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CONTENTS

1 Statistical Physics

1 **Lukas Einkemmer**, *University of Innsbruck (Austria)*
A Hamiltonian splitting for the Vlasov-Maxwell system
Co-authors: Erwan Faou; Nicolas Crouseilles

It is well known that the Vlasov-Maxwell system can be considered as an infinite dimensional Hamiltonian system, where the Hamiltonian structure is non canonical and depends on the solution itself (Poisson structure), see e.g. [1] and [2]. This is of interest, as contrary to the Vlasov-Poisson system for which the natural splitting between spatial advection and velocity advection is also a Hamiltonian splitting, it is not clear from the structure of the Vlasov-Maxwell system which choice of splitting scheme yields good conservation properties. The splitting methods for the Vlasov-Maxwell system constructed in the literature have exclusively focused on two-term splittings (motivated by the two transport terms in space and in velocity) and therefore have used rather ad-hoc procedures in order to obtain methods of second order (see e.g. [3]).

We propose a new splitting method that is based on the Hamiltonian structure of the Vlasov-Maxwell system. In addition to the fact that methods of arbitrary high order can be constructed by composition, we show that if a spectral method is employed for the spatial discretization, the charge is exactly preserved and the numerical solution satisfies Poisson's equation without explicitly solving it.

In addition, we present numerical simulations in the context of the time evolution of a number of electromagnetic plasma instability (including the Weibel instability and a two-stream instability driven by a perturbation in the magnetic field) which emphasizes the excellent behavior of the new splitting compared to methods from the literature. This presentation is based on [4].

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2 **Adriana Gomes Dickman**, *Pontifícia Universidade Católica de Minas Gerais (Brazil)*
Simulation of an epidemic model with vector transmission
Co-author: Ronald Dickman

We study a lattice model for vector-mediated transmission of a disease in a population consisting of two species, A and B, which contract the disease from one another. Individuals of species A are sedentary, while those of species B (the vector) diffuse in space. Examples of such diseases are malaria, dengue fever, and Pierce's disease in vineyards. The model exhibits a phase transition between an absorbing (infection free) phase and an active one as parameters such as infection rates and vector density are varied. We study the static and dynamic critical behavior of the

model using initial spreading, initial decay, and quasistationary simulations. Simulations are checked against mean-field analysis. Although phase transitions to an absorbing state fall generically in the directed percolation universality class, this appears not to be the case for the present model.

3 **Lucila Alvarez Zuzek**, *IFIMAR-CONICET (Argentina)*
Theory and simulations of Epidemics in partially overlapped Multiplex Networks
Co-authors: Camila Buono; Pablo A Macri; Lidia A Braunstein

Many real networks exhibit a layered structure in which links in each layer reflect the function of nodes on different environments. These multiple types of links are usually represented by a multiplex network in which each layer has a different topology. In real-world networks, however, not all nodes are present on every layer. To generate a more realistic scenario, we use a generalized multiplex network and assume that only a fraction q of the nodes are shared by the layers. We develop a theoretical framework for a branching process to describe the spread of an epidemic on these partially overlapped multiplex networks. This allows us to obtain the fraction of infected individuals as a function of the effective probability that the disease will be transmitted. We also theoretically determine the dependence of the epidemic threshold on the fraction q > 0 of shared nodes in a system composed of two layers. We find that in the limit of q -> 0 the threshold is dominated by the layer with the smaller isolated threshold. We perform extensive simulations of the SIR model using the Montecarlo method with synchronic updates. Our theoretical results are in excellent agreement with our numerical results.[1]

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4 **Sitangshu Bikas Santra**, *Indian Institute of Technology Guwahati*
Random rotational sandpile model: Crossover from rotational to stochastic universality class
Co-authors: Himangsu Bhaumik; Jahir Abbas Ahmed

Random rotational sandpile model (RRSM) is constructed assigning randomly anti-clockwise rotational toppling rule to p fraction of the lattice sites of a rotational sandpile model (RSM)[1] with fully clockwise rotational toppling rule. RRSM is studied varying the fraction p of the lattice sites having ACR toppling rule within RSM with fully CR toppling rule. The steady state as well the values of the critical exponents of RRSM are found to have strong dependence on p. A continuous crossover from RSM with fully CR toppling rule at p=0 to that with fully ACR toppling rule at p=1 is observed. As p changes from 0 to 1, the system passes through a series of non-universal models at each value of p with a stochastic one at p=0.5. A scaling theory for such a continuous crossover is developed and numerically verified. The critical state of RRSM at p=0.5 is finally compared with that of the stochastic sandpile model (SSM) [2]. Though values of certain macroscopic parameters characterizing the steady states are found drastically different for these two models it is interestingly noted that the universality class of RRSM at p=0.5 is that of the SSM. Not only the

critical exponents of SSM are independently measured and compared with those of the RRSM at p=0.5 but also universal scaling functions for avalanche size distribution and two point toppling number difference are obtained for these models by estimating non-universal metric factors of the respective models. Though the origin of stochasticity in these models and the macroscopic parameters identifying the critical states of the models are very different, both the models evolve to a unique universality class, the so called Manna class, of the stochastic sandpile models. The study confirms the existence of Manna class in the context of RRSM with controlled randomness.

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5 **Amin Najafi**, *Islamic Azad University (Iran)*

The study of Binder Cumulant's behavior in two-dimensional anisotropic of Ising models with foreign-neighbor interactions by SAPBC method

The fourth-order cumulant of the magnetization,the Binder cumulant is determined at the different temperature phases of Ising models on two-dimensional anisotropic lattices with various ferromagnetic foreign-neighbor couplings by the Screw-Antisymmetric Periodic Boundary condition (SAPBC Method) of Monte Carlo techniques. The SAPBC Method, actually, is an extended mixed method of Screw (helical) and Antisymmetric periodic boundary conditions. Here, instead of considering the nearest and next-nearest neighbor interaction of the main lattice, we act on interaction of foreign-neighbors. The Binder Cumulant's value is completely dependent on new boundary condition. We study the non-universal behavior of Binder Cumulant with thermodynamic limit of size at different temperature phases. The data get of Monte Carlo simulation is consistent with approach of phenomenological order parameter probability distributions augmented by finite-size scaling (FSS) extrapolations to the thermodynamic limit. At low and high temperature, we will have a relatively good agreement with thermodynamic limit of PBC method. But, at critically with SAPBC,we will clearly realize the critical Binder Cumulant is not independent of size of lattice, confirming of non-universal behavior of Binder Cumulant.

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6 **Gonzalo Suarez**, *IFIMAR-CONICET (Argentina)*
Transport with hard-core interaction in a chain of asymmetric cavities.
Co-authors: Miguel Hoyuelos; Hector O Martin

We studied the transport process of overdamped Brownian particles, in a chain of asymmetric cavities, interacting through a hard-core potential. When a force is applied in opposite directions a difference in the drift velocity of the particles inside the cavity can be observed. Previous works on similar systems deal with the low-concentration regime, in which the interaction is irrelevant. In this case it was found that large particles show a stronger asymmetry in the drift velocity when a small force is applied, allowing the separation of different size particles [1]. We found that when the interaction between particles is considered, the behavior of the system is substantially different. Simulating this system with the Monte Carlo method, we proved that, when the concentration increases the small particles are the ones that show a stronger asymmetry. For the case where the jump length is equal to the size of the particles, we took advantage of the particle-vacancy analogy to predict that the left and right currents are almost equal in a region around concentration 0.5 despite the asymmetry of the cavity. We also introduced a modified Fokker-Planck equation to describe this system analytically.

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7 **Ronald Dickman**, *Universidade Federal de Minas Gerais (Brazil)*
Intrinsic convergence properties of entropic sampling algorithms
Co-authors: Rolando Elio Belardinelli; Victor Daniel Pereyra; Bruno Jeferson Lourenço

We study the convergence of the density of states and thermodynamic properties in three flat-histogram simulation methods, the Wang-Landau (WL) algorithm [1], the 1/t algorithm [2], and tomographic sampling (TS) [3]. In the first case the refinement parameter f is rescaled (f -> f/2) each time the flat-histogram condition is satisfied, in the second f ~ 1/t after a suitable initial phase, while in the third f is constant (t corresponds to Monte Carlo time). To examine the intrinsic convergence properties of these methods, free of any complications associated with a specific model, we study a featureless entropy landscape, such that for each allowed energy E = 1,...,L, there is exactly one state, that is, g(E)=1 for all E. Convergence of sampling corresponds to g(E,t) -> const. as t -> infinity, so that the standard deviation &sigma of g over energy values is a measure of the overall sampling error. Neither the WL algorithm nor TS converge: in both cases &sigma saturates at long times. In the 1/t algorithm, by contrast, &sigma decays ~ 1/t1/2. Modified TS and 1/t procedures, in which f ~ 1/t&alpha, converge for &alpha in the interval (0,1]. There are two essential facets to convergence of flat-histogram methods: elimination of initial errors in g(E), and correction of the sampling noise accumulated during the process. For a simple example, we demonstrate analytically, using a Langevin equation, that both kinds of errors can be eliminated, asymptotically, if f ~ 1/t&alpha for &alpha in (0,1]. Convergence is optimal for &alpha

= 1. For &alpha less than or equal to zero the sampling noise never decays, while for &alpha > 1 the initial error is never completely eliminated.

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8 **Zhenjiu Wang**, *Beijing Normal University (China)*

Phase transitions in A nonlinear XY model with symmetry-breaking field in two dimensions

Co-authors: Wenan Guo; Anders Sandvik

We study the phase transitions in the nonlinear XY model with four-fold symmetry-breaking field using Monte Carlo simulation method.We show that, without the symmetry-breaking field, the transition is still KT-like when the nonlinearity is not strong, but turns to first order when the nonlinearity is strong enough. With four-fold symmetry-breaking field present, the transition turns to continuous but not KT-like in the weak nonlinearity. For Strong nonlinearity, the transition also turns to continuous with a small filed.

9 **Manabu Hasegawa**, *University of Tsukuba (Japan)*

Functionality limit of classical simulated annealing

An optimization function of simulated annealing (SA) [1] is reexamined in the solution process for the random traveling salesman problems [2-4]. A functional defect is revealed by applying a computational physics approach, the mapping-onto-minima approach [5] (see also [3,4]) used for studies on liquid and glass: the functionality limit beyond which the method is defeated by a simple local search emerges in the size-time plane. The impact of this limitation on the scalability test is demonstrated in the standardized framework of SA. The results draw the attention again to the appropriate implementation and competition of the SA and SA-related algorithms (see [4] for the case of generalized SA) and further to an illuminating aspect of computational physics analysis in the optimization algorithm research [3].

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10 **Henio Rego**, *CPS/Boston University and IFMA (USA)*
Percolation-Like Complexity in a 2 Dimensional Long Range SIR O-Lattice Model
Co-authors: Lidia Braunstein, H.E. Stanley

We present a Monte Carlo study of a 2 dimensional o-lattice Susceptible-Infected-Recovered (SIR) Model system with connections ruled by a long-range probability distribution of occurence given by a power law decreasing funtion with a characteristic exponent alpha. We considered several situations by fixing the probability of recovery "Pr" and the populational density "d" of the system, in order to determine the critical values for alpha in which the system becomes an outbreak. We finally discuss the results in terms of a long-range percolation problem.

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11 **Antonina Fedorova, Michael Zeitlin**, *IPME RAS (Russia)*
Pattern Formation: From Local Hidden Symmetries to Global Dynamics

We present universal framework for generation, analysis and control of non-trivial states/patterns in the complex systems like kinetic/BBGKY hierarchies describing general set-up for non-equilibrium dynamics and their important reductions [1]. We start from the proper underlying functional spaces and their internal hidden symmetries which generate all dynamical effects. The key ingredients are orbits of these symmetries, their representations, and Local Nonlinear Harmonic Analysis on these orbits. All that provides the possibility to consider the maximally localized fundamental generic modes, non-linear (in case of the non-commutative underlying symmetry) and non-gaussian, which are not so smooth as gaussians and as a consequence allowing to consider fractal-like images and possible scenarios for generation chaotic/stochastic dynamics on the level of representation theory only. The analytical consideration and modeling are based on some set of variational principles generating the so-called Generalized Dispersion Relations, which are the key and pure algebraic instrument for the realizable control, at least on the qualitative level, for the type of pattern we are interested in our applications. As a main example we consider the modeling of fusion dynamics in plasma physics.

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http://math.ipme.ru/zeitlin.html
http://mp.ipme.ru/zeitlin.html

12 **Atsunari Katsuki**, *Nihon University (Japan)*
Numerical simulation of dune morphology deformed by multiple flow conditions

Sand dunes are found in many places such as deserts, the sea bottom and the surface of Mars. They are formed through interplay between sand and air flow or water flow. When a strong flow blows, sand grains are dislodged from the sand surface. The entrained sand grains collide with the ground and are sometimes deposited. This process takes place repeatedly, resulting in the formation of a dune. The profile of the wind flow is modified by dune topography. We reproduced some dune morphology in numerical simulations and investigate the dynamics, changing the environmental condition such as the direction of winds. The motion of sand grains is realized by two processes: saltation and avalanche. Saltation is the transportation process of sand grains by flow. The saltation length and saltation mass are denoted L and q, respectively. Saltation occurs only for cells on the upwind face of dunes. The saltation length L and the amount of transported sand q are modeled by the following rules,L = a+bh(x,y,t)-ch(x,y,t)2, where a=1.0, b=1.0, and c=0.01 are phenomenological parameters. The last term is introduced for L not to become too large. Note that L is used only in the range where L increases as a function of h(x,y,t). In the avalanche process the sand grains slide down along the locally steepest slope until the slope relaxes to be (or be lower than) the angle of repose which is set to be 34 degrees. The dune pattern is classified by the amount of initial sand and directions of flow. For simulating multidirectional flow, wind direction is changed in a certain period Pch from one direction to the other. When the wind is unidirectional and the sand bed is thin barchans appear. When the wind is unidirectional and the sand bed is deeper, transverse dunes appear. As the amount of sand mass increases, the transverse dunes become wider. Linear dunes appear when the wind direction is two and sand bed is thick. As the amount of sand mass decrease, the linear dunes become drop dunes. When the number of wind direction is four Pch=100, star dunes appear.

13 **Altan Allawala**, *Brown University (USA)*
Equal-time PDF of the stochastically forced Lorenz-63 attractor using a Fokker-Planck description
Co-author: Brad Marston

We investigate the Fokker-Planck description of the equal-time probability distribution function (PDF) of the three-dimensional Lorenz-63 attractor [1] modified with the addition of stochastic forcing. The steady-state PDF is found by time-evolving an initial PDF forward in time under the action of the linear Fokker-Planck operator. The PDF is compared to that obtained by the traditional method of accumulating statistics using direct numerical simulation (DNS). Another method of accessing the steady-state PDF is then tested that is based upon finding the the ground state of a linear self-adjoint differential operator using sparse-matrix techniques. Theoretical and computational issues of both approaches will be discussed.

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14 **Zheng Zhu, Andrew Ochoa**, *Texas A&M University (USA)*
Efficient sampling of ground-state configurations for quasi-two-dimensional Ising spin glasses
Co-author: Helmut Katzgraber

Spin glasses are the archetypal benchmark problem when developing and characterizing optimization algorithms. In particular, the recent development of quantum annealing machines has increased the demand for ground-state test instances on (quasi) two-dimensional lattices. The scaling with the number of spins (i.e., size of the input) when determining the minimum of a spin-glass Hamiltonian (i.e., the value of a cost function) represents a first stringent metric when evaluating the quality of a novel optimization approach. However, verifying that an optimizer can sample all solutions that minimize the Hamiltonian is a far more stringent test for any newly-developed algorithm. While most solvers easily compute the minimum of a cost function for small to moderate input sizes, equiprobable sampling of all ground-state configurations (within Poissonian fluctuations) is much harder to obtain. Most notably, methods such as quantum annealing fail in passing this test for certain highly-degenerate problems [1]. Here we present an attempt to sample ground states for (quasi) two-dimensional Ising spin glasses with a space dimension below 3. The method is based on a combination of low-temperature parallel tempering Monte Carlo [2] used to sample ground-state configurations as introduced by Moreno et al. [3], combined with the rejection-free cluster algorithm by Houdayer [4] run at finite temperature. After generating an initial population of ground-state configurations via parallel tempering sampling [3], we exploit the symmetry of the Hamiltonian, as well as degeneracies due to zero local fields. These configurations are then fed to the Houdayer cluster algorithm. Because the latter is rejection free and obeys details balance, the ground-state manifold is efficiently sampled. We illustrate the approach for Ising spin glasses on the D-Wave Two quantum annealer topology, known as the Chimera graph [5], as well as two-dimensional Ising spin glasses with bimodal disorder.

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15 **Nagendra Panduranga**, *Boston University (USA)*
k-Core percolation in interdependent networks
Co-authors: H.E. Stanley, Jianxi Gao, Shlomo Havlin

Complex networks have been proven to be an important tool to study complex systems. Moreover, the study of interdependent substructures of complex networks attracted much interest recently. The k-core percolation approach is one way to identify the highly connected sub-structures and has been extensively studied for single networks [1]. In reality, diverse critical infrastructures are coupled together and depend on each other, including systems such as water and food supply, communications, fuel, financial transactions, and power stations. Recently, a mathematical framework for studying percolation of "network of interdependent networks" has

been developed. This framework [2,3], can help to extend the k-core percolation approach to interdependent networks. Here, we study the percolation properties for various k-cores in a system of two fully or partially interdependent networks.. In particular, we find that percolation transition of k-core in two interdependent ER network changes from a continuous second order phase transition to a discontinuous first order phase transition as the coupling strength increases.

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16 **Na Xu**, *Boston University (USA)*
Dynamics of 2D Ising Model in linearly varying magnetic field
Co-authors: Anders Sandvik, Cheng-Wei Liu, Anatoli Polkovnikov

We consider non-equilibrium dynamics of systems driven out of equilibrium at some finite rate near phase transitions. In previous work [1] on systems with varying temperature, scaling behaviors have been tested in great detail. Here with Monte Carlo simulations, we investigate the 2D Ising Model with linearly varying magnetic field and demonstrate the applicability of similar scaling functions when approaching the critical point. Moreover, we have found an interesting power-law scaling behavior in this system also below the critical temperature (even close to T=0).

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17 **Bolun Chen**, *Boston College (USA)*
Scaling of spiking neural network for mammalian olfaction

We are interested in how cognitive function can emerge from the collective behaviour in biologically inspired networks of neurons. In particular we use the dynamics of stable attractors in the form of subsets of neurons that (transiently) synchronize when a very particular sensory stimulus is presented as a many-body pattern recognition algorithm. We test these notions in a model of olfaction and show: (1) coupled neurons rapidly develop correlations in spike times, (2) biologically inspired network recognizes odors using synchrony, (3) reliability of the network scales dramatically with system size, and (4) inhibitive feedback can tune the relative performance of different cognitive tasks.

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implementation, PNAS 96: 12505 (1999).

18 **Alejandro Lage Castellanos**, *Universidad de la Habana (Cuba)*
Bayesian inference of epidemics on networks via Belief Propagation
Co-authors: Alfredo Braunstein, Luca Dall'asta, Riccardo Zecchina, Fabrizio Altarelli

We study several bayesian inference problems for irreversible stochastic epidemic models on networks from a statistical physics viewpoint. We derive equations which allow to accurately compute the posterior distribution of the time evolution of the state of each node given some observations. Unlike with most existing methods, we allow very general observation models, including unobserved nodes, state observations made at different or unknown times, and observations of infection times, possibly mixed together. Our method, which is based on the Belief Propagation algorithm, is efficient, naturally distributed, and exact on trees. As a particular case, we consider the problem of finding the "zero patient" of a SIR or SI epidemic given a snapshot of the state of the network at a later unknown time. Numerical simulations show that our method outperforms previous ones on both synthetic and real networks, in some cases by a very large margin.

19 **Alejandro Lage Castellanos**, *Universidad de la Habana (Cuba)*
Region graph approximations to free energy in finite dimensional spin glasses.
Co-authors: Federico Ricci-Tersenghi, Tommaso Rizzo, Roberto Mulet, Eduardo Dominguez

We study the Cluster Variational Method (Region Graph Approximation to free energy, or Generalized Belief Propagation) in the case of 2D and 3D Edwards Anderson model. We show how Replica Symmetric calculations can be implemented at this level to obtain thermodynamic limit predictions of this kind of systems to a certain accuracy level. Statistical mechanics of disordered systems is an active research area. It has produced many interesting results, both conceptually and as a tool for interdisciplinary applications, in the past 40 years. Within this area, disordered spin glass models in finite dimensions remain unsolved in many senses. We focus specially on the 2D Edwards Anderson model, where we show that not only average case predictions can be done with the Cluster Variational Method, but also single instance characterization. In particular, CVM finds a (thermodynamically wrong) spin glass phase at non-zero temperatures, that, however, is connected to metastable states of the Monte Carlo dynamics, and can be exploited to infer non trivial parameters like the replicas overlap P(q).

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2 Soft Matter and Biological Physics

1 **Shourjya Sanyal**, *University College Dublin (Ireland)*

Simulations On The Designing Rationale of FRET Based Uni-Molecular Probes

Co-authors: David Coker, Donal Mackernan

Bio-sensors based on the detection of FRET (Foster Resonance Energy Transfer) luminescence are extensively used in molecular biology to identify spatio-temporal protein interactions invitro towards understanding biochemical pathways.[1] FRET bio-sensing systems generally consist of two interacting proteins in solution that carry different FRET donor and acceptor chromophores which can exchange excitation energy when brought to within mesoscopic distances due to protein-protein interaction. Subsequent acceptor fluorescence thus in principle signals that this protein-protein interaction enhancement process has taken place.[2] To increase protein-protein interaction probability in solution, peptide linkers made of flexible amino acids are attached to the FRET pair, known as uni-molecular FRET probes. However it still remains a open question, if the flexible linker systems are the best choice of linkers or more structural linkers like hinges could give better intensity and/or signal to noise ratio. Idealised models consisting of macroparticles and simple mechanical linkers have been developed and applied to investigate the linker role in uni-molecular FRET based bio-sensors.[3] The statistical properties of these models have been investigated by Monte Carlo sampling. The results help us to understand the properties of floppy linkers (poly-Glycine type) currently used in experiments, and give key qualitative insight into the possibilities of designing structural linkers like hinges. These linker systems selectively restricts the motion of the macroparticles (proteins), to enhance the intensity and/or the signal to noise ratio of FRET probes. In this work we have shown that in case of low binding energy between the protein-protein system, structural linkers can be ideally up to twice as good as flexible linkers.

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2 **Amid Ranjkesh Siahkal***, University of Maribor (Slovenia)*

Computer simulation of domain patterns in randomly perturbed Nematic liquid crystal

Co-authors: Tim Sluckin, Milan Ambrozic, Samo Kralj

Glassy liquid crystalline systems are expected to show significant history-dependent effects. Two model glassy systems are the Random Anisotropic Nematic (RAN) and sprinkled Silica Spin (SSS)lattice models. The RAN model is a Lebwohl-Lasher lattice model[1] with locally coupled nematic spins, together with uncorrelated random anisotropy fields at each site, while the SSS model has a finite concentration of impurity spins frozen in random directions. Here Brownian simulation is used to study the effect of different sample histories in the low temperature regime in a three dimensional model intermediate between SSS and RAN, in which a finite concentration p < pc (pc the percolation threshold) of frozen spins interacts with neighboring nematic spins with coupling W.Simulations were performed at temperature T TNI /2 (TNI the bulk nematic-isotropic transition temperature) for temperature-quenched and field-quenched histories (TQH and FQH respectively), as well as for temperature-annealed histories (AH). The first two of these limits represent extreme histories encountered in typical experimental studies. Using long-time averages for equilibrated systems, we calculate orientational order parameters and two-point correlation functions. Finite size-scaling was used to determine the range of the orientational ordering, as a function of coupling strength W; p and sample history [2-5]. Sample history plays a significant role; for given concentration p, as disorder strength W is increased, TQH systems sustain quasi-long-range(QLRO) and short-range-order (SRO). The data are also consistent with a long-range order(LRO) phase at very low disorder strength. By contrast, for FQH, only LRO and QLRO occur within the range of parameters investigated. The crossover between regimes depends on history, but in general, the FQH phase is more ordered than the AH phase, which is more ordered than the TQH phase. In the weak-disorder limit the Larkin-Imry-Ma [6] scaling is observed.

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3 **Emine Deniz Tekin**, *University of Turkish Aeronautical Association (Turkey)*

Molecular Dynamics Simulation of Self-Assembled Peptite-Amphiphiles

Self-Assembly is the basic mechanism through which structural organizations (both organic and inorganic), are formed from the scale of molecules to the galaxies. Peptide amphiphiles form 1-dimensional nanostructures via the mechanism of Self-Assembly. These nanostructures, in the context of regenerative medicine and tissue engineering, have the potential to be used in the construction of blood vessels and cytoskeleton mimicking the extra cellular matrix (ECM). There is

a vast amount of literature on the experimental side of Self-Assembly at the molecular level. Experimentalists have had great success in getting self-assembled supramolecules, yet their success is always limited by the fact that their measurements are at best as good as their measuring devices. It is clear that, without having a fundamental understanding of the Self-Assembly mechanism, one has to just rely on experience and intuition in synthesizing new materials. Therefore, theoretical studies (computer simulations) are imperative to understand the processes involved in the Self-Assembly mechanism and to find the connections between the properties of the product materials and the involved molecules. In this study, a detailed molecular dynamics study of cylindrical nanofibers formed by self-assembling peptide amphiphiles is carried out. Molecular Dynamics is known to be very efficient in understanding the dynamics of large bio-molecules. With the same method, the effects of changing the temperature of the environment on the configuration and properties (such as stiffness) of the formed supramolecules as well as the role of the molecular interactions is studied. It is expected that these suggested theoretical studies will help experimentalists to synthesize materials with the desired properties.

4 **Freddie Salsbury**, *Wake Forest University (USA)*

All-atom GPU-enabled simulations of therapuetic nucleic acids and their effects on DNA-binding proteins

Co-authors: Ryan Melvin, William Thompson

Fluorouracil is a modified nuclear acid and a common chemotherapuetic, yet much remains to be known about its molecular properties. We will present initial results on long-time simulations of two fluorouracil systems. The first is the polymeric form, F10, where we present initial results on various conformations that our microsecond-scale simulations have discovered. The second, will be fluorouracil incorporated into DNA, where we will compare the conformational effects of binding to the mismatch repair protein complex MSH2/6 to the effects of binding other types of DNA damage, as obtained from 250nanosecond-length simulations.

5 **Julio Rocha**, *UFMG (Brazil)*

Identifying transitions in finite systems by means of partition function zeros and microcanonical inflection-point analysis: A comparison for elastic flexible polymers

For the estimation of transition points of finite elastic, flexible polymers with chain lengths from 13 to 309 monomers, we compare systematically transition temperatures obtained by the Fisher partition function zeros approach with recent results from microcanonical inflection-point analysis. These methods rely on accurate numerical estimates of the density of states, which have been obtained by advanced multicanonical Monte Carlo sampling techniques. Since both the Fisher zeros method and microcanonical inflection-point analysis yield very similar results, we conclude that these methods are equally useful for the identification of transition points in finite systems and outperform conventional canonical analysis of thermodynamic behavior.

6 **Danh-Tai Hoang**, *Asia Pacific Center for Theoretical Physics (Korea)*
Conserved rule for pancreatic islet organization
Co-authors: Vipul Periwal, Hanami Hara, Junghyo Jo

Morphogenesis, spontaneous formation of organism structure, is essential in life. In pancreas, endocrine alpha, beta, and delta cells are clustered to form islets of Langerhans, the critical micro-organ for glucose homeostasis. The spatial organization of endocrine cells in islets looks different between species. Based on the three-dimensional positions of individual cells in islets, we computationally inferred the relative attraction between cell types, and found that the attractions between homotypic cells were slightly stronger than the attractions between heterotypic cells commonly in mouse, pig, and human islets. The difference between alpha-betacell attraction and beta-beta cell attraction was minimal in human islets, maximizing the plasticity of islet structures. Our result suggests that although cellular composition and attractions of pancreatic endocrine cells are quantitatively different between species, the physical mechanism of islet morphogenesis may be evolutionarily conserved.

7 *Cancelled*

8 **Sarra Douah**, *Université des Sciences et de la Technologie d'Oran (Algeria)*
Partition function zeros for semi-flexible homopolymers
Co-authors: Daniel Seaton, David Landau

We present a partition function zeros analysis for semi-flexible homopolymers considering chain lengths from 10 to 55 monomers. The zeros were calculated from the estimate density of states obtained by a two-dimensional variant of Wang-Landau sampling. We aim to verify weather this method is capable or not of finding the indications of the same transitions as we have already identified using means of "peaks" and "shoulders" of fluctuating energetic and structural quantities as function of the canonical temperature. Since the transitions points are simple to identify we also demonstrate the importance of understanding the zeros of partition function from the viewpoint of statistical physics.

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9 **Shuhei Kawamoto**, *Temple University (USA)*
Free energy analysis of membrane fusion
Co-authors: Wataru Shinoda, Michael Klein

Phosphatidylethanolamine (PE) lipid is a fusogenic lipid, encouraging the membrane fusion when incorporated into a lipid membrane. The propensity to a fusion should be measured as a

decrease of free energy barrier to the membrane fusion in a molecular dynamics simulation. In order to calculate the free energy along a fusion process, we need to control the membrane morphology along a plausible fusion pathway. In a previous study of a simple soft-core model membrane, the membrane morphology was controlled by using particle density field [1]. This method, however, gives a large uncertainty of free energy, when used for a molecular model, due to the inherent large density fluctuation of a molecular system. We propose here a new free energy method, which controls the membrane morphology along the stalk mechanism of membrane fusion using an external guiding wall potential [2]. The free energy barrier is estimated by thermodynamic integration with respect to the controlling parameter,λ. Using the SDK coarse-grained model [3], we have successfully obtained a well converged free energy profile along the stalk mechanism of membrane fusion. The effect of PE lipid on the free energy barrier of fusion was evaluated. The energy barrier was reduced by 30% for stalk formation and 40% for fusion pore formation. The effect of curvature on the free energy was also investigated using vesicular systems.

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10 **Abdiravuf Dzhurakhalov**, *University of Antwerp (Belgium)*

Monte Carlo parameterization in the VirtualLeaf framework

Co-authors: Gerrit Beemster, Dirk De Vos, Jan Broeckhove

Monte Carlo (MC) methods are useful for simulating systems with many degrees of freedom, such as cellular structures and plant tissues. The recently developed simulation framework VirtualLeaf [1] uses a MC method with Metropolis dynamics for studying plant tissue morphogenesis. In VirtualLeaf the cell and tissue behavior is represented within a generalized energy, i.e. Hamiltonian. It includes the terms responsible for the intracellular turgor pressure and the cell wall resistance to this pressure. In this formalism the stable state of the system, i.e. the balance between turgor pressure and cell wall resistance at a certain time is defined by the minimization of a generalized potential energy. Minimizing the energy of the tissue is done by an energy evaluation-only method. The Hamiltonian used is a multi-variable function as it consists of the contributions to the energy from a large number of cells and cell walls. Although the energy evaluation-only method used in VirtualLeaf is more appropriate for multi-variable functions, it is a non-derivative method and reaching a desirable state or a local/global energy minimum of the system cannot be evaluated safely by a fixed energy threshold value. We have developed a more robust criterion for the energy minimization method of this type of multivariable and complex systems where the use of a gradient norm is impossible. The proposed sliding window criterion is based on the continuous checking of a threshold value within some energy difference window sliding along the energy change of the system. We show that with this method the resulting stable solution increases drastically in comparison with the fixed energy difference method

previously used in VirtualLeaf. The advantages of the sliding window criterion are discussed and results obtained by this method are presented. Parameterization effects for various models of the VirtualLeaf framework are analysed and current features and possible extensions of VirtualLeaf for plant growth studies are demonstrated.

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11 **Rui Travasso**, *University of Coimbra (Portugal)*

Validity of the contact order-rate correlation in the folding of small, single domain proteins: A Monte Carlo simulation

Co-authors: Heinrich Krobath, Patricia Faisca

The use of extensive Monte Carlo simulations of coarse- grained protein models allows an accurate study of both equilibrium thermodynamics and folding kinetics. The ability to efficiently and rapidly simulate complete folding trajectories, and to observe thousands of folding-unfolding events, unravels the role played by certain protein properties in the folding process. Here we employ replica-exchange Monte Carlo simulations of simple lattice models with folding energetics modeled by different interaction potentials to study the folding transition of topologically distinct proteins. In doing so we are able to identify the physical roots of the empirical correlation found between the contact order (CO) parameter, a metric of topological complexity, and protein folding rates. We further assess the interplay of native topology as measured by the CO and non-native interactions in the folding of surface-tethered proteins, a physical constraint that occurs in co-translational folding and in many single molecule experiments. We find that the excluded volume effect imposed by the tethering plane together with abundant non-native interactions can drive a low CO topology into misfolding, whereas a high CO native topology, dominated by long-range interactions, still folds correctly, although not necessarily via a strict two-state transition. Our results thus indicate that the empirical correlation between folding rate and contact order may not apply to surface-tethered protein folding, and, likewise to folding in vivo.

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12 **Busara Pattanasiri**, *University of Georgia (USA)*

Effect of surface attractive strength on structural transitions of a confined HP lattice protein

Co-authors: David Landau,Ying Wai Li, Thomas Wust

We investigated the influence of surface attractive strength on structural transitions of a hydrophobic-polar (HP) lattice protein model [1] confined between two parallel attractive walls. Thermodynamics and structural properties have been determined by employing Wang-Landau sampling [2, 3] together with efficient Monte Carlo updates (pull moves [4] and bond-rebridging moves [5]). The simulations were performed on a HP sequence with 48 monomers (PHPHP4HPHPHP2HPH6P2H3PHP2HPH2P2HPH3P4H), where there are equal number of H- and P-monomers. This sequence has been designed by Yue et al [6] for algorithm testing purpose. The effect of surface attraction has been studied by varying the ratio between the surface attractive strength and the attraction between the monomers. For simplicity, we only considered those surfaces that attract all monomers with the same strength. To identify conformational transitions, we analyzed the specific heat together with several structural quantities, such as the number of surface contacts, the number of hydrophobic pairs, and radius of gyration. We found that such a comprehensive analysis of these structural quantities is essential to distinguish different conformational transition processes since the specific heat alone is unable to give distinct signals in some cases. In general, when a HP protein is confined between two attractive surfaces, some of these four transition processes are observed upon cooling: adsorption, flattening of adsorbed structure, debridging process and hydrophobic core formation. Depending on the surfaces' attractive strength, these transitions take place at different temperatures, while the ground state configurations show structural variations. These scenarios are confirmed by snapshots of typical states of the systems.

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13 **N. Atamas**, *National Kyiv Taras Shevchenko University (Ukraine)*

Study of ionic liquids+aromatic mono-substituted benzene strongly diluted solutions by molecular dynamics at t = 400k

Co-authors: V. Kovalchyk

The big class of solvents with are considered promising to replace organic solvents in industrial processes, are ionic liquids and the use them as solvents for different processes on industrial and pilot plant scale gains more and more interest. The study showed that an ionic liquid based process can be economical more beneficial than conventional processes. In the present study

includes we report results from MD simulations study of three-component systems ionic liquids (dimethyl-imidazolim chloride) – polar (tholuene, phenole and anisole) and ionic liquids (dimethyl-imidazolim chloride) -nonpolar molecule (benzene) at T=400K. Conducted calculations allowed us to obtain information on the structural characters of the three-component solutions. From radial distribution functions (RDF) the analysis of the local structure, energetic and dynamic of solutions were done. The parameters of hydrogen bonds and the size of first and second hydrations shape ware determined. The influence of polar and non-polar solvent molecule on ionic liquids local structure, the hydrogen bonds nets and energetics at T=400K ware analyzed.

14 **Amir Azadi**, *University of Massachusetts Amherst (USA)*
Emergent structure of multi-dislocation ground states in curved crystals
Co-authors: Gregory M Grason

We study the structural features and underlying principles of multi-dislocation ground states of a crystalline spherical cap. In the continuum limit where the ratio of crystal size to lattice spacing W/a diverges, dislocations proliferate and ground states approach a characteristic sequence of structures composed of radial grain boundaries (``neutral scars"), extending radially from the boundary and terminating in the bulk. Employing a combination of numerical simulations and asymptotic analysis of continuum elasticity theory, we prove that an energetic hierarchy gives rise to a structural hierarchy, whereby dislocation number and scar number diverge as a/W -> 0 while scar length and dislocation number per scar become {\it independent} of lattice spacing. We characterize a secondary transition occurring as scar length grows, where the n-fold scar symmetry is broken and ground states are characterized by polydisperse, forked-scar morphologies[1].

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15 **Kang Liu**, *Boston University (USA)*
Physiologic Networks: Topological and Functional Transitions
Co-Authors: Ronny Bartsch, Plamen Ivanov

The human organism is a complex network of interconnected organ systems, where the behavior of one system affects the dynamics of other systems. Due to these interactions, failure of one system can trigger a breakdown of the entire network. With transitions across physiologic states (e.g., sleep-stages), the dynamics of physiologic systems as well as their interaction may change. Identifying and quantifying dynamical networks of diverse systems under varied physiologic conditions is a challenge due to the complexity in the dynamics of individual systems and the transient and non-linear characteristics of their coupling.

We introduce a novel computational method based on the concept of time delay stability, and we utilize complex network approaches to identify and quantify dynamic links among physiologic

organ systems. We analyze large data bases of continuously recorded multi-channel physiologic data from healthy young subjects during hours of night-time sleep. This allows us to track the dynamics and evolution of the physiologic network across well-defined physiologic states (e.g., sleep stages). We study the network of interactions for an ensemble of key integrated physiologic systems (cerebral, cardiac, respiratory, ocular and muscle activity). We focus on transitions in the topology and dynamics of the network and their association to physiologic function.

We develop the first map of dynamic network interactions between key physiologic systems in the human organism. We find that each physiologic state is characterized by a specific network structure, demonstrating a robust interplay between network topology and function. Across physiologic states the network undergoes topological transitions associated with fast hierarchical reorganization of network links on time scales of a few minutes, indicating a remarkable network flexibility in response to perturbations.

With this computational network approach, we demonstrate for the first time on real data a direct association between network topology and network function.

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16 **Ronny Bartsch**, *Boston University (USA)*

Phase Synchronization and co-existing forms of non-linear coupling between physiologic systems

Co-authors: Kang Liu, Plamen Ivanov

Multiple-component physiologic systems, such as the cardiac and respiratory system, exhibit complex dynamics that are further influenced by intrinsic feedback mechanisms controlling their coupling. The nature of cardio-respiratory coupling, and whether it changes with transitions across different states and conditions is not understood. Since key scale-invariant, fractal, linear and nonlinear properties of the cardiac and the respiratory system change across different sleep stages, we expect that also the cardio-respiratory coupling would be influenced by those transitions. We develop an algorithm suitable to identify phase-synchronization and non-linear coupling between oscillators in chaotic regime. We apply this algorithm to analyze continuous 8-hours multi-channel recordings of 200 healthy subjects during sleep. We quantify the adjustment of rhythms between heartbeat and breathing signals, and we investigate how cardio-respiratory synchronization changes with sleep-stage transitions and with aging. We find pronounced phase transitions in cardio-respiratory coupling and a significant decline of synchronization with age.

Specifically, cardio-respiratory coupling abruptly changes up to 400% with transition from one sleep stage to another, reminiscent to phase transitions in physical systems. Moreover, we find that the degree of coupling strongly depends on the specific sleep stage, forming a robust sleep-stage stratification pattern observed for all subjects and over all age groups. Finally, we uncover that cardio-respiratory phase synchronization coexists with other forms of non-linear coupling between the cardiac and respiratory system, indicating an a-priory unknown non-linear mechanism of simultaneous communication through different channels of interaction.

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17 **Kristina Streu**, *Boston College (USA)*

Stability of stapled p53 peptides bound to MDM2

Co-authors: Zuojun Guo, Goran Krilov, Udayan Mohanty

The stabilization of secondary structure is believed to play an important role in the peptide-protein binding interaction. In this study, the α-helical conformation and structural stability of single and double stapled all-hydrocarbon cross-linked p53 peptides when bound and unbound to MDM2 are investigated. We determined the effects of the peptide sequence, the stereochemistry of the cross-linker, the conformation of the double bond in the alkene bridge, and the length of the bridge, to the relative stability of the α-helix structure. The binding affinity calculations by WaterMap provided over one hundred hydration sites in the MDM2 binding pocket where water density is greater than twice that of the bulk and the relative value of free energy released by displacing these hydration sites. In agreement with experimental data, potential of mean forces (PMFs) by weighted histogram analysis method (WHAM) indicated the order of peptides from lowest to highest binding affinity. Our study provides a comprehensive rationalization of the relationship between peptide stapling strategy, the secondary structural stability, and the binding affinity of p53/MDM2 complex. We hope our efforts can help to further the development of a new generation of p53/MDM2 inhibitors that can reactivate the function of p53 as a tumor suppressor gene.

18 **Johannes Bock**, *University Leipzig ITP (Germany)*
Semi-flexible polymers in disordered media
Co-authors: Wolfhard Janke

We report computational studies of the behavior of semi-flexible polymers in disordered media. An off-lattice chain growth algorithm based on the Monte Carlo method is used to examine configurational properties of the polymers such as the end-to-end distance and tangent-tangent correlation. Particular attention is paid to the effects of the disordered environment on the properties of the polymers. These studies are validated by comparison with previous work done in our group in two dimensions, which is now expanded into the third dimension.

19 **Alemayehu Mengesha Cherkos**, *Instituto Superioro Tecnico (Portugal)*
Effect of viscosity on Propagation of MHD Waves in Astrophysical Plasma

We have investigated the sixth-order dispersion relation and we determine the general dispersion relation for the propagation of magnetohydrodynamic (MHD) waves in an astrophysical plasma by considering the effect of viscosity with an anisotropic pressure tensor. Basic MHD equations have been derived and liberalized by the method of parturition to develop the general from of the dispersion relation equation. We discussed the solutions of the dispersion relation in various special cases corresponding to the standard wave mode of stability and instability zero β, low β and high β plasmas. Our finding indicates that the presence of viscosity in a strong magnetic field gives reasonable physical meaning for stability and instability of different modes with considerable wavelength and for different limits of β.

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20 **Sumantra Sarkar**, *Brandeis University (USA)*
Shear Induced Rigidity in Athermal Solids
Co-authors: Bulbul Chakraborty

Shear plays a dominant role in shaping the collective behavior of systems where thermal fluctuations are irrelevant. Recent studies of athermal systems such as dry grains and dense, non-Brownian suspensions have shown that shear can lead to solidification through the process of shear jamming in grains and discontinuous shear thickening in suspensions. The similarities observed between these two distinct phenomena suggest that the physical processes leading to

shear-induced rigidity in athermal materials are universal. In this talk, we present a model that provides a unified statistical mechanics framework for these shear-driven transitions. The model exhibits the phenomenology of shear jamming and discontinuous shear thickening in different regions of the predicted phase diagram. Our analysis identifies the crucial physical processes underlying shear-driven rigidity transitions, and clarifies the distinct roles played by shearing forces and the density of grains.

21 **Yoelvis Orozco-Gonzalez**, *BGSU/USP (USA)*

Implementation of the free energy gradient to the geometry optimization of molecular systems in complex environments

Co-authors: Sylvio Canuto, Massimo Olivucci

In this work a methodology is developed for performing the geometry optimization in the free energy surface of molecular systems surrounded by complex environments like the protein cavities and solvents. This methodology is based on the idea of Nagaoka et al. [1] and allows determining the gradient and Hessian of a hybrid QM/MM Hamiltonian [2] of a molecular system embedded in an average external field. Here this external field is generated by a set of superimposed uncorrelated configurations which mimics the configurational ensemble of the system into thermodynamic equilibrium, ASEC model [3]. Therefore, the free energy geometry optimization is performed here using an iterative procedure where the superimposed ensemble selected in a molecular dynamics simulation step is then used to calculate the gradient and Hessian of the free energy with respect to the coordinate of the quantum subsystem (e.g. a protein chromophore) and optimize it. The improved geometry and charges of the quantum subsystem are then updated and used in the next iteration. This methodology was successfully applied to the geometry optimizations of two transition states and ground state of the 11-cis retinal chromophere of bovine Rhodopsin and of two isomers of the Anabaena Sensory Rhodopsin containing the 13-cis and all-trans chromophores. The spectroscopic properties of the optimized structures and the height of the barriers show good agreement with the experimental and previous theoretical results.

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22 **Md Zulfikar Ali**, *Clark University (USA)*
In silico evolution of biochemical networks
Co-authors: Ned S Wingreen, Ranjan Mukhopadhyay

We are studying in silico evolution of complex, oscillatory network dynamics within the framework of a minimal model of protein-protein interactions. We consider N protein species, each with the same total concentration. Each species is either a kinase (activator) or a phosphatase(inhibitor). Each protein can either be phosphorylated(active) or unphospphorylated (inactive). Active proteins bind to and can then modify their target based on their interaction strengths. As the system is evolved the interaction strength is modified. This model can be studied for non-trivial behavior e.g. oscillations, chaos, multiple stable states. We are trying to relate evolution to design principles of biochemical oscillatory networks with desired amplitude, frequency etc. We also study network drift in 3-component system where each component is a protein species. Starting with 2 component system third component is added with zero interaction. The system is then allowed to evolve with the constraint that it continues to oscillate and the behavior of the network is studied.

3 Materials Science and Nanoscience

1 **Victoria Mazalova**, *Southern Federal University (Russia)*
The combined XANES and DFT approach for study of nanomaterials.

As most properties depend on the fine details of local atomic structure, the diagnostic methods to control structural parameters, such as the distances between the atoms, with very high precision are required. In this research X-ray absorption spectroscopy is used to study the geometry of several types of nanomaterials. In addition, a detailed interpretation of the experimental XAS (X-ray Absorption Spectroscopy) data requires strong theoretical support, which will be provided in the present study by model spectra, based on non-muffin-tin (full potential) framework and DFT (Density Functional Theory) calculations. The main goal of the research is to apply recently developed cutting-edge method for the determination of 3D local geometry and electronic structure of condensed materials without long range order of atoms for studying of modern nanomaterials. This approach includes x-ray absorption spectroscopy in EXAFS (Extended X-Ray Absorption Fine Structure) and XANES (X-ray Absorption Near Edge Structure) regions followed by advanced theoretical analysis of XANES data using both real space self-consistent full-multiple scattering theory and very recently developed non-muffin-tin (full potential) framework, Molecule Dynamics and advanced DFT scheme to initial geometry optimization. As a result of the research important novel insight into structure – properties relationship in of modern nanomaterials can be done.

2 **Edwin Mapasha**, *University of Pretoria (South Africa)*
Van der Waals Density Functional Study Of LIthium on Bilayer Graphene
Co-authors: Nithaya Chetty

We have systematically investigated the effects of lithium (Li) on AA and AB stacking sequences of bilayer graphene using density functional theory (DFT). To accurately describe the bonding that occurs in bilayer graphene, the following van der Waals corrected exchange correlation functionals were used, namely, vdW-DF revPBE, vdW-DF C09x and vdW-DF2 C09x. Several configurations that contain two Li atoms were considered to examine the effects of the Li-Li interaction on bilayer graphene. For all configurations considered, we observe a variation in formation energies predicted by these functionals. The vdW-DF revPBE consistently predicts the highest formation energies, and vdW-DF2 C09x gives the lowest. One of the Li-configurations c10(AB) undergoes a spontaneous translation from the AB to AA stacking, and is found to be the most energetically stable configuration compared to the other configurations. It is found that the change in the interlayer distance caused by Li intercalation greatly depends on the exchange correlation functional used. The GGA-PBE shows a reduction in the interlayer distance while the van der Waals corrected exchange correlation functionals show an expansion. In the case of Li intercalated configurations, GGA gives nearly the same interlayer distances as vdW-DF revPBE, unlike in the pristine structures. The agreement of these two functionals is explicitly discussed. Even if the construction of these van der Waals corrected exchange correlation functionals was basically on the energetics (stability) and structural properties, our calculated workfunction for pristine bilayer graphene obtained using i.e vdW-DF2 C09x agrees very well with the experimental data compared to GGA-PBE.

3 **Sergei Zakharchenko**, *Moscow Institute of Physics and Technology (Russia)*
Algorithm of Shaping Multiple-beam Bragg's Acousto-optic Diffraction Laser Field Into 1D and 2D Patterns
Co-authors: Andrew Baturin

Precise shaping of laser beam has recently become of great technological importance due to its possible applications in various fields of science and technology [1-2]. For instance, the use of a multi-point laser in confocal laser scanning microscopy helps to improve overall performance of the method, which is crucial for investigation of ultra-fast processes in biology. Shaping the laser beam into confining potentials found its application for creation and subsequent manipulation of Bose-Einstein condensate. Laser beams shaped into 2D patterns can replace conventional micromirror scanning in stereolithography. These applications require new rigorous algorithms for near real-time data processing with the delay between the incoming pattern and calculated acoustic drive signal of up to a few seconds. A parallelizable computational algorithm is proposed to solve the direct problem of modeling acousto-optic interaction between laser emission and acoustic signal consisting of a set of equidistant frequency components. The infinite system of coupled wave differential equations is reduced to sparse eigenvalue problem by limiting the highest rediffraction order taken into the model and summing the components related to

appropriate trajectories in the phase space. The contribution of the higher rediffraction orders is analyzed separately. Inverse problem of finding an optimal set of equidistant frequency components of the driving acoustic signal to form the desired diffraction pattern in Bragg field efficiently (up to 95%) is also considered and a few optimization approaches are analyzed. Heuristic method of splitting 2D pattern into subframes, each suitable for simultaneous projection by a two-axis acousto-optical deflector with multifrequency acoustic driving signal, is developed.

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4 **Seiki Saito**, *Kushiro National College of Technology (Japan)*

Study on Hydrogen Plasma - Carbon Material Interaction by Molecular Simulation in Submicron Scale

Co-authors: Atsushi M Ito, Arimichi Takayama, Hiroaki Nakamura

Carbon material is employed for the plasma facing material in plasma experimental device. For example, isotropic graphite materials are used for the divertor plates of Large Helical Device (LHD) in National Institute for Fusion Science, Japan. Development of the control technique of the surface erosion and hydrogen retention processes are the key issue for the achievement of steady state operation of nuclear fusion reactor. Deep understanding of the erosion and retention processes are required for the development of the control technique. Molecular dynamics (MD) simulation is one of powerful tools for the investigation of carbon-hydrogen interaction in atomic scale. Although, grain size of graphite is submicron order, MD simulation is difficult to apply for such large scale system because of its computation time. A typical scale length of the MD simulation in our simulation is several nm. There is another method called binary-collision-approximation-based (BCA) simulation. BCA simulation can apply the system in submicron scale. However, BCA simulation is weak at low energy interaction. For the calculation of carbon material interaction with chemical interaction in submicron scale, we develop a hybrid simulation [1-3] technique of MD and BCA simulations. We perform a simulation of hydrogen injection into polycrystalline graphite by the hybrid simulation. Polycrystalline graphite is prepared by arranging single crystalline graphite with random crystal angle. From this simulation, it is seen that hydrogen atoms are trapped in an interlayer of graphene sheets when their kinetic energy becomes lower than 100 eV. This phenomenon is called "channeling". Moreover, the grain size dependence of the penetration depth from surface of the target material is also investigated. From the investigation, it is seen that the penetration depth becomes shorter as grain size becomes shorter. It is because the random structure of grain boundary causes dechanneling of hydrogen atoms.

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5 *Cancelled*

6 **Esam Abdul-Hafidh**, *Royal Commission (Saudi Arabia)*
Modulus of Spherical Palladium Nanoparticles by Chen-Mobius Lattice Inversion Method

Palladium is a precious and rare element that belongs to the Platinum group metals (PGMS) with the lowest density and melting point. Numerous uses of Pd in dentistry, medicine and industrial applications attracted considerable investment. Preparation and characterization of palladium nanoparticles have been conducted by many researchers, but very little effort has taken place on the study of Pd physical properties, such as, mechanical, optical, and electrical. In this novel study, Chen-Mobius lattice inversion method is used to calculate the cohesive energy and modulus of palladium. The method was employed to calculate the cohesive energy by summing over all pairs of atoms within palladium spherical nanoparticles. The cohesive energy has been calculated by inverting the potential energy function proposed by (Rose et al., 1981). The modulus is derived from the cohesive energy curve as a function of particles' sizes. Due to lack of experimental measurements for the modulus of Pd, the results are found to be comparable with previous predictions of Ag nanoparticles which lies in the same period of the periodic table.

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7 **Alexander Popov**, *Lomonosov Moscow State University (Russia)*
Multiscale simulation of thermal disruption in resistance switching process in amorphous carbon
Co-authors: Nikolay Nikishin, Georgiy Shumkin

The switching of material atomic structure and electric conductivity are used in novel technologies of making memory on the base of phase change. The possibility of making memory on the base of amorphous carbon is shown in experiment [1]. Present work is directed to simulation of the experimentally observed effects. Ab initio quantum calculations were used for simulation of atomic structure changes in amorphous carbon [2]. These simulations showed that the resistance change is connected with thermally induced effects. The temperature is supposed to be the function of time. In present report we propose a new multiscale, self-consistent model

combines three levels of simulation scales and takes into account the space and time dependencies of the temperature. On the first level of quantum molecular dynamic we provide the calculations of phase change in atomic structure with space and time dependence of the temperature. Noose-Hover thermostats are used for MD simulations to reproduce space dependency of the temperature. It is shown that atomic structure is localized near graphitic layers in the center of conducting dot. Structure parameter is used then in the next levels of the modeling. Modified Ehrenfest Molecular Dynamics is used on the second level. Switching evolution of electronic subsystem is obtained. In macroscopic scale level, the heat conductivity equation for continuous media is used for calculation space-time dependence of the temperature. Joule source depends on structure parameter evolution and electric conductivity profiles obtained on previous level of modeling. Iterative procedure is self-consistently repeated combining three levels of simulation. Increase of the space localization of Joule heat source leads to the thermal disruption. Obtained results are permitted to explain S-form of the volt-ampere characteristic observed in experiment. Simulations were performed on IBM Blue Gene/P supercomputer at Moscow State University.

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8 **Yasunari Zempo**, *Hosei University (Japan)*

Development of the SSPH Method for Real-Space Electronic Structure Calculation

Co-authors: Soichiro Sugimoto

The real-space approach is widely used for electronic structure calculations based on density functional theory [1]. In particular, it is used for large systems that include many atoms, because a real-space mesh is suitable for large-scale parallel computing. The real-space approach also allows the capture of a clear physical image because it does not use an explicit basis such as a plane wave or Gaussian basis sets. For the simplest real-space implementation, the higher-order finite-difference method is employed as the discretization technique. There are also real-space implementations using finite-element and meshfree methods. These methods have an advantage in their non-uniform distribution of computation points, which also reduces computational costs. Smoothed particle hydrodynamics (SPH) is a typical meshfree particle method, in which the system is represented by a finite set of arbitrarily distributed particles without using any mesh [2]. Since SPH is known for its low accuracy, various types of SPH methods have all been proposed as alternatives. These methods improve the accuracy of SPH using the Taylor series expansion. In this study, we employ the symmetric smoothed particle hydrodynamics (SSPH), because it is the simplest method in the higher-order series expansion [3]. This study evaluates the accuracy of SSPH for electronic structure calculation applications, whose solutions are well known such as

simple atoms and small molecules. The results are then compared to the higher-order finite-difference method. In this paper, we will demonstrate that the SSPH method based on the higher-order Taylor series expansion provides similar accuracy as the higher-order finite-difference method. We believe that SSPH can be readily applied in real-space electronic structure calculations that require high accuracy. The detail will be discussed in the presentation.

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Eigen Frequency Piezoelectric Resonance Modes in Terms of Longitudinal Temperature Gradient Stimulated by Second Harmonic Generation

Co-authors: Oleg Ryabushkin

Nowadays second harmonic generation (SHG) is widely used in order to extend spectral range of conventional laser sources. SHG efficiency depends on phase velocities of interacting waves. Refractive index of the crystal depends on its temperature. Crystal 3D temperature distribution is crucial [1,2]. For measurement of thermodynamic temperature of laser heated crystal we have introduced the concept of equivalent temperature [3]. Its determination is based on piezoelectric eigen frequencies dependence on temperature. Theoretical analysis of crystal piezoelectric resonance frequencies dependence on nonuniform temperature distribution was performed in [4]. However longitudinal temperature distribution was not taken into account. SHG effects crystal temperature distribution and in turn temperature has influence on SHG. Thereby we should solve problem of 3 equation systems. First refers to the SHG in crystal, second is 3D heat conduction equation and the last one relates to crystal acoustic vibrations, excited by external radiofrequency electric field. As far as crystal vibration amplitudes are relatively small the impact of vibration on SHG and crystal heating is negligible. So that just nonlinear-optical processes and crystal heating should be considered simultaneously and problem of finding crystal eigen frequencies can be solved separately. Simple 1D SHG model was considered assuming slow varying amplitude approximation. Crystal longitudinal temperature dependence was also taken into account. Rayleigh-Ritz variation method was employed for solving 3D heat conduction equation assuming convective cooling boundary condition. Both equation systems were solved separately. By substituting solution of each system as an initial condition for another one the equation iteration procedure was performed. Problem of crystal eigen modes was solved by minimization of Lagrangian (includes kinetic, elastic, piezoelectric and electric field energies).

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10 **Stylianos Karozis**, *National Center for Scientific Research "Demokritos" (Greece)*
A non-stochastic computational approach for the determination of the surface area of microporous solids
Co-authors: Georgia Ch Charalambopoulou, Theodore A Steriotis, Michael E Kainourgiakis

The accurate, fast and reliable determination of the surface area and pore volume of microporous materials is receiving great attention due to the extensive applications of such materials (e.g. zeolites, Metal-Organic Frameworks (MOFs) etc.) in highly important industrial processes (catalysis, adsorption etc.). The most popular method for deriving the surface area of a porous solid is based on a standard protocol where the BET theory is used for the analysis of nitrogen adsorption data at 77 K. This approach can be virtually replicated with a Grand Canonical Monte Carlo (GCMC) simulation, which is essentially a digital experiment. Alternatively one can consider the use of geometric shapes, such as spheres, to represent the van der Waals surface of the atoms constructing the porous media. Measuring stochastically the free surface of the spheres gives the surface area of porous material. In the present work, we present a new methodology for creating and calculating the surface area of microporous media. In brief, the surface area is assumed to be the result of the interaction of atoms subjected to an atomistic forcefield (e.g. Lennard-Jones), and subsequently is shape independent. The structure is discretized with voxels which are filtered according to certain criteria (i.e. whether a voxel is occupied by a gas molecule or not) in order to produce a "phase" function representing the spatial distribution of matter in the biphasic porous medium. The specific surface area is then calculated by the correlation function of the phase function, a method well established for the calculation of the specific surface area in mesoporous media. In order to validate our method we chose as case studies well-established MOF structures, a new class of microporous materials with high surface areas and extremely interesting properties for a great number of applications. The obtained calculation results are compared with experimental and GCMC simulation literature data.

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11 **Tom Underwood**, *University of Edinburgh (UK)*
Which crystal structure? Lattice-switch Monte Carlo can tell you
Co-authors: G J Ackland

One of the primary aims of theoretical materials science is the accurate determination of the phase diagram of a given substance. Put another way: for a given substance, where in phase space do the phase transitions occur? This question is difficult to answer for solid-solid transitions. Surprisingly, the difficulty is by no means limited to 'realistic' models of solids: the location of the hcp-fcc transition for the Lennard-Jones solid – an archetype of a 'simple' model of a solid – remained contentious until relatively recently [1]. The method which resolved the Lennard-Jones dispute – lattice-switch Monte Carlo (LSMC) [2,3] - is the subject of this work. In LSMC a type of move is introduced which 'switches' the underlying crystal lattice, while leaving the displacements of the particles from their lattice sites unchanged. Furthermore, one preferentially biases microstates from which 'lattice switches' are more likely. The result is that microstates pertaining to both crystal structures are explored in a single simulation of reasonable duration. Information gathered during the simulation is then used to evaluate the free energy difference between the crystal structures – which is zero at a transition point. As well as being both computationally efficient and relatively simple to implement, one crucial benefit of this method is that it provides an uncertainty for the free energy difference. As with other Monte Carlo methods, this uncertainty can of course be reduced by increasing the simulation time. LSMC is a general technique, and can be applied to a variety of crystal lattices and particle interactions; our ultimate aim is to interface the technique with ab initio codes. The method has even been applied to a solid-fluid transition [4]. Here, I will focus on describing the technique, but will also present some preliminary results pertaining to the iron fcc-bcc transition examined using embedded atom potentials.

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12 **Zenan Qi**, *Boston University (USA)*
Highly Ductile Graphene Kirigami
Co-authors: David Campbell, Harold Park

Graphene's exceptional mechanical properties have been exploited for various structural applications. However, graphene is also known to be brittle, with experimentally measured tensile fracture strains that do not exceed a few percent. Using classical molecular dynamics simulations, we introduce the notion of graphene "kirigami," which can dramatically enhance the ductility of graphene. Whereas the more familiar graphene "origami" involves solely folding of the graphene layer, with kirigami both folds and cuts are allowed. Specifically, we show that the yield and fracture strains of graphene can easily be doubled or tripled using kirigami as compared

to standard graphene nanoribbon. Yield stress, Young's modulus and toughness are also studied. This special mechanical response in graphene kirigami should open up interesting opportunities in both mechanical and electronic behaviors. Authors thank NSF, Boston University Mechanical Engineering and Physics Departments.

13 **George Lithoxoos**, *National Center for Scientific Research "Demokritos" (Greece)*

Determination of partial charges in inorganic-organic clusters based on DFT calculations

Co-authors: Stylianos N Karozis, Georgia Ch Charalambopoulou, Theodore A Steriotis, Nikolaos I Papadimitriou

Nanostructured materials are of major interest in many sectors such as environment, energy and biosciences as they find numerous applications (e.g. as carriers, sorbents, composites etc.) in processes of high industrial significance. On the molecular level, the determination of partial charges on such materials is necessary for the estimation and explanation of their unique properties. In the present study we have calculated the partial charges in atomic inorganic – organic clusters that can be met as key structural components of a wide range of materials, spanning from nanoporous matrices (such as Metal Organic Frameworks) to systems of biological relevance. In order to study these clusters we have used ab initio calculations on the DFT level of theory. In such studies the proper definition of the atomic cluster is important since the results will play a significant role in the construction of the forcefield that later will be used for the estimation of particular properties of the system. We have used several model clusters in a systematic way in order to show these differences and locate the most appropriate one. For the saturation of these clusters methyl, phenyl and carboxylic groups were used. The B3LYP functional was chosen for the calculations while the 6-31G* basis set was used for all except the heavy atoms [1]. When heavy metals (such as Zn and Zr) are considered, the LANL2DZ was used for the reduction of the computational time. LANL2DZ belongs to the effective core potential (ECP) basis sets that are largely used for heavy transition metals. The calculations were performed using the nwchem program [2]. For the derivation of the partial charges the ESP module was chosen that uses grid points in order to fit the quantum mechanical electrostatic potential. In all cases it is seen that the distribution of the partial changes is greatly affected by the respective chemical environment.

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14 **Katsuhiko Higuchi**, *Hiroshima University (Japan)*

Electronic structure calculations for materials immersed in a uniform magnetic field via the relativistic tight-binding approximation method

Co-authors: Dipendra Hamal, Masahiko Higuchi

The softening in elastic constants of the silicon has attracted much attention because the density of silicon vacancies can be evaluated from it[1]. It is also reported that the elastic softening is suppressed by an external magnetic field in the boron-doped silicon[1]. Several papers concerning such phenomena have been published so far, and it is pointed out that the spin-orbit interaction plays an important role on them as well as the Zeeman effect[2-5]. In this study, we develop the relativistic tight-binding (TB) approximation method that enables us to calculate electronic structures of materials immersed in a uniform magnetic field, in order to reveal the mechanism of the suppression of the elastic softening. As compared with the previous work by Hofstadter[6], in which the TB approximation method for Bloch electrons in the uniform magnetic field is based on the so-called Peierls substitution, the present method has two striking features. One is that it is applicable not only to a simple model such as a s-band model[6] but also to various kinds of real materials. Another one is that the present method takes into account the relativistic effects fully. The validity of the present method is confirmed by revisiting the so-called Hofstadter butterfly diagram. Namely, if the present method is applied to the s-band model in the two-dimensional square lattice, and if relativistic effects and the Zeeman effect are neglected, then the present method reproduces the Hofstadter butterfly diagram. We also apply the present method to silicon. The characteristic gap structures (deformed butterfly diagram) can be seen in the energy diagram if the wavevector of the magnetic Bloch function, which lies in the magnetic Brillouin zone, is restricted in the plane perpendicular to the magnetic field. It is expected that the present method would be useful to the investigations of electronic states of silicon vacancies and the elastic constant softening.

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15 **Grigory Kolesov**, *Harvard University (USA)*

Methoxy photo-dissociation on TiO2 surface: ab initio excited-state dynamics

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Photocatalysis on semiconductor surfaces is a subject of extensive research in the quest for renewable energy and green materials. Photocatalytic methoxy splitting on rutile TiO2 (110) surfaces has previously been observed in experiments in vacuum [1]. Here we study the excited-

state dynamics of this process using the Ehrenfest approximation within time-dependent density functional theory (TDDFT). To overcome the technical challenge of simulation of the dynamics of large extended systems at long times, we develop a methodology based on atom-centered localized basis functions which allows for order of magnitudes faster simulation times in comparison to the existing implementations, while providing essentially the same results. We demonstrate that while methoxy splitting does not occur spontaneously during normal thermal motion, it does occur at about ~70 fs after the photoexcitation. A complex, dynamic polarization pattern is observed to emerge at the absorbed methoxy group and to ultimately drive the transition of a hydrogen atom from the methoxy group to the bridging oxygen on the surface.

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16 **Nicolas Sawaya**, *Harvard University (USA)*

Computational Design of Excitonic Structures with DNA: Beyond Förster Resonance Energy Transfer

Recently many researchers have used DNA as a scaffold for the accurate placement of molecules and for the design of arbitrary supramolecular structures. Functional mechanical devices have even been designed and synthesized. The specificity, addressability, and predictability of DNA structures allow for the placement of light-absorbing dyes in arbitrary patterns with sub-nanometer precision. In the Förster limit, theoretical methods have been successful in predicting excitonic behavior when dyes are well separated. Here we present a computational scheme that is valid when close dye spacing causes the Förster approximation to break down, for use in designing and predicting the properties of DNA-based excitonic structures. In such structures, it is necessary to consider the coherent effects between the dyes' excited states. Our multi-level scheme uses molecular dynamics simulations and quantum chemical calculations to obtain accurate dye couplings and noise parameters. The resulting excitonic Hamiltonian is then used to simulate exciton diffusion as well as absorption and circular dichroism spectra. We propagate the excitonic wave function with a stochastic Schrodinger equation formalism and with a variation of the Redfield theory. We have used this method to design a light-harvesting structure that mimics a photosynthetic complex found in nature. This computational pipeline is a step towards allowing researchers to design nanoscale structures with tunable excitonic properties.

17 **Khellil Bouamama**, *University Setif 1 (Algeria*

Ab-initio calculation of the structural and elastic properties of ternary metal nitrides TaxMo1-xN and TaxW1-xN

Co-authors: Mohamed Benhamida, Philippe Djemia

First-principles pseudopotential calculations of the lattice constants and of the single-crystal elastic constants for ternary metal nitrides TaxMo1-xN and TaxW1-xN alloys were carried out. The cubic B1-rocksalt structure is considered. These calculations were performed using density functional perturbation theory (DFPT). For the exchange-correlation potential, we used the generalized gradient method (GGA). For the treatment of the disordered ternary alloy, we have used the virtual crystal approximation VCA in which the alloy pseudopotentials are constructed within a first-principles VCA scheme. The supercell method (SC) was also employed in order to check the reliability of the VCA results. We find that the formation energy remains negative for both TaxMo1-xN and TaxW1-xN alloys in the whole composition range which implies that these cubic TaxMo1-xN and TaxW1-xN ordered solid solutions are stable. The calculated equilibrium lattice parameters exhibit a deviation from the Vegard's rule with a bowing parameter that depends on the transition metal. We have investigated the effect of alloying Mo and W on the trend of the mechanical properties of TaN. The shear elastic constant C44 and the Cauchy pressure (C12–C44) are used to discuss the mechanical stability of the structure and the brittle/ductile behavior. We have also investigated the effect of alloying the Ta on the trend of the elastic properties of MoN and WN to determine the onset transition from unstable structure to the stable B1-rocksalt one. Moreover, in the frame work of the anisotropic elasticity, we have estimated, by the homogenization methods, the averaged stiffnesses <Cij>, dtheirection dependent Young's moduli and the Poisson's ratios of some polycrystalline TaxMo1-xN and TaxW1-xN alloys considering a {111} crystallographic fiber texture.

18 **Nikolaos Papadimitriou**, *National Center for Scientific Research "Demokritos" (Greece)*

Evaluation of the Efficiency of Clathrate Hydrates in Storing Energy Gases

Co-authors: Ioannis Tsimpanogiannis, Ioannis Economou, Athanasios Stubos

Clathrate hydrates are crystalline materials made of water molecules. Their crystal lattice consists of cavities where gas molecules can be entrapped. As such, they have attracted extensive interest as potential materials for the storage of energy-related gases (e.g. hydrogen, methane, carbon dioxide). We have used Monte Carlo simulations to examine the efficiency of several hydrate structures in storing hydrogen or methane. The simulations are performed in the Grand Canonical ensemble (GCMC) with the MCCCS Towhee code. In this way, the hydrate lattice is treated a solid substrate where gas adsorption takes place. The most common hydrate structures (sI, sII, sH) are examined over a wide range of temperature (200 - 300 K) and pressure (up to 500 MPa). Different water models (SPC/E, TIP4P/Ice, TIP5P) have been used to examine the effect of the selected model on the simulation results. Moreover, several gas models for hydrogen and methane were tested. Special focus is given to the study of multiple occupancy, i.e. the presence of more than one gas molecules in the same hydrate cavity. This effect occurs in the case of

hydrogen hydrates and may drastically increase their storage capacity. In close agreement with the literature and regardless of which water model is used, the small cavity of hydrates cannot store more than one hydrogen molecule. However, the large cavities of sI and sII structures as well as the medium cavity of sH structure can store up to 4 molecules while the large cavity of sH structure can reach an occupancy of 8 molecules. Moreover, a parametric analysis is carried out to quantify the correlation between lattice constant and storage capacity since small changes in the size of the crystal unit cell may induce large changes in the storage capacity, especially in cases with multiple occupancy.

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19 **Asanka Weerasinghe**, *University of Massachusetts Amherst (USA)*
Multiphonon Raman scattering in monolayer WSe2
Co-authors: Jun Yan

We present our experimental studies of two dimensional Tungsten Diselenide (WSe2) atomic films grown on 0001 plane of sapphire substrate with vapor-solid transport method in a 3 feet long three zone horizontal tube furnace. Room temperature Raman scattering and photoluminescence measurements are performed to characterize the sample. We observe well resolved photoluminescence peaks at around 750nm with intensity more than two orders of magnitude higher than the sapphire luminescence, indicating high crystalline quality. Absence of the Raman peak at around 307cm-1 further confirms that the sample is a monolayer. To our surprise the sample exhibits very efficient multiphonon Raman scattering and we observe up to fifth order in harmonics. These intriguing results provide new insights on the assignment of Raman bands that appear in atomically thin WSe2 layers. This work is supported in part by NSF-MRSEC at UMass (DMR-0820506).

20 **Seyedeh Nazanin Khatami**, *University of Massachusetts Amherst (USA)*
Optimizing Si1−xGexSi1−yGey Superlattices for Thermoelectric Efficiency by Minimizing thermal Conductivity
Co-authors: Zlatan Aksamija

Waste heat can be considered as a major resource of energy. In this case we are able to design next generation of thermoelectric converters that enable us to recover large amounts of waste heat back into useful electric energy [1]. Thermoelectric efficiency is given by a dimensionless figure of merit ZT defined by S2σ/(κe+κL). ZT depends on Seebeck coefficient (S), electrical conductivity (σ) and thermal conductivity (κ). κ e is the thermal conductivity for electron and κ L is the thermal conductivity for lattice. In semiconductors charge is carried by electron while heat is

carried by phonons therefore lattice contribution to thermal parts (kL) dominates the electronic counterparts (ke). Si as a widely available semiconductor has vast investigation in thermoelectric power generation. Recent experiments focused on nanostructured superlattices and varying composition which demonstrate significantly lower thermal conductivity [2]. Solving the single-mode phonon Boltzmann transport equation in the relaxation-time approximation, full thermal conductivity tensor in Si1−xGex/Si1−yGey superlattices was calculated. Interfaces between materials become increasingly important on small scales [3]. Additionally phonon scattering rate and the scattering probability of each phonon at the interface were calculated. Hence we develop a model that accurately predicts the cross-plane and in-plane transport in the superlattices [4]. In summary, by varying thickness and compositions, a result of thermal conductivity 3 to 5 times lower than the bulk form was obtained. As a result an alloy/alloy superlattice has a lower thermal conductivity than bulk SiGe with the same alloy composition. The results are in line with the data provided in reference [5].

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21 **Sanjay Kumar Singh**, *Jiwaji University (India)*

Investigation of high pressure phase transition and electronic properties of Lutetium Nitride

Co-authors: U P Verma

We have systematically investigated the structural, electronic and phase transition properties of the heaviest lanthanide lutetium nitride (LuN) compound using an ab initio calculations based on the density functional theory with Perdrew, Burke and Ernzerhof generalized gradient approximation (PBE-GGA) and Engel-Vosko(EV)-GGA as implemented in WIEN2k code. The basic ground state properties viz., lattice constants (a), bulk modulus (B0) and its pressure derivative (B0') and total energy (E0) are calculated. The calculated values of lattice constant is 4.76 Å which is good agreement with experimental value a= 4.76 Å [1] and other theoretical value [2]. The relative stabilities of LuN at high pressures in the NaCl (B1), CsCl (B2), zinc blende (B3) and body centred tetragonal (BCT) structures are analysed. At compressed volumes, this compound is found to favour the CsCl phase rather the body centred tetragonal phase and zinc blende as observed in other lanthanum pnictides, which has been predicted by the total energy minimization. Under compression LuN undergoes a transition from NaCl to CsCl type structure at around 250.81 GPa with a volume collapse of 3.75%. To see the effect of functional we have also computed the band structure and density of states in B1 and B2 structure. Obtained result on band structure shows that LuN are semimetal by GGA while depicts semiconducting behaviour by EV-GGA. It shows metallic nature in B2 phase. It is obvious from energy versus volume curves that the B1 structure is the most stable at ambient pressure, which is consistent with the experimental results. Due to small band gap in LuN can be used as infrared detector.

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22 **Genri Norman**, *JIHT RAS (Russia)*

On the difference and similarity between plasma-plasma and liquid-liquid first-order phase transitions

Co-authors: Ilnur Saitov, Vladimir Stegailov

A first-order plasma phase transition was predicted by Norman and Starostin [1,2] similar to the Van der Waals equation from the competition of short-range quantum repulsion, long-range effective Coulomb attraction and temperature. The hypothesis initiated theoretical works, see e.g. [3,4]. Experimental evidences are obtained for shock-compressed hydrogen [5-7] and at static pressures [8]. The liquid-liquid phase transition was observed experimentally by Brazhkin et al [9]. The transition was attached to the liquid-solid coexistence curve. The similar triple point is considered for liquid hydrogen [8]. The transitions [9] and [1] supplement each other. The first manifests itself in the vicinity of the triple point, another – in the area near the critical point. Such a coexistence curve was predicted in [2]. The transition [9] was announced as semiconductor-metal transition. Two phases [1] differs by degrees of ionization. Ab initio quantum modeling is applied to check the ideas of [1] and [9] and to analyze both similarity and difference between transitions [1] and [9] as well as with the Wigner metallization. Density of electron states (DOS) is investigated to verify the nature of the transition [9]. The concepts of “degree of ionization” and “free electrons” do not work in dense plasmas. Electron states cannot be classified as only free and bound, contrary to the ideal plasmas. The wide range of the intermediate multi-particle non-stationary fluctuation states spans between free and bound states, the borders being rather diffuse [10]. The range width expands with the increase of plasma density. The excited bound states disappear. Free electrons number density is not an observable value. An approach is developed to study two liquid phases along the coexistence curve. Not only conductivity but also plasma frequency is calculated since the latter is an observable value in any plasmas. A calculation method is developed for dense plasmas and warm dense matter.

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23 **Rabab Zahira**, *University of Agriculture Faisalabad (Pakistan)*
Co-precipitation synthesis, physical and magnetic properties of manganese ferrite powder
Co-authors: Irfan Elahi, Kiran Mehmood, Arifa Jamil

On account of their diverse and fascinating applications in wide technological and scientific fields, the synthesis and characterization of nano-sized magnetic materials have emerged as an important subject during last several years. Among these, ferrites, ferromagnetic having cubic spinel structure (MFe22O4) are complex versatile materials have been extensively investigated by the scientists in view of their unique optical, electrical and magnetic properties [1]. Magnetic manganese ferrite powder was synthesized via chemical co-precipitation techniques using metallic chlorides of manganese and iron. Sodium hydroxide (NaOH) base was used as precipitant agent. The ratio between Fe and Mn was kept at 2:1 respectively. The calcinations were performed at 600°C for 5 h [2]. The structural investigation of the prepared sample was performed with X-ray diffractometer (XRD) and scanning electron microscope (SEM). Magnetic properties were studied by vibrating sample magnetometer (VSM) at room temperature [3, 4]. The crystallite size was 26.53 nm calculated using Sherrer formula. The SEM results clearly indicates that microstructure of the grains of the sample is ultra-small, having an average grain size of 10 μ m. Result indicates that powder exhibited clear hysteresis showing typical magnetic behavior, ferromagnetic, having a non-zero coercivity and remanance. The value of magnetic saturisation 16.36 emu/g, is at B is equal to 6.7 kOe.

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24 **Lin-Lin Wang**, *Ames Laboratory (USA)*
High-throughput Screening of Doped MnBi for Better Permanent Magnets

MnBi has the unique property of increasing coercivity with increasing temperature. As such, MnBi is potentially an excellent material for a permanent magnet up to ~200 C. To explore if we can improve its magnetic properties and stability, we use density functional theory (DFT) calculations to explore the effects of doping on MnBi properties with transition metals (TM). We have studied three types of point defects: a substitutional impurity on a Mn site, an interstitial impurity on a bipyramidal site, and a combination of the two. The high-throughput screening from DFT calculations identifies trends across the TM series in impurity formation energy, magnetic and structural properties – trends explained by both the d-band filling and atomic size effects of the

TM series occupying the larger substitutional site and smaller interstitial site with different coordination. Although no enhancement is found for the magnetization with TM-doping, we find that the increased in-plane lattice constant can be used to enhance the magnetic anisotropy in improving MnBi for a better permanent magnet, which explains the increased coercivity due to thermal expansion effects.

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25 **Berk Onat**, *Harvard University (USA)*
Artificial Neural Networks for Representation of Potential Energy Surface of Li-Si Alloys
Co-authors: Ekin Cubuk, Brad Malone, Efthimios Kaxiras

There is an increasing demand to model the structural evolution of Li-containing Si electrodes, because this is an attractive candidate for the anode of Li-ion batteries. Investigating structural phenomena such as phase transitions and nano-scale dynamics of the Li-Si systems are inaccessible by first-principles approaches because realistic simulations require large numbers of atoms and long time scales. These phenomena can be modeled by interatomic potentials that can capture the dependence of structure on chemical composition. To construct the potential energy surface of Li-Si alloys, we developed a high-dimensional artificial neural network interaction (ANNI) potential based on environment-dependent atomic energy contributions. Compared with the conventional empirical potentials, ANNI potentials generally offer a promising approach to extend the time scales of simulations without sacrificing the accuracy. In our implementation of the ANNI potential for Li-Si alloys we used the feed-forward method of training the network with ab-initio density functional theory data of the systems. Our results show that the potential can predict accurate structures and total energies both for pure Li, Si and for Li-Si alloys with various concentrations of Li.

26 **Farzaneh Shayeganfar**, *Ecole Polytechnique de Montreal (Canada)*
Electronic Properties of Self-Assembled Trimesic Acid on Graphene
Co-authors: Alain Rochefort

In order to study the effect of adsorbed molecules on the electronic structure of graphene, trimesic acid (TMA) in an isolated form, or within a hydrogen-bonded layer and multilayers has been investigated using scanning tunneling microscopy (STM) simulations and density functional theory (DFT) calculations. Carboxylic groups are of particular interest because of their combined donor and acceptor character with respect to hydrogen bonding that can significantly alter π-π interactions between graphene surface and the adsorbed molecules. In terms of charge transfer, the projected density of states indicates that the contribution of π-orbitals to the total charge density is more important than sigma-orbitals. The medium-range attractive forces contribute to bring the COOH groups closer to the surface, hence improving the overlap between π-electron clouds of both species. We will show that both DFT and STM simulations can describe quite subtle

interactions occuring between weakly bonded species and graphene. Most of the STM simulations were performed with the in-house but static Flex-STM package that is based on first-order perturbation theory, and which takes into account different tip geometries. The poster presentation will put emphasis on the using STM simulation images supported by DFT calculation to analysis electronic properties of TMA isolated and self-assembled TMA dimer and trimer adsorbed on graphene.

27 **Sholeh Alaei**, *METU (Turkey)*

Study of Structural, Electronic and Magnetic Properties of (Fe2O3)n Clusters Using Density Functional Theory

Co-authors: Sakir Erkoc, Seifollah Jalili

In this study, the electronic and magnetic properties of (Fe2O3)n (n = 2-5) clusters were studied using Density Functional Theory. It came out that the most stable structures for n = 2, 3 and n = 4, 5 were ferrimagnetic and antiferromagnetic, respectively. The states with completely geometrical symmetry were spin-symmetric also, i.e. had equal atomic magnetic moments. It was found that by increasing 'n', the binding energy (Eb) increased, while such an observation was not seen for n = 4 and n = 5 and the binding energies were equal in these cases. An interesting result was that one of the states for n = 4 (n4-1) was a half-metallic antiferromagnet, which is important in spintronics applications. The most of the considered clusters were semi-metal or half-metal due to presence of Fe atoms.

28 **Angelo Ziletti**, *Boston University (USA)*

Exciton transport and charge separation in artificial light harvesting systems: merging quantum non-adiabatic dynamics with electronic structure theory

Co-authors: David Coker

The semi-classical mapping of the second-quantized many-electron Hamiltonian proposed by Miller and coworkers [1,3] is being merged with the Partial Linearized Density Matrix (PLDM) scheme [2], a quantum dynamical method for the evolution of the density matrix. The combination of the two approaches will allow us to accurately describe electron correlations through real time dynamics. This new approach wants to be a reliable alternative to the cumbersome GW-Bethe-Salpeter approaches[8] used in the solid-state community. The Maximally Localized Wannier Functions[4] are the optimal (and minimal) basis set to accurately describe both electronic and vibrational properties. The method will be applied to exciton transport and charge-separation in artificial light harvesting systems, although it could be applied to a large variety of systems (e.g. strongly correlated systems, metals, semiconductors, insulators, molecules, biological systems).

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29 **Ali Khaledi Nasab**, *Ohio University (USA)*

Localization of Envelop Functions in InAs/GaAs Dome-Shaped Quantum Dots

Co-authors: Roderick Melnik, Mohammad Sabaeain

We have analyzed the localization of envelop functions in dome-shaped InAs/GaAs quantum dots (QDs) under presence/absence of the wetting layer, size variations, and the Woods-Saxon (WS) potential. The Schrödinger equation was solved numerically using the finite element method for a three-level system. The radius of QDs was varied from 1 to 30 nm, both in the presence and absence of wetting layer (WL, thickness of 3nm). In the presence of WL in QDs with increasing radii, WL (quantum well) states are transformed to be QD states and the complete transition (of three states) occurs for a particular radius (R=16nm). A similar event happens for a QD without WL. In particular, it was found that the conversion from unconfined states to confined states in QDs occurred suddenly once the dome radius reaches a specific value (R=10nm) that differs from the one in the case of WL. Analyzing confined QD states for each situation (ground, first, and second excited states), we concluded that there is a critical radius. Additionally, in the absence of WL, the envelop function at low radii is distributed inside GaAs matrices and the localization appears noticeably at the critical radius. Finally, we examined the effect of WS potential on the InAs/GaAs QD system with WL. For the first excited state the leakage of envelop function towards the GaAs matrix was observed. Moreover, the second excited state moves towards the bottom of GaAs matrices (this state used to be completely inside the QD with wetting layer in the case of constant potential). We have also analyzed the feasibility of control over the distribution of envelop function and the amplitudes of energy eigenvalues.

30 **Ali Khaledi Nasab**, *Ohio University (USA)*

Shape-dependent Properties of InAs/GaAs Quantum Dots in Presence and Absences of Wetting Layer

Co-authors: Mostafa Mohammad Rezaee, Amina Alipour, Iman Khazrak

We have carried out a numerical simulation to investigate the optical and electronic properties of InAs/GaAs Quantum dots (QDs). The main contribution of this paper is investigating linear and nonlinear optical properties as well as distribution of envelope functions on different shape of QDs in presence and absence of wetting layer. In absence of wetting layer the dome, conical, cylindrical, ellipsoidal and spherical QDs are being modeled, afterward the wetting layer was added to models for the aim of comparison. It is found the shape as well as presence/absence of wetting layer plays a crucial role in overall properties in QDs. The localization of envelope functions and the amplitude of energy eigenvalues are being investigated versus shape of QDs as well.

31 **Xukun Xiang**, *Michigan State University (USA)*
Atomistic simulation of systems driven through phase transitions by hot electron distributions
Co-authors: Jenni Portman, Phillip Duxbury

A variety of pump-probe experiments are emerging to monitor the ultrafast structural response of materials. Typically a hot electron distribution is generated by an ultrafast laser pulse or by high energy particle beams, such as swift heavy ions. The hot electron distribution then thermalizes relatively quickly, on timescales in the 100fs range, while the lattice response is slower. Structural probes such as ultrafast electron diffraction or ultrafast X-ray diffraction, are able to image the structural response typically on timescales of 100fs to nanoseconds. By integrating molecular dynamics simulations with the two-temperature model[1] that governs the electron and lattice temperatures, we are able to simulate the time evolution of this ultrafast structural response. Our results show the presence of temperature shock waves propagating in the bulk of the material and energy and thickness dependent track formation and healing. We have used this combined model in the simulation of titanium, graphite and phase-change materials (such as Ge2Sb2Se5) using either a Lennard-Jones potential or the Modified Embedded Atom Model (MEAM).

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32 **Nick Materise**, *Northeastern University (USA)*
Evaluation of Periodic Green's Functions on Graphics Processing Units
Co-authors: Hossein Mosallaei, Davood Ansari Oghol Beig, David Kaeli

The evaluation of Green's Functions is at the core of computational electromagnetics (CEM) simulations. Method of moments (MoM) is a popular and effective computational method widely used for numerical solution of problems arising in CEM and optics. MoM solution of problems involving periodic lattices, e.g. optical metamaterials and crystals, requires the evaluation of the so called periodic media Green's functions (PGF). Many methods have been used for evaluation of PGF that by nature involve slowly converging series representations. Among these methods, a simple yet robust technique based on windowed summation has been recently presented which, owing to its simplicity, lends itself to massive parallelization. The intrinsic data and thread parallelism of this algorithm lends itself well to computation on massively parallel devices such as graphics processing units (GPUs). We present the implementation of a PGF, highlighting the relative performance gains, discussing the challenges in porting the algorithm to GPUs, and offering an example computation now afforded by the GPU-optimized PGF.

33 **Aram Shirinyan**, *Kiev University and National Academy of Science (Ukraine)*
The nanophase diagrams of thin films based on molecular static simulations and the size effect
Co-authors: Yuriy Bilogorodskyy, Volodymyr Makara

The energy stability of binary crystalline thin film is investigated taking into account the size dependence of atom-atom interaction [1]. We use the modified atomic hypothesis that the atom-atom interactions in thin solid films are different depending on the thickness and construct the nanophase diagrams based on Gibbs thermodynamics [2]. Due to computer molecular static simulations based on the Morse and Sutton-Chen potentials the effective free energy densities and the size dependence for potential energy of the interaction between neighbour atoms in thin films at zero temperatures is substantiated. The corresponding methodology of phase diagram construction of binary thin nanofilms is offered. The result has been applied for thermodynamic calculations and designing diagrams of metallic Bi-Sn and Bi-Pb nanosystems phases. The results yield the shift of solubility curves and two-phase regions on phase diagrams in thin Bi-Sn and Bi-Pb films due to size effect. Keywords: size effect, atom-atom interaction energy, molecular static simulation, phase diagram, Bi-Sn and Bi-Pb nanofilms.

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34 **Guiping Zhang**, *Renmin University of China*
Effects of Strain on Electronic Transport Property of Graphene Nanoribbons between metallic contacts
Co-authors: Jing Wang, Xiaoqun Wang

Strain in graphene is very common as graphene samples are integrated to substrate and it can affect the electronic structure and transport properties of graphene. In a sample of graphene from chemical vapor deposition, the resistance remains around 7.5KΩ under less than 3% strain, while sharply enhances to 25KΩ under 5% strain [1]. Based on enhancement in the resistance by strain, graphene-based strain sensor was designed in a study in 2013[2]. We study the effects of uniaxial strain on electronic structure and transport properties through graphene nanoribbons (GNRs) between quantum wire contacts by transfer matrix method[3,4,5]. As the stress is along x axis, a zigzag-shaped oscillating band gap occurs in narrow armchair GNRs (AGNRs)[6]. A stable gap in AGNRs converges at thermodynamic limit as the stress is perpendicular to the armchair edge and exceeds a critical value, while all strained zigzag GNRs (ZGNRs) are gapless. Consistent with observations, the conductance through AGNRs and ZGNRs monotonically decreases, when the stress is parallel to the transverse direction. As the stress is perpendicular to the transverse direction, the conductance increases till the gap opens in AGNRs, while monotonically increases

in ZGNRs. Gap in strained AGNRs causes zero conductance around neutral region, and the transmission peak of neutral strained AGNRs is determined by the edge state of strained ZGNRs. The topology of the structure and energy dispersion of GNRs and quantum wire leads to positive and negative correlation between transport through GNRs and bonds parallel to and perpendicular to the transverse direction respectively. Our work provides a comprehensive understanding on the effect of strain on transport through graphene-based materials.

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4 Fluid Dynamics

1 **Yao Shi**, *Northwestern Polytechnical University (China)*
Numerical Simulation of Cavitation Characteristics for Pump-jet Propeller
Co-authors: Guang Pan, Qiaogao Huang

With k-e turbulent model, non-cavitating performance of a pump-jet propeller was obtained by calculating RANS equations. The cavitating hydrodynamic performance of it was calculated and analyzed with mixture homogeneous flow cavitation model based on Rayleigh-Plesset equations and sliding mesh. The effects of different inlet velocity ratio, cavitation number and flow velocity on cavitation characteristics of pump-jet were studied. When the cavitation occurred on the blades, the propeller thrust and torque decreased significantly, thereby causing open water efficiency reduced 15%. For the same cavitation number, as the inlet velocity ratio decreased, the pump-jet propeller blade cavitation phenomenon was more obvious. While for the same ratio, the smaller the number of cavitation, cavitation phenomenon was more remarkable. The more significant was that while the cavitation number was greater than a certain value, the blade cavitation phenomenon disappeared.

2 **Guang Pan**, *Northwestern Polytechnical University (China)*
Numerical Simulation of Drag and Flow Noise Property on Structure for Carrier of Multi-loads AUV
Co-authors: Yao Shi, Qiaogao Huang

The LES with Smagorinsky model and the FW-H equation based on Lighthill acoustic theory were adopted to simulate the sound and flow field with different kinds of structures. Based on the analysis of field, drag and flow noise reduction mechanism of the structures with different shapes and sizes was gotten. The result demonstrate preliminarily that the match between the length and diameter of the cylindrical structure has different effect on the drag and flow noise

reduction. The drag and noise reduction of the model studied in the paper with a length ratio of 0.1 and a diameter ratio of 0.55 is best. The relationship between hemispherical structure diameter and its drag and flow noise reduction effect is monotonic positive.

3 **Aydogan Ozdamar**, *Ege University (Turkey)*
Computational Investigation of Flow Control by Means of Tubercules on Darrieus Wind Turbine Blades
Co-authors: Utku Senturk, Gokhan Ozdamar

This study presents the computational fluid dynamics simulations of the boundary layer control by modifying the blade geometry of a Darrieus Turbine blade for use in wind energy conversion following the tubercule geometry of a humpback whale. The blade is designed for a constant cross section H-type Darrieus turbine. Finite-volume based software ANSYS Fluent was used in the simulations. Using the optimum control parameters for a NACA 0015 blade section with the help of former experimental and numerical studies on tubercule implementation, three dimensional, unsteady, turbulent simulations for the blade were conducted to look for a possible improvement on the performance of the turbine. The effect of several turbulence models were investigated and time-dependent flow phenomena such as separation and stall were examined to understand their impact on the overall performance of the machinery. Turbomachinery performance curves were shown comparatively.

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4 **Lev Barash**, *Landau Institute for Theoretical Physics (Russia)*
Dependence of the fluid convection in an evaporating sessile droplet on the properties of the substrate

Number of vortices in an evaporating droplet essentially depend on the thermal conductivity and the thickness of the substrate, on the contact angle and on the parameters of the fluid. In this work we perform detailed numerical calculations of the effect and find the temperature distribution and vortex structure in a droplet. We present "phase diagrams", which contain information on the number, orientation and spatial position of the vortices. Our results substantially expand the results of a recent paper [2].

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5 **Jinwang Tan**, *Boston University (USA)*
Modeling the growth and morphology of dendrites in Lithium air batteries
Co-authors: Emily Ryan

Dendrite formation on the anode surface of lithium (Li) air batteries plays a significant role in their performance and safety. We use predictive computational methods to model and investigate the growth and morphology of these dendrites within these complex battery systems. Initially, a simple one-dimensional model was developed to study the effects of local mass transport properties on dendrite growth. The one-dimensional system is modeled by the transient mass transport equation. To investigate the effects of dendrite growth on the transport properties of the electrolyte, we implement a functional diffusion coefficient, which simulates the changes in transport properties as the dendrites grow into the electrolyte. A uniform diffusion coefficient model shows good correlation to experimental data of sparse dendrite growth in low current cases; while simulation results of a functional diffusion model could help in understanding dense dendrite growth, which occurs under high current conditions. To further improve the understanding of dendrite growth, a two-dimensional reactive transport model is being developed which uses the smoothed particle hydrodynamics (SPH) method to model the 2-D dendrite morphology. This 2-D SPH model simulates the diffusive transport of lithium ions in the electrolyte, and the reactions of the lithium ions with the anode surface to form dendrites. The complex physics of the systems, such as heterogeneity of the electrode surface, potential/current distribution effects and anisotropic mass transport properties, are included in the model to understand the driving forces of dendrite growth and how they affect the morphology of the dendrites. These studies will help guide the investigation of novel liquid electrolyte solutions to reduce dendrite growth in lithium air batteries.

6 **Ilias Tolias**, *National Center of Scientific Research (Greece)*
CFD simulation of hydrogen deflagration in a vented room
Co-authors: Alexandros Venetsanos, Nikolaos Markatos, Christos Kiranoudis

Hydrogen is a very promising alternative fuel which is expected to play a significant role in the near future. Hydrogen is considered as an excellent alternative fuel due its potential to lead to significant reductions in greenhouse gas emissions and significant improvements in energy efficiency. On the other hand, significant safety issues are associated with it. In the case of an accidental release, hydrogen mixes with air and can form a flammable mixture over a wide range of concentrations. A possible ignition could lead to slow or fast deflagrations, or even detonations. In the present work, CFD simulations of hydrogen deflagration in a vented room are performed. A uniform hydrogen/air mixture with concentration 18% by volume fills a 64m3 chamber. Two square vent sizes were examined: one with 2.7 and one with 5.4 m2 area. The ignition point is located at the wall opposite to the vent (back-wall ignition). Overpressure time series and flame front positions measured in experiment are compared with the computational results. The combustion model is based on the turbulent flame speed concept. The turbulent flame speed is a modification of Yakhot's equation, in order to account for additional physical

mechanisms which involve in hydrogen deflagrations. Special attention is paid to the simulation of Rayleigh-Taylor instability. This instability occurs at the vent area and results in sudden explosion of the mixture that has been pushed outside the chamber at the initial stage of the explosion. The importance of this external explosion to the generated overpressures inside the chamber is highlighted. CFD simulations are based in Large Eddy Simulation (LES) using the ADREA-HF code. The agreement between experimental and computational results is satisfactory in both vent size cases.

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7 **William Lane**, *Boston University (USA)*

Efficient simulations of heated gas-particle flows with immersed horizontal cylinders

Co-authors: Avik Sarkar, Sankaran Sundaresan, Emily M Ryan

In the field of Computational Fluid Dynamics (CFD), scientists are frequently faced with an ultimatum, use a fine mesh at the expense of computational resources or use a coarse mesh at the expense of accuracy. Typically an optimum, medium mesh is chosen to minimize computational time while maximizing accuracy; however, certain problems are highly sensitive to mesh size, e.g., turbulent and multiphase flows, necessitating the use of fine mesh simulations. The Large Eddy Simulation (LES) [1] method was developed to solve this problem for turbulence modeling. In LES the system is simulated using a coarse mesh coupled with a constitutive term in the governing equations that approximates the unresolved physics. We extend these methods to efficiently simulate heated gas-particle flows in fluidized bed reactors, with applications to carbon capture systems. A campaign of highly-resolved, periodic-domain simulations are used to filter the results and constitute a model to predict the cylinder-suspension heat transfer based on the flow conditions and cylinder geometry. This model is then added to the energy conservation equation and employed with coarse grid simulations to efficiently model the heat transfer in gas-particle flows without explicitly resolving the physics of geometry.

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8 **Shreyas Mandre**, *Brown University (USA)*
A reduced model for vortex shedding from a body using matched asymptotics
Co-authors: Xinjun Guo, Ponnulakshmi V K

Flow around a solid body at high Reynolds number is often computed efficiently using inviscid vortex methods, if the distribution of vorticity shed from the surface of the body can be predicted accurately. The only method currently available for predicting the shed vorticity is by the application of the Kutta condition, which applies to slender wings at the leading and trailing edges. This limits the application of vortex methods to cases where the Kutta condition is applicable. Otherwise, computational complexity of vortex methods, which determine the distribution of shed vorticity by explicitly applying the no-slip condition on the surface of the body, is comparable to that of direct numerical solution of Navier-Stokes equations. Therefore, benefit from the high Reynolds numbr approximation is limited to situations where the Kutta condition is applicable. We present a method based on matched asymptotic analysis to compute the strength and distribution of vorticity shed from rigid bodies of arbitrary shape executing arbitrary motion in a uniform far-field flow. The method decomposes he flow domain in an inviscid outer region and a thin viscous boundary layer near the solid body. The flow is approximated by inviscid vorticity dynamics in the outer region and Prandtl's boundary layer theory in the boundary layer. The treatment of the boundary layer dynamics may be considered analogous to the Kutta condition, which yields am approximation to the shed vorticity. An approximately 100-fold increase in computational speed may be achieved using this method compared to direct numerical simulations.

5 Quantum Many-Body Physics

1 **Ying Tang**, *Boston University (USA)*
Monte Carlo studies of spinon deconfinement in two dimensions
Co-authors: Anders Sandvik

In this poster, I will first introduce a quantum Monte Carlo method [1,2] to characterize spinons (emergent S = 1/2 excitations) by their size and confinement length. I will then use this method to look for spinon deconfinement in 2D resonating-valence-bond (RVB) spin liquids and in a J-Q model hosting a quantum phase transition from an antiferromagnet to a valence-bond solid (VBS) at zero temperature [3]. The results confirm that spinons are deconfined in the RVB. Based on results near the critical point of the J-Q model, and comparing with a bilayer Heisenberg model and a 1D spin chain, the spinon deconfinement is marginal in the lowest-energy state in the spin-1 sector, due to weak attractive spinon interactions. Deconfinement in the vicinity of the critical point should occur at higher energies.

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2 **Zhi Wang**, *Sun Yat-sen Univerisity (China)*
Rectification effect in Majorana fermion SQUID

We investigated a SQUID structure formed by a spin-orbit coupling nanowire Josephson junction which contains Majorana fermions, and a conventional superconductor-insulator-superconductor junction [1], motivated by a recent experimental progress in realizing Majorana fermions in a heterostructure of a spin-orbit coupling nanowire and superconductor [2]. It is shown that the critical current of the SQUID is different for two flowing directions, due to the unconventional current-phase relation of the nanowire junction. This asymmetric critical current serves as a simple and direct signature of the Majorana fermion existence. Since the asymmetric Josephson current forms a ratchet potential for the dynamics of superconducting phase [3], a rectification effect is expected when the SQUID is driven by an ac current. That is, a rectified dc voltage appears when a pure ac current is applied. This rectification effect is expected to be useful for probing the Majorana fermion dynamics.

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3 **Adam Iaizzi**, *Boston University (USA)*
1D Valence Bond Solids in a Magnetic Field

A Valence bond solid (VBS) is a kind of long-range nonmagnetic order that can appear in certain quantum spin systems. Recent innovations in models and simulation techniques have enabled large-scale numerical studies of the quantum phase transition from a power-law quasi-Neel-ordered state to the VBS-ordered state. These studies have found evidence for the fractionalization of triplons into deconfined or nearly-deconfined spinons (spin-1/2 bosons) in the VBS phase. We study the VBS order and magnetization as a function of magnetic field in a J-Q2 model using stochastic series expansion (SSE) quantum monte carlo with directed loop updates.

4 **Zhao Liu**, *Princeton University (USA)*
Matrix-Product-State Algorithm for Finite Fractional Quantum Hall Systems
Co-authors: Ravindra Bhatt

Exact diagonalization (ED) has been shown to be a powerful tool to study fractional quantum Hall (FQH) systems. However, its capability is limited by the exponential increase of computational cost with size. In order to overcome this difficulty, Density Matrix Renormalization Group (DMRG)

based algorithms were developed to study larger system sizes. Very recently, it was realized that some model FQH states have exact matrix-product-state (MPS) representation. Motivated by this observation, we have developed an MPS code for finite FQH systems with open boundary conditions, which is closely related to, but different from traditional DMRG schemes. With single-site update and density matrix correction, we show that our code can perform an efficient search of the ground state of various FQH systems. We also compare the performance of our code with traditional DMRG schemes. Compared with the MPS code for infinite FQH systems [Phys. Rev. Lett. 110, 236801], our code is more suitable for studying the physics in finite systems, such as the overlap between wavefunctions and finite-size scaling. Possible generalization of our code to infinite systems is also discussed.

5 **Nils Blümer**, *Gutenberg University Mainz (Germany)*

Tunable nanomagnetism in moderately cold fermions on optical lattices

Co-authors: Elena Gorelik

Localized defects, unavoidable in real solids, may be simulated in (generically defect-free) cold-atom systems, e.g., via modifications of the optical lattice. We study the Hubbard model on a square lattice with single impurities, pairs of nearby impurities, or lines of impurities using numerically exact determinantal quantum Monte Carlo simulations. In all cases, correlations on the "impurity" sites are enhanced either by larger on-site interactions or by a reduced coupling to the environment. We find highly nontrivial magnetic correlations, which persist at elevated temperatures and should be accessible in cold-atom systems with current experimental techniques. With improved cooling techniques, these features could be followed towards generic quantum antiferromagnetism in the homogeneous limit. More generally, tunable crossing points between different correlation functions could be used, in a quantum steelyard balance setup, as robust thermometers [1]. At the heart of this phenomenology are nonlocal dynamical correlations, i.e. physics beyond dynamical mean-field theory (DMFT). Therefore, the observed spin correlation patterns cannot be approximated, let alone reproduced, by real-space DMFT, which is otherwise a quite successful technique in the cold-atom context [2]. They also differ substantially from patterns previously observed in the Heisenberg model [3], for which similar physics has already been explored within the last two decades.

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6 **Nils Blümer**, *Gutenberg University Mainz (Germany)*
Fate of the false Mott-Hubbard transition in two dimensions
Co-authors: Daniel Rost

We have studied the impact of non-local electronic correlations at all length scales on the Mott-Hubbard metal-insulator transition in the unfrustrated two-dimensional Hubbard model. Combining dynamical vertex approximation, lattice quantum Monte-Carlo and variational cluster approximation, we demonstrate that scattering at long-range fluctuations, i.e., Slater-like paramagnons, opens a spectral gap at weak-to-intermediate coupling -- irrespectively of the preformation of localized or short-ranged magnetic moments. This is the reason, why the two-dimensional Hubbard model is insulating at low enough temperatures for any (finite) interaction and no Mott-Hubbard transition is observed [1]. This new finding is one example illustrating that paramagnetic phases with sufficiently strong antiferromagnetic (AF) correlations can "look and feel" like long-range ordered AF phases in many respects, with properties completely unlike (hypothetical) nonmagnetic phases. Interestingly, the relevant temperature scale is the (dynamical) mean-field ordering temperature, both in two and three dimensions. This has important consequences for cold-atom experiments [2,3]. All of these studies depend crucially on our methods for eliminating systematic (Trotter and/or finite-size) errors from the results of quantum Monte Carlo simulations [4].

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7 **Cheng-Wei Liu**, *Boston University (USA)*
Imaginary-time quench quantum Monte Carlo algorithm and its applications to spin-glass transitions
Co-authors: Anatoli Polkovnikov, Anders Sandvik

We demonstrate the application of a quantum Monte Carlo algorithm that carries out finite-velocity quenching in the imaginary time direction to approach the phase transition point. The algorithm has been established and well tested on quantum Ising models Refs. [1,2] along with a generalized scaling that is based on Kibble-Zurek mechanism Ref.[3]. We first make a distinction between the imaginary-time quench and simulation time quench, the latter has often been misleadingly referred to as quantum annealing. We then demonstrate the application of this algorithm on antiferromagnetic transverse-field Ising model on 3-regular random graphs, which is a spin-glass system. We extract the spin-glass transition point as well as the critical exponents to high numerical precisions.

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8 **Edgar Josué Landinez Borda**, *Universidad Estadual de Campinas (Brazil)*
Mechanical Properties of Solid Helium 4 by Path-Integral Monte Carlo Calculations
Co-authors: Wei Cai, Maurice De Koning

By means of path-integral Monte Carlo simulations we compute the ideal shear strength [1] and Peierls Stress in HCP Helium 4, the prototypical bosonic quantum solid. The ideal strength represents a theoretical upper bound of material strength, being defined as the minimum stress required to destabilize a defect-free crystal and produce a plastic deformation. We find that the ideal strength limit is reached by homogeneously nucleating a stacking fault. In addition, the strength is anisotropic but follows Schmid's law of resolved shear stress. Comparing the ideal strength to that of many other crystals, we find that it closely fits the normalized Frenkel-Orowan model of ideal strength. This is an example of a situation in which classical mechanical models remain useful even for solids dominated by quantum effects. Finally, we also determine the Peierls stress for a screw dislocation. It is defined as the minimum stress required to move this dislocation and it is an important parameter that largely controls the plastic behavior. We present the current estimate of this quantity and discuss it in terms of the plastic behavior.

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9 **William Putikka**, *Ohio State University (USA)*
Entropy and Thermopower in the 2D t-J Model

Results for the 2D tJ entropy at J/t=0.4 for all temperatures T and electron densities n are reported, along with a comparison to the properties of the thermopower in cuprate superconductors. The calculation is done by combining data from Monte Carlo calculations for the 2D Heisenberg AF energy as a function of T [1] with high temperature series calculated to 12th order in 1/T for the tJ entropy. Pade approximates are used to extrapolate the series for the difference ΔS(n)=StJ(n)-nSAF(J*), where J* is a density dependent modified energy scale for the AF. ΔS is small and is extended to T=0 by a power law fit assuming ΔS=0 at T=0. The most interesting aspect of the tJ entropy is the density derivative at fixed T (∂S/∂n)T, which is strongly T and n dependent for temperatures less than T∼5J. The features present in (∂S/∂n)T can be understood in terms of competition between AF spin fluctuations and d-wave pair fluctuations [2] by comparing the thermodynamic properties to the properties of the corresponding correlation functions. In addition, (∂S/∂n)T is an approximation for the thermopower [3]. The thermopower has been experimentally measured in the cuprates [4]. The n and T dependence of (∂S/∂n)T=0 broadly correspond to what is

observed in experiments on the cuprates [4,5]. In this analysis the sign change in the thermopower is given by a maximum in the entropy as a function of density [3] which is determined by the order parameter fluctuations present in a doped AF.

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10 **Hidemaro Suwa**, *University of Tokyo (Japan)*

Gap Estimation and Level Spectroscopy for Quantum Spin Systems by Monte Carlo Method

Co-authors: Arnab Sen, Anders Sandvik

We have developed a precise gap estimation method by the worldline quantum Monte Carlo method and applied the spectral analysis to the bilayer Heisenberg model and the two-dimensional J-Q model with the 4-spin interaction. The moment method for the excitation-gap estimation using the Fourier-transformed imaginary-time correlation is generalized to an asymptotically unbiased gap estimators[1,2]. Each excitation sector is unambiguously specified by quantum numbers, e.g., a total S, a total Sz, and a wave number, in the projection Monte Carlo scheme. For the bilayer model, the excitation velocity at the quantum phase-transition point was precisely calculated from the excitation gaps at several wave numbers. The quantum critical behavior at low temperatures was investigated and quantitatively compared to the field-theoritical prediction by using 1/N expansions for SU(N) spins. For the J-Q model, which has caught much attention as one of simplest models exhibiting the deconfined criticality, we precisely obtained the transition point between the Neel and the valence-bond solid phases by the lowest excitation-gap crossing. We found that the crossing point has the 1/L2 scaling and the finite-size correction is much smaller than that of the order parameters. As a non-trivial property, it is observed that not only the ordered sectors but also additional sectors become gapless at the transition point, which is expected if the transition is continuous. The velocity and the scaling dimension around the multiple gapless sectors were calculated. Our result is consistent to the continuous phase transition and the deconfined criticality scenario. Moreover, our Monte Carlo gap estimation and the spectral analysis can be applied to general quantum models in any dimension.

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11 **Masahiko Higuchi**, *Hiroshima University (Japan)*

Validity of the kinetic energy functional based on the coupling-constant expression in the pair-density functional theory

Co-authors: Katsuhiko Higuchi

The diagonal element of the 2nd-order reduced density matrix, which is referred to as the pair-density (PD), essentially contains more information on the electron correlation than the electron density. Therefore, the PD functional theory[1-6] that can in principle reproduce the ground-state PD is considered as one of the promising theories to go beyond the conventional density functional theory. In order to develop the PD functional theory, there exist two kinds of well-known problems. One is how we devise to extend the search region of PDs within the set of N-representable PDs. We have attempted to utilize as the search region of PDs the set of PDs that come from some kind of antisymmetric wave functions[6]. Recently, we have proposed the PD functional theory utilizing the electron-coordinates scaling of the PD[6]. This method can substantially extend the search region of PDs without heavy calculation tasks, and is called the "scaling method" [6]. The other problem is how we develop the approximate form of the kinetic energy (KE) functional. Namely, some approximation is needed for the KE functional of the PD functional theory since it cannot be expressed only by using the PD. In this study, we present approximate KE functionals that are derived on the basis of the rigorous expression with the coupling-constant integration[6]. These approximate KE functionals consist of the noninteracting KE and correlation energy terms, which have no adjustable parameters. In order to check the validity of such approximate forms, we perform atomic structure calculations by means of the scaling method[6]. It is shown that the correlation energy term is indispensable for the reduction of the KE error, i.e., reductions of both inappropriateness of the approximate functional and error of the resultant PD. Judging from the calculation results, the KE expression with the coupling-constant integration seems to be a good starting point for developing the approximate form.

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12 **Kyle Robertson**, *University of Vermont (USA)*

Monte Carlo Simulation of Superfluid Helium-4 in Mesoporous Silica

Co-authors: Adrian Del Maestro

Recent advances in nanofabrication techniques now allow for the creation of well ordered porous materials based on silicon [1] that provide a route to dimensional confinement of quantum fluids. As the spatial dimension is reduced, we expect enhanced thermal and quantum fluctuations, and

such substrates may allow for the experimental study of quasi one dimensional superfluids [2]. It is thus important to develop a theoretical understanding of how the geometry of a confining material affects the properties of a fluid flowing inside it. To this end, we have computed the Lennard-Jones potential experienced by an uncharged atom, such as helium-4, proximate to a semi-infinite polarizable medium [3]. We have studied the infinite half-plane, where a simple closed form is obtained for the potential, as well as cylindrical and elliptical cavities which must be evaluated numerically. Our results will ultimately be included in first principles quantum Monte Carlo simulations of confined quantum nanofluids.

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13 **Krissia de Zawadzki**, *Universidade de São Paulo (Brazil)*
Alternative numerical renormalization-group method to compute magnetic relaxation rates in dilute magnetic alloys

The interaction of a localized magnetic moment with the conduction electrons in a metallic host defines a problem with numerous facets. At sufficiently low temperatures, below the Kondo temperature T_{K}, this interaction gives rise to the Kondo effect and forms a spin-polarized region known as the Kondo screening cloud. Previous theories suggest that the radius of the cloud is R_K = \hbar v_F / k_B T_K, which for typical T_{K}'s and Fermi velocities v_{F}'s reaches mesoscopic distances. Numerous measurements of R_K have been attempted, but the results have been inconclusive. For example, NMR experiments have been unable to measure R_K because the signal decays fast with distance. Here, we present a computational alternative to the experimental NMR procedure, one that is based on the numerical renormalization-group (NRG) method and can probe distances on the scale of R_{K}. We consider a magnetic probe at a distance R from the impurity and calculate the spin-lattice relaxation rate 1/T_1 as a function of R and the temperature T. The computation involves a large number of matrix elements of the spin-flipping Hamiltonian representing the NMR probe between eigenstates of the model Hamiltonian. The NRG procedure having been designed to compute local properties of the impurity, the standard way of computing such matrix elements is overwhelmingly expensive. To reduce the cost, we have developed an alternative procedure that is substantially less costly, more straightforward to implement, and equally accurate. With this procedure we find a crossover in the T-dependence of 1/T_1 as R grows past R_K. What is more, both the phase and period of the Friedel oscillations change as we cross R_K. Our results confirm the expression R_K \propto T_K^{-1}. Nonetheless, they also show that a fuzzy shell around R=R_K marks the border of the screening sphere. We conclude that NMR measurements would be unable to precisely determine R_K.

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14 **Mohammad Soltanieh-ha**, *Northeastern University (USA)*

Interplay of charge, spin and lattice degrees of freedom on the spectral properties of the one-dimensional Hubbard-Holstein model

We calculate the spectral function of the one dimensional Hubbard-Holstein model using the time dependent Density Matrix Renormalization Group (tDMRG), focusing on the regime of large local Coulomb repulsion, and away from electronic half-filling. We argue that, from weak to intermediate electron-phonon coupling, phonons interact only with the electronic charge, and not with the spin degrees of freedom. For strong electron-phonon interaction, spinon and holon bands are not discernible anymore and the system is well described by a spinless polaronic liquid. In this regime, we observe multiple peaks in the spectrum with an energy separation corresponding to the energy of the lattice vibrations (i.e., phonons). We support the numerical results by introducing a well controlled analytical approach based on Ogata-Shiba's factorized wave-function, showing that the spectrum can be understood as a convolution of three contributions, originating from charge, spin, and lattice sectors. We recognize and interpret these signatures in the spectral properties and discuss the experimental implications.

15 **Shainen Davidson**, *Boston University (USA)*

SU(3) classical representation of quantum dynamics of interacting spins

Co-authors: Anatoli Polkovnikov

We present a formalism for simulating quantum dynamics of lattice spin-one systems first introducing local hidden variables and then doing semiclassical (truncated Wigner) approximation in the extended phase space. In this way we exactly take into account the local on-site Hamiltonian and approximately treat spin-spin interactions. In particular, we represent each spin with eight classical SU(3) variables. Three of them represent usual spin components and five others are hidden variables representing local spin-spin correlations. We argue that this method becomes asymptotically exact in high dimensions. This method allows for access to both non-equal time and spatial correlations. We compare our formalism with exact quantum dynamics of fully connected spin systems and find very good agreement. As an application we discuss quench dynamics of a Bose-Hubbard model near the superfluid-insulator transition for a 3D lattice system consisting 1000 sites. We argue that these ideas can be extended to other interacting systems.

16 **Thomas Lang**, *Boston University (USA)*
Dynamic scaling from non-equilibrium quenching of correlated Dirac fermions
Co-authors: Anders Sandvik

We present recent advances in the study of the evolution from the weak-coupling semimetal into the strong-coupling, insulating regime by means of unbiased quantum Monte Carlo simulations of the Hubbard and related models on the honeycomb lattice at half filling. Employing a novel approach to quantum phase transitions, we perform non-equilibrium imaginary time quenches of the Hubbard model in (zero temperature) projective quantum Monte Carlo simulations. This allows us to efficiently access order parameters on a finite size lattice for a wide range of coupling values in a single run. We show how to extract reliable estimates for the scaling properties and critical exponents of the semimetal-insulator quantum phase transition.

17 **Alberto Nocera**, *Northeastern University (USA)*
Pairing and nanoscale phase separation in Bose-Fermi mixtures

We determine the ground state phase diagram of a one dimensional Bose-Fermi Hubbard model with spin-full fermions using the Density Matrix Renormalization Group (DMRG) method. We focus on the regime with one fermion per site, and deep into the superfluid bosonicphase. We study the effects of the boson-fermion attraction on the fermionic pairing, as a function of the interaction strength, hopping, andbosonic density. We identify the regime in which fermionic superfluidity dominates, and analyze the structure of the Cooper pairs and thebosonic cloud that acts as the glue. At sufficiently large boson-fermion attraction, the system presents instability towards a nanoscale phase-separated phase, where one has “bubbles” of atoms separated by either empty sites or by a bosonic superfluid. The fermions form a band-insulating state inside the bubbles, while the bosons remain superfluid. We present a simple hydrodynamic argument to explain the energetic stability of this phase and study the size of the “bubbles” and of the superfluid background as a function of the boson-fermion and boson-boson interaction.

18 **Daoxin Yao**, *Sun Yat-sen Univerisity (China)*
Quantum Monte Carlo study of Disordered Spin Systems
Co-authors: Nvsen Ma, Yurong Shu, Anders Sandvik

We use quantum Monte Carlo methods to study the disordered quantum spin systems. Firstly, we use the SSE QMC to study the disordered S=1/2 quantum spins on the square lattice with three different nearest neighbor interactions J1, J2 and J3. Here J1 represents weak bonds, and J2 and J3 correspond to stronger bonds which are randomly distributed on columnar rungs forming coupled 2-leg ladders. By tuning the average value of J2 and J3, the system undergoes Ne´el-glass-paramagnetic quantum phase transition. A wide range of Mott glass phase has been found. We notice that its uniform susceptibility in the glass phase follows $\chi \sim \exp(-b/T^{\alpha})$, where $0<\alpha<1$.This dimerized disordered quantum spin system shows the violation of Harris criterion. Secondly, we use the Projector QMC and strong-disorder renormalization-group method to study

a disordered quantum spin chain. We find the system shows a power law decay for the dimer-dimer correlation function. The corresponding exponent is given.

19 **Chia-Min Chung**, *National Tsin Hua University (Taiwan)*
Entanglement spectroscopy using quantum Monte Carlo
Co-authors: Lars Bonnes, Pochung Chen, Andreas Lauchli

We present a numerical scheme to reconstruct a subset of the entanglement spectrum of quantum many body systems using quantum Monte Carlo. The approach builds on the replica trick to evaluate particle number resolved traces of the first n of powers of a reduced density matrix. From this information we reconstruct n entanglement spectrum levels using a polynomial root solver. We illustrate the power and limitations of the method by an application to the extended Bose-Hubbard model in one dimension where we are able to resolve the quasidegeneracy of the entanglement spectrum in the Haldane-insulator phase. In general, the method is able to reconstruct the largest few eigenvalues in each symmetry sector and typically performs better when the eigenvalues are not too different.

20 **Hitesh Changlani**, *University of Illnois at Urbana-Champaign (USA)*
Stochastically Projecting Tensor Networks
Co-authors: Bryan Clark

We apply a series of projection techniques on top of tensor networks to compute energies of ground state wave functions with higher accuracy than tensor networks alone with minimal additional cost. We consider both matrix product states as well as tree tensor networks in this work. Building on top of these approaches, we apply fixed-node quantum Monte Carlo, Lanczos steps, and exact projection. We demonstrate these improvements for the triangular lattice Heisenberg model, where we capture up to 57 percent of the remaining energy not captured by the tensor network alone. We conclude by discussing further ways to improve our approach.

21 **Michael Zeitlin**; Antonina Fedorova, *IPME RAS (Russia)*
Quantum Mechanics: Beyond Gaussians
Co-authors: Antonina Fedorova

We construct some universal picture for re-consideration of base states and generic phenomena, like entanglement, in Quantum Mechanical set-up. Our main goal is related to the analytical continuation of the standard zoo of solutions/base states from trivial ones, like plane waves or gaussians to novel states, possibly realizable, which permit more realistic (re)interpretation of the base folklore of Quantum Mechanics as well as more proper analytical/numerical modeling on the whole qualitative scale from entanglement to decoherence. Definitely, there is a set of experimental features as well as theoretical prerequisites demanding the appearance of new usefulness images. We start from some simple categorification procedure allowing to consider generic states as sheaves but not functions, after that we look for internal hidden symmetries on the level of the underlying "categorified" Hilbert space of extended states. The orbits of these

symmetries create the arena where we can model the novel features of our generalization of Quantum Mechanics. The analytical instruments allowing us to model both qualitative and quantitative aspects are Nonlinear Local Harmonic Analysis on the representations of orbits of hidden symmetries of underlying generalized Hilbertian spaces and variational principles which permit the algebraization of the subsequent control of the type of behaviour. It seems that reasonable extension of the zoo of possible (realizable) states can simplify the search of prototypes for realizable quantum devices as well as provide the more realistic (re)interpretation of the long-living standard "quantum folklore".

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22 **Phillip Weinberg**, *Boston University (USA)*

Using Local Updates to Evaluate Real Time Dynamics of Manybody Lattice Models

Co-authors: Anders Sandvik, Anatoli Polkovnikov

For local lattice Hamiltonians, the total number of nonzero matrix elements between manybody states in the worst case scenario scales as the number of sites in the lattice. Therefore the number of operations it takes to apply H to a state should scale as L^d*N. by Acting with H "on the fly" one can produce the sequence of states H^n|psi_0> which can be used to produce the evolved state any time later. This series is notorious for being plagued by round off error. We derive a lower bound on the maximum time at which the series accurately provides unitary evolution, given the number of digits kept. We apply this method to the real time evolution of hardcore bosons and compared with exact diagonalization. We find that if one breaks up the evolution into small intervals the exact evolution can be achieved for all times, but for a single starting point the series fails to converge shortly after the bound that we derive.

23 **Hui Shao**, *Beijing Normal University (China)*

Topological properties of valence-bond-solid states of the JQ3 model

Co-authors: Wenan Guo, Anders Sandvik

By using the ground-state projector quantum Monte Carlo simulations[1-2], we study the topological properties of the valence-bond-solid states of the JQ3 model on the square lattice[3-4]. The topological winding number is shown to be an emergent quantum number in the thermodynamic limit for the JQ3 model in the VBS state.

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24 **Lu Liu**, *Beijing Normal University (China)*
The effects of bond-disorder in the two-dimensional JQ_3 model
Co-authors: Wenan Guo, Anders Sandvik

We use the ground-state projector quantum Monte Carlo and the stochastic series expansion quantum Monte Carlo methods to study the bond-disordered JQ_3 model on the square lattice. The effects of disorder are investigated by measuring the dimer order parameter, the square of the staggered magnetization, dimer-dimer correlation and spin-spin correlation.

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8 Astrophysics and Space Plasma Physics

1 **Ke-Jung Chen**, *UCSC (USA)*
Supernovae at the Cosmic Dawn

One of the frontiers in modern cosmology is understanding the end of cosmic dark ages, when the first luminous transformed the simple early Universe into a state of ever-increasing complexity. We present multidimensional simulations of the thermonuclear supernovae from the first stars. Numerical and theoretical study of the primordial star formation in the early Universe suggest that these stars could have been very massive and may have died as energetic thermonuclear supernovae. We model the explosion of the supernovae by using a new radiation-hydro code, CASTRO and find the fluid instabilities driven by nuclear burning and hydrodynamics during the explosion. These instabilities are sufficient to break down the spherical symmetry of the supernova ejecta and can affect their observational signatures.

2 **Pramod Kumar Purohit**, *National Institute of Technical Teachers' Training & Research (India)*
Evaluation of geomagnetic storms effects on the GPS derived total electron content (tec)
Co-authors: Azad A Mansoori, Parvaiz Ahmad Khan, Roshni Atulkar, Sharad C Tripathi

The geomagnetic storm represents the most outstanding example of solar wind- magnetospheric interaction, which causes global disturbances in the geomagnetic field as well as the trigger ionospheric disturbances. We study the behaviour of ionospheric Total Electron Content (TEC) during the geomagnetic storms. For the present investigation we have selected 47 intense geomagnetic storms (Dst ≤ -100nT) that were observed during the solar cycle 23 i.e. during 1998-2006. We then categorized these storms into four categories depending upon their solar sources

like Magnetic Cloud (MC), Co-rotating Interaction Region (CIR), SH+ICME and SH+MC. We then studied the behaviour of ionospheric TEC at a mid latitude station Usuda (36.13N, 138.36E), Japan during these storm events produced by four different solar sources. During our study we found that the smooth variations in TEC are replaced by rapid fluctuations and the value of TEC is strongly enhanced during the time of these storms belonging to all the four categories. However, the greatest enhancements in TEC are produced during those geomagnetic storms which are either caused by Sheath driven Magnetic cloud (SH+MC) or Sheath driven ICME (SH+ICME). We also derived the correlation between the TEC enhancements produced during storms of each category with the minimum Dst. We found the strongest correlation exists for the SH+ICME category followed by SH+MC, MC and finally CIR. Since the most intense storms were either caused by SH+ICME or SH+MC while the least intense storms were caused by CIR, consequently the correlation was strongest with SH+ICME and SH+MC and least with CIR.

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3 **Pramod Kumar Purohit**, *National Institute of Technical Teachers' Training & Research (India)*

The statistical investigation of amplitude Scintillations at Indian high latitude Station Maitri, Antarctica

Co-authors: Prakash Khatarkar, P A Khan, Roshni Atulkar, Shivangi Bhardwaj

We have investigate the occurrence characteristics of ionospheric scintillations, using dual frequency GPS, installed and operated at Indian scientific base station Maitri (71.45S and 11.45E) Antarctica, during December 2009 to December 2010. The scintillation morphology is described in terms of S4 Index. The scintillations are classified into four main categories as Weak (0.2<S4<0.4), Moderate (0.4<S4<0.6), Strong (0.6<S4<1.0) and Saturated (S4>1.0). From the analysis we found that the percentage of weak, moderate, strong and saturated scintillations were 96%, 80%, 58% and 7% respectively. The maximum percentage of all types of scintillation was observed in the summer season, followed by equinox and the least in winter season. As the year 2010 was a low solar activity period, consequently the maximum occurrences of scintillations were those of weak and moderate and only four cases of saturated scintillation were observed.

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4 **Carlos Arturo Soto-Campos**, *Autonomous University of Hidalgo State (Mexico)*
An alternative model to cold dark matter for galactic rotation curves
Co-authors: Argelia Bernal-Bautista

The nature of the dark matter is one of the most intriguing and fundamental subjects in Modern Physics. The Scalar Field Dark Matter (SFDM) model, which assumes that dark matter is composed by bosonic particles that can be described by an scalar field, is an alternative model to the Cold Dark Matter (CDM) model and is as succesful as this one at cosmological scales, even more, the SFDM would be free from the controversies that the CDM has at small scales. In this work we investigate the behaviour of SFDM at small scales, specifically its viability in reproducing galactic rotation curves by fitting observational data from different galaxies. We build the SFDM galactic density profiles by solving a non linear system of ordinary differential equations for the scalar and the gravitational fields. Given the appropriate boundary conditions the system becomes in a eigenvalue problem which is solved by an inner-outer iteraction using an efficient computational method written partly in R. This method is faster than the predecessors, and could be implemented in parallel computing.

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5 **Juan Hinojosa**, *Texas A&M University (USA)*
The Surface Gravitational Expression of an Upwelling Thermal Mantle Plume: A Computational Model

Thermal mantle plumes in the Earth and other terrestrial planets are responsible for hot spots on the surface. Thermal plumes in the mantles of the terrestrial planets provide an important mechanism for the transfer of heat from the planet's interior. Theory and experiment both determine the structure of thermal plumes as having a large plume head and a long and narrow plume tail. The gravitational effects at the surface of the plume head are easily observable due to the large mass anomaly. However, the small lateral dimensions of the plume tail make the tail difficult to resolve. An axially symmetric mantle plume is modeled using spheres or disks for the plume head, and a long and narrow cylinder for the tail. The gravitational potential, gravitational equipotential surface, gravitational acceleration, and vertical gravity gradient of an upwelling thermal mantle plume are calculated. The results indicate that the plume tail may be indirectly observed using the vertical gravity gradient. The vertical gravity gradient presents a novel technique for detecting the plume tail, and can also be used to determine the lateral dimensions of both the plume head and plume tail from the signal at the surface.

9 Computational Physics Education

1 **Felix Garcia-Clemente**, *University of Murcia (Spain)*
EjsS: A JavaScript library which makes computational-physics education simpler
Co-authors: Francisco Esquembre

Nowadays, the teaching in computational physics is based on the usage of powerful instructional tools (e.g. Mathematica) and the programming in several software languages (e.g. Java) to do algebraic and numerical calculations, graphics and animations for a variety of mathematics and physics problems. However, the deployment of these animations requires that the author have training and skills in graphics programming, which could be too demanding in teaching scenarios. In this sense, we propose EjsS (Easy JavaScript Simulations) is a new Javascript library which makes the simulation of physics phenomena very easy. While a simple movement of a spring in raw programming language (e.g. WebGL or Java) would turn out hundreds of lines, an EjsS equivalent is only a fraction of that. Moreover, EjsS does not require that the author must have advanced knowledge in software programming because it includes an authoring tool, called EjsS Editor [1], to make the definition of simulations easier. The author uses EjsS Editor to define the physics model and to link model definitions to the components of the view. The editor includes 2D, 3D and UI elements, which include properties that can be linked to simulation variables. Also it is possible to define groups or sets to apply transformations to several elements together. Finally, the editor includes the automatic generation of code that integrates the simulation definition into the EjsS library. In relation to the technologies, EjsS is based on JavaScript and HTML5 and uses WebGL and SVG. Note it does not require other graphical libraries (e.g. Three.js) or UI library (e.g. jQuery), so EjsS is an independent library optimized to graphically show physics simulations. Therefore, it can be used in any web browser with HTML5 and WebGL support (currently, most of them) in any kind of device, such as smartphones or tablets. Moreover, the user could use the app EjsS Reader (available at iTunnes and Google Play) to organize his/her simulations and connect directly to the OSP Collection [2].

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2 **Samuel Castle**, *Davidson College (USA)*
A Parallel Computational Model of Orbiting N-Body Clusters
Co-authors: Wolfgang Christian

The study of N-body dynamics is a common practice with many realistic applications and examples, yet the ability to accurately model the interactions of large, dynamic planets via computer simulation remains an area of current research.1 We report the results from a parallel

computational model using long-range gravitational attraction and short-range, hard-sphere Hooke's law interactions between particles to model planetary and satellite motion. We show that our model obeys the conservation of energy and angular momentum and we use our model to investigate the development of tidal locking between two clusters over the course of many orbits. We were able to simulate several thousand particles and achieved thousands of Verlet time steps per second on a 12-core CPU with 24 parallel threads running Java 7. In future work, we intend to study planet-asteroid collisions, eventually examining the popular giant impact hypothesis—the conjecture that Earth's moon formed when a large asteroid collided with Earth. We created our model using Alan Kaminsky's Parallel Java library2 distributed with the Easy Java/JavaScript Simulations modeling tool. Easy Java/JavaScript Simulations is a part of the Open Source Physics3 project sponsored by the National Science Foundation and Davidson College and is available from Francisco Esquembre4 and the ComPADRE Open Source Physics digital library at http://www.compadre.org/OSP/" target="_blank.

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3 **Jay Wang**, *University of Massachusetts Dartmouth (USA)*

Computational physics with meshfree methods

In computational physics we often need to solve problems expressed in partial differential equations, such as the Laplace and Schroedinger equations. One approach involves discretizing space into regular grids, or meshes, over which the differential operators are approximated. There is another class of meshfree methods. In the meshfree approach, rather than discretizing space, the solutions are interpolated over a chose set of basis functions which are scattered over the domain. We discuss one meshfree method, namely, the radial basis function (RBF) method. The advantage of the RBF method is that it is efficient, simple to implement, and can easily handle irregular domains or higher dimensions. We present the application and results of the meshfree method to several problems, including the Poisson equation for electrostatics, string displacement under a load, and time-dependent quantum systems.

4 **Hartmut Ruhl**, *LMU (Germany)*

An effective PIC-solver for radiation reaction of electrons and radiation

Co-authors: Constantin Klier

Radiation reaction is one of the self-field effects on electrons that become important at large radiation efficiencies of the latter. Radiation reaction is typically important when ultra-strong fields interact with electrons. With the help of mean-field transport equations for electrons and

photons the Particle-In-Cell (PIC) method can be applied to integrate the radiation reaction force and to obtain the associated radiation spectrum. To overcome the soft photon problem a probabilistic summation methods is employed for the soft part of the radiation spectrum that creates effective soft photons but is highly efficient. Hard photons are created in a detailed way. It is shown that the correct trajectories of radiating electrons are obtained. Both, the energy loss of electrons and the corresponding radiation spectrum are predicted correctly.

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10 Novel Computing Paradigms

1 Kewei Du, *Institute of Software*

Heterogeneous Beam Dynamic Simulations for Linear Accelerator

Co-authors: Ruifeng Zhao, Jin Xu

Tracking huge number of charged particles in linear accelerator is important for high current linear accelerator's design and optimization. In this paper, a 3D heterogeneous parallel beam dynamic simulation software LOCUS3DG is introduced. It uses CPU as well as GPU on heterogeneous computers. It is designed to simulate the beam dynamics in high current linear accelerator by tracking billions of particles simultaneously. It uses a 3D parallel particle-in-cell (PIC) method, which captures the space charge field around the particle bunch by solving Poisson's equation on a regular grid. In order to achieve high performance, the particles are distributed in both CPUs and GPUs in some ratio to reach high performance. An effective parallel 3D Poisson's equation solver is developed using Fast Fourier Transform (FFT) method and 2D domain decomposition method, which makes it easy to use thousands of processors. Periodic boundary condition has been implemented in z and DIRICHLET zero boundary conditions in x and y directions. It has been parallelized using Message Passing Interface (MPI), and the particle charge information is collected from both GPUs and CPUs. Parallel frame, initialization and I/O have been developed to use GPU efficiently. Furthermore efficient post-processing tools have been developed to process beam information while the simulation is ongoing. Detailed benchmark results have been obtained on GPU cluster at SCCAS and TIANHE-1 at NSCC-TJ. Currently, It can simulate standard accelerator devices and new devices can be easily extended to it. At the end, a Radio Frequency Quadrature (RFQ) device has been simulated on TIANHE-1 at NSCC-TJ. Two-term formula of RFQ has been used to provide approximate electromagnetic fields in each RFQ cell, and detail statistics as well as information on lost particles have been obtained. This provides an advanced platform for accelerator physicists to conduct more sophisticated beam dynamics simulations.

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2 **Yun-Da Hsieh**, *National Taiwan University*
Implementation of the Universal Tensor Network Library on GPU using Cuda
Co-authors: Ying-Jer Kao

GPU programming plays an important role nowadays in scientific computation. In light of past successes building accelerated algorithms using Nvidia Cuda, we use GPU to accelerate tensor network based numerical methods. We develop a general purpose tensor network library called "the Universal Tensor Network Library", Uni10. In addition to its elegant user interface, applications on uni10 can be easily accelerated using GPU without the user knowing GPU programming. So far, we have benchmarked several common tensor network based algorithms such as DMRG, iTEBD and MERA. All these results show great extent of acceleration compared with the CPU version.

3 **Andrew Pochinsky**, *MIT (USA)*
Data parallel scientific programming with Qlua
Co-authors: Sergey Syritsyn

Physics applications consume considerable portion of supercomputing resources. As computers grow in capabilities, programming complexity grows as well. Complexity of programing large computing clusters needs to be addressed. Qlua is a revival of the data parallel programming paradigm based on a popular programming language Lua. The current implementation is tailored to Lattice QCD needs with domain-specific data types, operations, and layout primitives. Qlua provides seamless access to high-performance libraries as well. Local nature of Lattice QCD maps well into the data parallel model. Qlua is successfully used for large scale production as well as for exploration of algorithms.

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https://usqcd.lns.mit.edu/w/index.php/QLUA

11 General Computational Physics

1 **Brian Burrows**, *Staffordshire University (UK),*
Confined Systems

It is shown that the usual model for confined one-centre systems can be extended to two-centre systems and the theory is used to treat H2 and HeH++ . It is convenient to use spheroidal coordinates for the two-centre problems and we use this formalism to compare hydrogen-like systems confined spheroidally with the more standard spherical confinement. A discussion of confinement by both penetrable and impenetrable barriers is given together with a new technique for describing the effect of the external region

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Physical Review A 88 052511 (2013)

2 **Mitsuki Toogoshi**, *Hosei University (Japan)*
Maximum Entropy Method for Optical Spectrum Analysis of Real-Time TDDFT
Co-authors: Satoru Kano, Yasunari Zempo

In computational materials science, Time-Dependent Density Functional Theory (TDDFT) is a powerful tool for calculating the excited states of molecules. In our calculations, the real-time and real-space technique is adopted in solving equations by the finite difference approach [1, 2]. Within the framework of this approach, the wave functions are evolved with the perturbed initial wave function. In the traditional method, the optical strength function is obtained from the frequency Fourier transform of the dynamic dipole moment. In the frequency domain, the maximum entropy method (MEM) is well known for obtaining a fairly high resolution and accuracy in spectral estimation with a relatively small number of time-series data. MEM is based on the Fourier transform relationship between the power spectrum and the autocorrelation function. We apply this method to the spectrum analysis of the dynamic dipole moment, which is calculated by using TDDFT. MEM provides a similar spectrum for the peak position to that of FFT with almost half of the time evolution for small molecules [3]. To obtain a better spectrum, however, we have to choose a suitable number M for the lag of the autocorrelation function. In general, larger values of M yield unphysical results such as pseudo-peaks and splits, while smaller values of M give broad peaks. Thus, an appropriate value of M is required for good spectra. We investigate how to obtain an appropriate value of M that can be applied to several molecules. In the presentation, we will show how to use MEM effectively.

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3 **Ronald White**, *James Cook University (Australia)*
A method for the accelerated numerical solution of fractional diffusion equations
Co-authors: Peter Stokes, Bronson Philippa

Kinetic equations containing fractional derivatives are a useful approach for the description of transport in complex systems which exhibit anomalous diffusion and memory effects. It is this non-Markovian nature which results in increased computational complexity when solving these equations numerically. For an N-point finite difference discretisation this corresponds to accessing the entire history of the system at every time step, increasing the time complexity from O(N) to O(N2). We present here a relationship between the solution of the Caputo fractional diffusion equation of order 0<α<1 and the solution to the normal diffusion equation This relationship takes the form of the linear mapping in time alone where U and V are, respectively, matrices representing numerical solutions of u(t,x) and v(t,x) and A is the mapping matrix, which depends solely on α. It is from this mapping which arises a method for improving the time complexity of solving the considered fractional diffusion equation numerically. The method involves performing the above matrix multiplication partially by removing negligible terms from the mapping. After a precomputation of the mapping matrix in O(N1+αlnN), the fractional diffusion solution can be found using this method in O(Nα). We successfully apply this method to accelerate the fitting of a fractional advection diffusion model for the current in a time-of-flight experiment.

4 **Ronald White**, *James Cook University (Australia)*
The application of pseudo-spectral methods to low-energy positron transport gases
Co-authors: Greg Boyle, Wayne Read

The modeling of positron transport is important in a variety of areas ranging from astrophysics to medical imaging [1]. Positron-specific process such as annihilation significantly modify transport behaviour [2]. In this work we model positron transport using kinetic theory via the Boltzmann equation. The standard approach is to represent the velocity-space by a series of Spherical Harmonics or Legendre Polynomials based on symmetry considerations [3], then decomposing the Boltzmann equation into a hierarchy of coupled differential equations. Further progress is generally made numerically. Pseudo-spectral methods, particularly those employing Chebyshev polynomials, have become the adopted method for many numerical problems in mathematics and physics [4]. The rate of convergence of spectral and pseudo-spectral approximations depends only on the smoothness of the solution, a property known as “spectral accuracy”. Given their exceptional convergence properties and efficient use of computational time and memory, it is the authors’ belief that pseudo-spectral methods have been under-utillized for modeling charged particle transport. Finite difference methods, on the other hand, have been used extensively in the literature. In this work we compare the finite difference method with two pseudo-spectral methods, one based on Chebyshev polynomials and the other on Laguerre functions, when

applied to low-energy positron transport. At low energies, only elastic and annihilation processes are operative. Inelastic processes lead to regions of sharp variation, reducing the effectiveness of global approximation schemes. The three numerical schemes are applied to a simple benchmark model with cross-sections represented by power laws, then to real Argon gas with accurate elastic and annihilation cross-sections.

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5 **Arman Kussainov**, *al-Farabi National University (Kazakhstan)*
Neutron monitor data analysis through quantum transformation operator's eigenvalue statistics
Co-authors: Natalya Pya, Sain Kussainov

The considerable interest in studying the Hamiltonians associated with the quantum state evolution has been generated while implementing the work of a quantum computer. In this work, we interpret time series data in terms of the objects specific to the quantum computations, namely using unitary transformation matrices and their eigenvalues. We analyze a case of relating two n-qubit long quantum states, constructed from a single original time series, to each other by a direct analytical computation of a single rotation in infinite-dimensional Hilbert space. Kernel smoothing is applied to estimate the density functions [1] of the eigenvalues of the transformation matrices and of the spacing between the ordered eigenvalues. It is claimed to be a useful approach for examining the variations of the eigenvalues and reflecting the properties of the original data. The proposed approach is used on the data collected over 9 months period from a single registration channel of the 18NM64 neutron monitor hosted at Tian-Shian high elevation research station, 3340 m above the sea level in Kazakhstan mountains.

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6 **Sul-Ah Ahn**, *KISTI (Korea)*
Research Activity in High Performance Computational Physics: Co-authorship Network Analysis
Co-authors: Youngim Jung

The research activities of the high-performance computational physicists are analyzed by scientometric approaches. This study aims at providing high-performance computational physicists and policy planners with useful scientometric results for an assessment of research activities. In order to achieve this purpose, we carried out a co-authorship network analysis of journal articles to assess the research activities of researchers for high-performance

computational physics as a case study. For this study, we used journal articles of the Scopus database from Elsevier covering the time period of 2004-2013. We extracted the author rank in the high-performance computational physics field by the number of papers published during ten years from 2004. Finally, we drew the co-authorship network for 50 top-authors and their coauthors, and described some features of the co-authorship network in relation to the author rank. Suggestions for further studies are discussed.

7 **Henio Rego**, *CPS/Boston University and IFMA (USA)*

When a Text is Translated Does the Complexity of Its Vocabulary Change? Translations and Target Readerships

Co-authors: Sasuke Miyazima, Lidia Braunstein, HE Stanley

In linguistic studies, the academic level of the vocabulary in a text can be described in terms of statistical physics, by using a "temperature" concept related to the text's word-frequency distribution. Here, we propose a "comparative thermo-linguistic" technique to analyse a text and to determine what academic level and thus what target readership its vocabulary is focused toward in any given language. We apply this technique to a large number of books by several authors and examine how the vocabulary of a text changes when it is translated from one language to another. Unlike the uniform results produced using the Zipf law, using our "word energy" distribution technique we nd variations in the power-law behavior. We also examine some common features that span across languages and identify some intriguing questions concerning how to determine when a text is suitable for its intended readership.

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