recent rapid advances in computational power, it is now possible to perform such calculations on a desktop PC or laptop (or even, in some cases, on a mobile phone!) With little need for infrastructure, this is an area of advanced research that can be easily embraced by students and scientists in the developing world.

In this talk, I will share some of my experiences in teaching the necessary basics of solid state physics, as well as the theory and practice of density functional theory, in a number of workshops held in

developing countries over the past decade. (Most of these workshops were organized in partnership with the developers of the QUANTUM ESPRESSO package.)

I will discuss the advantages of supplementing the usual formal equation-based teaching methods, characteristic of graduate courses, with the use of visual imagery and analogies. I will also discuss ways in which one can encourage students to make the transition from the rote-memory-based learning patterns that are characteristic of much of the developing world, to more adventurous, creative and critical ways of thinking that are needed in order to be successful in research.
Thus, in the workshops we have held, we include discussions on such
topics as what makes a good paper and how best to present one's results.

I will also describe one successful experiment we carried out, at a summer school held in Bangalore, which resulted in a joint publication co-authored by 67 lecturers and students participating in the school [1].

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Wolfgang Christian, *Davidson College (USA)*
Parallel Programming Using Easy Java Simulations

Parallel programing is of great importance for computational practitioners but it is almost never incorporated into introductory computational physics courses. This paper describes the adaption of Alan Kaminsky's parallel Java code library for use in the Easy Java Simulations (EJS) authoring and modeling tool. Using EJS instructors can easily introduce parallel programming techniques such as spatial decomposition and data replication in any computational physics course. EJS provides graphical elements to manage parallel teams, parallel regions, and parallel loops and we demonstrate how students use these objects to parallelize 3D Ising and 3D molecular dynamics simulations. These and other parallel programming examples are hosted on and distributed from the Open Source Physics (OSP) Collection of the ComPADRE National Science Digital Library http://www.compadre.org/osp/.

Rachele Dominguez, *Randolph-Macon College (USA)*
The role of computational physics in the liberal arts curriculum

I will discuss a new computational physics course at Randolph-Macon College and my attempt to identify where it fits into the larger liberal arts curriculum and why. In doing so, I will describe the goals of the course, the challenges I faced in teaching it, and some lessons learned.

Werner Krauth, *ENS Paris (France)*
Statistical Mechanics: Algorithms and Computations - A High-Level Massive Open Online Course (2014)

My ten-week MOOC on the Coursera platform, that ran in early 2014, focused on subjects such as Monte Carlo sampling, molecular dynamics, phase transitions in hard-sphere liquids, simulated annealing, classical spin models, quantum Monte Carlo algorithms, and Bose-Einstein condensation, etc. It familiarized a huge international crowd of students with cutting-edge subjects in computational physics.

In this talk I will present the topics of the course, its basic design ideas, its scope and challenges, and compare it with my earlier attempts in online teaching.

Thursday, Parallel Sessions 1, 8:30-10:15

Materials Science and Nanoscience 5

Markus Eisenbach, *Oak Ridge National Laboratory (USA)*
Magnetic Materials at finite Temperatures: thermodynamics and combined spin and molecular dynamics derived from first principles calculations
Co-authors: Dilina Perera , David P. Landau, Don M. Nicholson, Jungqi Yin, Gregory Brown

We will present a unified approach to describe the combined behavior of the atomic and magnetic degrees of freedom in magnetic materials. Using Monte Carlo simulations directly combined with first principles the Curie temperature can be obtained ab initio in good agreement with experimental values. The large scale constrained first principles calculations have been used to construct effective potentials for both the atomic and magnetic degrees of freedom that allow the unified study of influence of phonon-magnon coupling on the thermodynamics and dynamics of magnetic systems. The MC calculations predict the specific heat of iron in near perfect agreement with experimental results from 300K to above Tc and allow the identification of the importance of the magnon-phonon interaction at the phase-transition. Further Molecular Dynamics and Spin Dynamics calculations elucidate the dynamics of this coupling and open the potential for quantitative and predictive descriptions of dynamic structure factors in magnetic materials using first principles derived simulations.

This Work is sponsored by the U.S Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, “Center for Defect Physics,” an Energy Frontier Research Center, and by the Office of Advanced Scientific Computing Research, This research used resources of the Oak Ridge Leadership Computing Facility at the ORNL, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

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Van An Dinh, *Osaka University (Japan)*
Origin of ferromagnetism in GaMnAs: A hybrid density functional study
Co-authors: Kazunori Sato, Jiroshi Katayama-Toshida

Previously, the ferromagnetism in GaMnAs has been known to be induced by the p-d exchange interaction of the valence holes and localized d-electrons of Mn atoms [1,2]. Recently, some experiments have reported that the Fermi level locates in the d-band inside the band gap [3], which suggests that the ferromagnetism in GaMnAs would be caused by the ferromagnetic double exchange between d-electrons of Mn atoms. Theoretically, until now, the above-mentioned confliction of the experimental conclusions is still an open question and needed to be solved. The fact that the previous calculations obtained by using KKR-CPA, or pure DFT show an impurity band of the d-electrons of Mn atoms being overlapped with the valence band, leads to the conclusion that the ferromagnetism in GaMnAs is originated from the p-d exchange interaction. It is necessary to employ a more reasonable method to deal with this problem.

In this talk, we present our calculated results of the electronic structure of GaMnAs obtained by employing HSE06. The most preferred configurations of Mn atoms at various concentrations were obtained by a full optimization calculation. The interaction between the interstitial, anti-site and substitutional Mn atoms was studied. The possibility of diffusion of Mn atoms from the interstitial shells to the other site was also addressed. In order to explore the dominant mechanism of ferromagnetism in the system, the dependence of the impurity band and Fermi level on the Mn concentration is investigated. Our results show an overlap of the impurity band and valence band at the dilute concentrations of Mn atoms (<1%), which suggests a possibility of ferromagnetism originated from the p-d exchange interaction. On the contrary, at a higher concentration of Mn dopants, the separation of the impurity band from the valence band was found. These pictures suggest that the origin of ferromagnetism in GaMnAs would change depending on the concentration of magnetic dopants.

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Tiago de Campos, *Universidade de São Paulo (Brazil)*
Diagonalization of very large dense electronic structure matrices: an out-of-core iterative method
Co-authors: Guilherme M. Sipahi

Electronic structure determination is the first step towards theoretical modeling of optical properties such as absorption and emission spectra of low dimensional semiconductor. A possible theoretical approach for these band structure calculations is the k.p method in reciprocal space [1], a perturbative model that describe the energy bands around a high symmetry point. In the case of quantum confinement, each confinement direction increases the order of the matrices and we have to deal with very large dense matrices leading to problems on the order of tenths of millions of elements (1D) or even tenths of billions of elements (0D) . In this scenario it becomes clear that the use of direct diagonalization methods becomes a bottleneck either on computational execution time or memory requirements. Although iterative minimization methods are designed for large sparse matrices, we propose an out-of-core formulation of the LOBPCG [2] minimization method to improve the efficiency of the diagonalization of such very large dense matrices. In our tests we have implemented the Jacobi pre-conditioner and, even though it is the simplest one, we observe a speedup when the size of the matrices is greater then a total of 35 millions elements. Besides that, the out-of-core procedure reduces the memory requirements allowing very large systems to be realized on a common desktop. Furthermore, a better choice of pre-conditioner can lead to better convergence rates but this is a problem at its own, as we will point out. Summarizing, we developed a new methodology that can simulate sophisticated systems such as radial nanowire heterostructures and colloidal core-shell quantum dots [3-6] with low computing and memory requirements.

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Qiao-neng Guo, *Zhengzhou University (China)*
Temperature dependence of tensile properties of nano-Cu films: Molecular dynamics simulation
Co-authors: Qiao-Neng Guo, Ernie Pan, Shi-E Yang, Mingxing Wang, Qiang Sun, Jie-Fang Wang, Yu Jia

Though nano-Cu films used extensively in Microelectro Mechanical Systems (MEMS) have been the subject of widespread experimental [1-4] and theoretical [5-7] research, the mechanisms of plastic deformation of them have not fully understood up to the present. Moreover, only a limited portion [2,3] of studies published has been concerned with the aspect of various temperatures. Thus, in the isobaric-isothermal ensemble [8], molecular dynamics simulations are employed to simulate the mechanical responses of single-crystalline nano-Cu films under uniaxial tensile loading, using the embedded-atom method [9].

Firstly, the system temperature was taken as the parametric variable in analyzing the thermal effects on the failure process under tensile strain. With varying applied temperatures to the nano-Cu films, the variation of the maximum stress, Young's modulus and maximal potential energy is characterized and three critical temperatures for the transition of plastic flow mechanism in a wide temperature range from 40 to 460 K are identified.

Secondly, the plastic deformation mechanisms are then analyzed by examining the variation of the atomic structure of the emerging defect using common neighbor analysis [10].

Thirdly, the different mechanisms of copper films in different temperature ranges are also explained via the continuum damage mechanics.

Fourthly, two important physical quantities, activation volume and activation free energy, can be calculated and used to determine the mechanisms of the strange temperature dependence of tensile deformation.

Fifthly, the present studies are compared with previous experimental [1-3] and theoretical [5,6] results, and the discrepancy between these results is discussed.

Finally, it is concluded that at temperatures above 370 K, the mechanism is dislocation climbing; when about 370 K, it is pipe diffusion; when the temperature is between 370 K and 200 K, normal slip process occurs; whereas at temperatures between 200 K and 100 K, both twin and slip processes; when below 100 K, twin nucleation process appears.

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Xavier Andrade, *Harvard University (USA)*

Application of compressed sensing to electronic structure simulations

Co-authors: Jacob N. Sanders, Thomas Markovich, Alan Aspuru-Guzik

Compressed sensing (or compressive sampling) [1,2] is a method originally developed by the signal analysis community to minimize the data required to reconstruct a signal, based on the ideas of incoherent sampling and sparse optimization.

In this talk we will discuss our effort to apply compressed sensing and related techniques to the computational simulation of atomic systems, and we will show why compressed sensing has great potential for computational science.

The talk will start with a brief introduction of compressed sensing,
followed by a discussion of the applications to obtain frequency resolved information from real-time simulations such as molecular dynamics and real-time electron dynamics, where compressed sensing outperforms the standard Fourier transform, allowing us to obtain accurate spectral information from much shorter
time signals [1,2].

Next, we will discuss the effort to integrate compressed sensing at the core of simulation methods to maximize the amount of information that can be obtained from each computation. Our first application is to accelerate the calculation of costly matrices, common in electronic structure. For example, we show that it is possible to combine compressed sensing and molecular mechanics methods to speed up first principles calculation of the Hessian matrix, required for the calculation of molecular vibrational modes.

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Soft Matter and Biological Physics 4

Shanadeen Begay, *Boston University (USA)*
The Thermodynamics and Structure of Methionine Enkephalin using the Statistical Temperature Molecular Dynamics-CHARMM algorithm

A key research area in the Keyes Lab is focused on studying protein folding and energy landscapes using statistical biophysics techniques. Kim, Straub, and Keyes introduced the Statistical Temperature Molecular Dynamics (STMD) algorithm which has been implemented into the biosimulation package CHARMM. Atomistic simulations using this enhanced sampling algorithm have been performed on the Methionine Enkephalin (Met-Enk) five-mer peptide with a methionine terminal cap in a droplet of 638 TIP3P water molecules; the system has 1917 water atoms and 84 peptide atoms, a total of 2001 atoms.

Chain thermodynamics is analyzed from the novel perspective of the statistical temperature as a function of energy, TS(U). Canonical averages are calculated via reweighting to the desired temperature. Thermodynamic signatures of folding, the native contacts, the radius of gyration, root-mean-square deviation, and energy order parameters are investigated. Both the minimum in the slope of TS(U), and the peak in the heat capacity, C(T), is calculated via reweighing, indicate a collapse transition at T&theta &cong 260K (Ref. Wales). Distributions of dihedral angles, as a function of temperature, reproduce low probability sampling with minimal deviation (Ref. Wodak). Efficiencies over a subset of enhanced sampling methods is demonstrated. STMD-CHARMM reliably reproduces results found with similar methods for a variety of temperatures using a single simulation run. Order parameters and long-time averages indicating a weak folding and folding temperature will be discussed.

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Xizhong An, *Northeastern University (China)*

Radical Tessellation and Microstructure Characterization of Binary and Ternary Hard Sphere Crystals

Co-authors: Defeng Wang

Quantitative characterization on the structure of granular matter has been more and more attracting materialists and physicists' eyes in the past decades. Even though mono-modal or multi-modal hard sphere crystals (the crystal is called in terms of the packing structure of largest particles) such as BCC, FCC, HCP and amorphous states can be constructed by dynamic method (e.g. DEM), however, for multi-modal hard sphere crystals, the densest packing structure is really hard to generate by dynamic methods, i.e. the pores formed by the large particles are difficult to be effectively filled by small particles. In addition, the quantitative characterization on the microstructure of various hard sphere crystals was less studied. Therefore, different perfect hard sphere crystals which generated by the effective filling of small particle into the pores left by large particles were created in this study based on geometrical modeling, and quantitative tessellation on the structure of each crystal was conducted by radical method. Here, we mainly focus on the filling of small particles into (1) tetrahedral pores in BCC crystal, and (2) tetrahedral or octahedral pores or both in FCC and HCP crystals. In addition to the characterization on the macro property such as packing density and the micro properties such as coordination number, radial and angular distributions, the topological and metrical properties of each radical polyhedron were systematically studied and compared. The results showed that different hard sphere crystals corresponding to different cells of radical polyhedra, for example, octahedra and

icosidodecahedra in BCC; octahedra, tetrakaidecahedra and polyhedral with 26 faces in FCC; octahedra, dodecahedra and polyhedral with 26 faces in HCP. Meanwhile, the orientations of the polyhedral cells which include the same sized spheres were influenced by their neighbors, and the analysis revealed the anisotropic properties of these crystals.

Zhenlu Cui, *Fayetteville State University (USA)*
Mesoscale structures and Rheology of Active Liquid Crystals

Active liquid crystals are a new and exciting class of soft matters in which energy is continuously being supplied by internal or external sources. Examples arise in both the physical and biological science realms including bacteria suspensions, active gels and assemblies of motors and filaments. These compound element systems are naturally multiscale as it is activity that yields its peculiar phenomena such as bacterial swarming, bio-convection phenomenon and the spontaneous flow even in the absence of externally applied forces, both stationary and oscillatory, in sharp contrast to their passive counterparts. In this talk, I will present a hydrodynamic model for such systems. Steady structures, instabilities and rheology in a shear will be explored and discussed.

Amandeep Sangha, *UT/ORNL Center for Molecular Biophysics (USA)*
Lignin polymerization in plant cell walls: Monolignol binding, oxidation and radical coupling reactions
Co-author: Robert Standaert, Mark Davis, Jeremy Smith, Jerry Parks, Brian Davison

Major challenge impeding cost-effective biofuel production from plant biomass stems from its recalcitrance nature towards degradation into biomass components. Lignin is the main cause of this resistance. In plant cell walls, lignin is derived form radical polymerization of substituted phenyl propylene units: p-coumaryl, coniferyl and sinapyl alcohol. Reducing lignin content or altering monomer composition can provide higher sugar yields from plant biomass. Identifying the factors that control the growth of lignin polymers is of particular interest because shorter lignin chains can be extracted more easily during biomass conversion for improved sugar accessibility. We investigated three main steps involved in growth of lignin polymers: relative binding affinity of monolignols to the active site of horseradish peroxidase enzyme, the intrinsic chemical reactivity of lignin precursors to undergo peroxidase-mediated radical formation, and the reactivity of the radicals thus formed to undergo coupling reaction forming various ether and C-C interunit linkages using both classical and quantum chemical simulation techniques. Results indicate that (i) Binding of monolignols to the peroxidase active site is weak and there exists an equilibrium between monolignol being in the aqueous phase and in the active site of the enzyme [1] (ii) presence of highest occupied electron density (HOMO) electron density on the phenolic oxygen correlates with the ability of lignin precursors to undergo peroxidase-mediated oxidation [2] and (iii) β-O4, β-β and β-5 inteunit linkages are enthalpically more favorable for self- and cross-coupling reactions among all monolignol radicals [3]. Our results are in agreement with experiments and explain for the first time that why incorporating H subunit in high abundance into G-rich lignin leads to shorter lignin chains. This study identified chemical factors intrinsic to the lignin oligomers that can potentially control lignin chain elongation.

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Nikolaos Papadimitriou, *National Center for Scientific Research "Demokritos" (Greece)*
Study of Ceramide Bilayers with Molecular Dynamics Simulations
Co-author: Michael Kainourgiakis, Stylianos Karozis, George Lithoxoos, Georgia Charalambopoulou

Ceramide bilayers constitute the lipid domain of stratum corneum, the outermost layer of the skin. Ceramides are a special class of lipids that consist of a polar head and two alkyl tails, one of which is sphingosine and the other is a fatty acid. The biological importance of the specific system arises from the fact that it has major contribution to the barrier function of the skin.
In this work, we have used Molecular Dynamics simulations to examine a wide range of structural, thermodynamic, and transport properties, such as: bilayer thickness, density profiles along the bilayer normal, area per lipid, order parameters, radial distribution functions, chain tilt, and hydrogen-bond network. The system under investigation is a fully hydrated bilayer that consists of 128 molecules of CER NS 24:0. Special focus is given to the study of the lateral packing of the alkyl chains since it determines the phase behavior of the bilayer. For this reason, a technique is developed that uses the radial distribution functions of the chains to derive information about their lateral arrangement. It was found that the chains adopt a strictly hexagonal arrangement, giving more evidence to an issue for which the available experimental data are contradictory. Moreover, the hydrogen-bond connectivity between water and lipids and between the lipids themselves is extensively investigated since this kind of information is of great significance but it is not easily accessible by experimental means.
All simulations have been carried out with five force fields (OPLS-UA, GROMOS, BERGER, CHARMM, GAFF) in an attempt to evaluate their performance in the study of ceramide bilayers considering that there is no force field that has been specifically parameterized for ceramides. For most of the examined properties, all force fields led to similar conclusions although in some cases (e.g. intramolecular hydrogen bonding) notable discrepancy occurred.

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Sunita Negi, *University of Delhi (India)*
Probing temperature dependent conformation change of Calmodulin protein using Molecular Dynamics simulations

With advancement in computing hardware and simulation techniques scientists have developed a substantial overlap between the timescales accessible to atomic-level simulations and those on which the fastest-biological actions take place. Here we demonstrate, using simulations of Calmodulin (CaM) protein, how molecular dynamics simulations can provide direct access to RMSD calculation and deviation in torsional angle ϕ and bending angle θ, since these are the fundamental calculations to appreciate folding or unfolding. Temperature dependent conformation changes in CaM protein are studied with extensive molecular dynamics simulations. A quantitative comparison of our simulation data with various forms of available experimental results is discussed. Earlier such kinds of studies have been performed experimentally using fluorescence measurements as in [1]. The calcium bound form of the protein CaM is observed to undergo a reversible conformation change in the temperature range 22-28 °C. The transition temperature was observed to depend on the calcium ion concentration of the protein. Leap-dynamics approach was used earlier to study the temperature dependent conformation change of CaM [2]. At 290 K, both the N- and C-lobes were stable, at 325 K, the C-lobe unfolds whereas at 360 K both the lobes unfold. In this work we performed extensive molecular dynamics simulations of 100 ns each at various temperatures ranging 280-360 K on the apo form of CaM. A remarkable dependence of folding and unfolding on the temperature is confirmed as reported in our earlier study [3].

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Christopher Cooper, *Boston University (USA)*
Implicit-solvent model using Python and GPUs for proteins interacting with charged surfaces
Co-authors: Lorena A. Barba

We present an implicit-solvent model for protein-surface interactions. Applying the theory of electrostatics in a domain divided into solvent and protein dielectric regions leads to a coupled system of PDEs. The Poisson-Boltzmann equation applies in the solvent region (water with salt), the Poisson equation with point charges in the protein region, and interface conditions at the solvent-excluded surface dividing both regions.

To solve the resulting system of PDEs efficiently, we wrote a fast boundary-element method (with a multipole-based treecode) in Python and CUDA. We call our code PyGBe, it is open-source under the MIT license and can be downloaded from https://github.com/barbagroup/pygbe.

Our current application looks at the preferred orientation of proteins adsorbed on a charged surface, a situation relevant in biosensing. Biosensors are designed to detect a target molecule when it binds to a ligand molecule, itself attached to the sensor through a self-assembled monolayer (SAM). It is key that the binding sites of the ligand molecule be adequately exposed to the flow that carries the targets, and hence the importance of orientation. In our model, surfaces with SAMs are represented by prescribing a charge distribution. We compute the free energy in various orientations, and the minimum corresponds to the preferred orientation.

We will present results for three test cases. The first case is used to verify the code; it compares the numerical result with an analytical solution derived by us, valid for spherical geometries. In the second case, we computed the preferred orientation for protein G B1 adsorbed on a charged surface and compared and matched the result with published molecular dynamics simulations and experimental observations. In the final case, we used a full antibody, a common ligand molecule that is larger than protein G B1 and would be difficult to simulate with MD. This test shows the capability of PyGBe to compute realistic bionsensing systems.

Lattice Field Theory 3

Simon Catterall, *Syracuse University (USA)*
Supersymmetry on a lattice

Attempts to formulate supersymmetric field theories on discrete spacetime lattices have a long history. However, until recently most of these efforts have failed. In this talk I will review some of the new ideas that have finally allowed a solution to this problem for certain supersymmetric theories. I will focus my attention, in particular, on N=4 super Yang-Mills which forms one of the pillars of the AdSCFT correspondence connecting gravitational theories in anti-deSitter space to gauge theories living on the boundary of that space.

I will present results on the first large scale lattice study of N=4 Yang-Mills using this new approach. Our results are consistent with the existence of a single deconfined phase for the theory in which the static potential shows only a Coulomb behavior. Unlike QCD there is no confining, chirally broken phase even at strong coupling. This is consistent with one loop calculations which show that
the beta function of the lattice theory vanishes just as expected in the continuum.

Frithjof Karsch, *Brookhaven National Laboratory (USA)*
Conserved charge fluctuations in strong interaction matter

Fluctuations of conserved charges, i.e. baryon number, strangeness and electric charge, are sensitive probes for the transition from the confined hadronic to the deconfined partonic phase of strong interaction matter. Rapid changes of, e.g. quadratic fluctuations of net baryon number, net strangeness as well as correlations between these conserved charges, signal the change of degrees of freedom that carry the corresponding quantum numbers. The magnitude of these charge correlations and fluctuations provides information not only on the mass of the carriers of these quantum numbers (hadrons or quarks). They also provide information on the abundance of hadronic degrees of freedom with different quantum numbers, and allow to determine the thermal conditions at the time of hadronization (freeze-out) in heavy ion collisions.

Evan Weinberg, *Boston University (USA)*
Targeting the Conformal Window: Measuring the 0++ Scalar
Co-author: Oliver Witzel, Claudio Rebbi, Rich Brower, Anna Hasenfratz

The light Higgs boson of the Standard Model could arise as the consequence of the weakly broken conformal symmetry in a strongly interacting gauge theory just below the conformal window. Here we present a novel idea to study the transition from conformal to confining behavior using an SU(3) gauge theory with four light and eight heavy flavors. This system interpolates between the 12 flavor conformal and the 4 flavor chirally broken theory as the mass of the heavy flavors are varied. We show first results on the determination of the isosinglet 0++ state as it interpolates between QCD-like and conformal behavior.

Rajamani Narayanan, *Florida International University (USA)*
Polyakov loops in two dimensional QCD

I will discuss recent results on correlations between Polyakov loops in two different directions on a finite torus for two dimensional QCD. Analytical results for SU(2) will be combined with numerical results for SU(N) with $N > 2$. The behavior at infinite N will also be discussed.

Astrophysics 2: Compact Objects and Gravitational Waves

Christian David Ott, *Caltech (USA)*
Petascale Simulations of Core-Collapse Supernovae
Co-author: Erik Schnetter, Philipp Moesta, Christian Reisswig, Sherwood Riches, Ernazar Abdikamalov

Core-collapse supernovae from massive stars are among the most energetic events in the universe. They liberate a mass-energy equivalent of ~15% of a solar mass in the collapse of their progenitor star's core. The majority (~99%) of this energy is carried away by neutrinos, while ~1% is transferred to the kinetic energy of the explosive outflow. A smaller, yet still tremendous amount of energy is emitted in

electromagnetic and gravitational waves. Core collapse and the subsequent supernova evolution towards explosion involves a broad range of physics: Boltzmann transport of neutrinos, weak interactions, nuclear reactions, the nuclear equation of state, magnetohydrodynamics, and gravity. The problem is also multi-scale and for modeling the supernova engine, one must generally resolve physical scales from ~10000 km down to below ~100 m. Due to its multi-physics multi-scale nature, the core-collapse supernova problem poses a formidable computational challenge that requires petascale resources of the caliber of the NSF Blue Waters system. I review the computational approaches employed by the core-collapse supernova modeling community and present an overview of recent results from the first set of full 3D simulations.

Deirdre Shoemaker, *Georgia Tech (USA)*
Numerical Relativity and Gravitational Waves

Gravitational waves deliver information in exquisite detail about astrophysical phenomena, among them the collision of two black holes, a system completely invisible to the eyes of electromagnetic telescopes. Models that predict gravitational wave signals from likely sources are crucial for the success of this endeavor. Modeling sources of gravitational radiation requires solving the Einstein equations of General Relativity using powerful computer hardware and sophisticated numerical algorithms. This talk presents where we are in understanding ground-based gravitational waves resulting from the merger of black holes and the implications of these sources for the advent of gravitational-wave astronomy.

Hyun Lim, *South Dakota State University (USA)*
A Time Parallalizable Numerical Approach for the Semilinear Wave Equation
Co-authors: Matthew Anderson, Jung-Han Kimn

For certain formulations of partial differential equations, proper time-parallel preconditioners can be successfully applied in space-time finite element simulations. Such an approach may enable the extraction of more parallelism to better utilize high performance computing resources. In this work, we examine the behavior of the semi linear wave equation in 1 + 1 dimensions using the space-time finite element method. We discretize space and time together for the entire domain using a finite element space which does not separate time and space basis functions. We also explore the effectiveness of the time additive Schwarz preconditioner for this problem, and use a non-uniform mesh in both space and time. We present the critical regime and self-similarity of the semi linear wave equation using p=7 for the nonlinear term.

R K Chhajlani, *Vikram University (India)*
Self-gravitational Instability in Interstellar Molecular Clouds with polarized dust and neutral collisions
Co-authors: Ramprasad Prajapati

The self-gravitational instability in interstellar molecular cloud is investigated considering the effect of dust-neutral collisions, magnetic field and polarization force. The modified dynamic of dusty plasma are

discussed and gravitational modes are obtained with a linear dispersion relation. The dynamics of self-gravitating charged dust grain and neutral particles are considered and low frequency waves and instabilities are discussed for the considered system. The normal mode analysis is used to derive the dispersion relation which is discussed for weakly and highly collisional dusty plasma medium. The condition of Jeans instability and expression for critical Jeans wave number are obtained which depend upon polarization interaction parameter. The structure formation in interstellar molecular cloud consisting charged dust particles is also discussed. Numerical calculations have been performed to study the effect of dust-neutral collision parameter, polarization interaction parameter and magnetic field on the growth rate of the Jeans instability.