20th Mardi Gras Conference

Petascale Many Body Methods for Complex Correlated Systems

Louisiana State University, Center for Computation & Technology

Baton Rouge, U.S.A., February 12^{th} to 14^{th}, 2015

Thursday, February 12^{th}, 2015

8:30	Registration & Coffee
9:00-9:15	Opening remarks

Session 1	**Chair: Juana Moreno** (Louisiana State University)
9:15-10:00	**Alexey Rubtsov** (Moscow State University & Russian Quantum Center, Russia), *Towards a numerically exact description of correlated open quantum systems*
10:00-10:15	Discussion
10:15-11:00	**Salvatore R. Manmana** (Universität Göttingen), *Matrix product state formulation of frequency-space dynamics at finite temperatures*
11:00-11:15	Discussion
11:15-12:00	**Randy S. Fishman** (Oak Ridge National Laboratory), *Using inelastic scattering measurements to determine the complex spin states of multiferroic materials*
12:00-12:15	Discussion
12:15-1:30	Lunch break: **Philip Adams** (Louisiana State University), *Hysteresis, Avalanches, and Slow Relaxation: Complex non-equilibrium spin dynamics in a Zeeman-limited superconductor*

Session 2	**Chair: Wei Ku** (Brookhaven National Laboratory)
1:30-2:15	**Rudolf Roemer** (University of Warwick), *Self-assembling tensor networks and holography in disordered spin chains*
2:15-2:30	Discussion
2:30-3:15	**Karen Tomko** (Ohio Supercomputer Center), *MPI+PGAS Hybrid Programming*
3:15-3:30	Discussion
3:30-4:15	**Erik Koch** (German Research School for Simulation Sciences, Jülich), *Stochastic sampling for the analytic continuation of imaginary-time data*
4:15-4:30	Discussion
4:30-6:00	Poster session

	Friday, February 13th, 2015
8:30	Registration & Coffee

Session 3	**Chair: Mark Jarrell** (Louisiana State University)
9:00-9:45	**Kieron Burke** (University of California, Irvine), *Why strong correlation is difficult in density functional theory*
9:45-10:00	Discussion
10:00-10:45	**Wei Ku** (Brookhaven National Laboratory), *Connecting real materials to low-energy effective Hamiltonian: applications of symmetry-respecting Wannier functions*
10:45-11:00	Discussion
11:00-11:45	**Ehsan Khatami** (San Jose State University), *Numerical Linked-Cluster Expansion Approach for Strongly-Correlated Electronic Systems*
11:45-12:00	Discussion
12:00-1:30	Lunch break: **Ilya Vekhter** (Louisiana State University), *Quasiparticle Étouffée: unconventional superconductors probed by magnetic field*

Session 4	**Chair: Václav Janiš** (Acad. Sciences, Czech Republic & Louisiana State Univ.)
1:30-2:15	**Martin Weigel** (Coventry University), *Simulating spin models on GPU: A tour*
2:15-2:30	Discussion
2:30-3:15	**Ka-Ming Tam** (Louisiana State University), *Simulations of Edwards-Anderson model using GPU*
3:15-3:30	Discussion
3:30-4:15	**Frank Marsiglio** (University of Alberta), *The Dynamic Hubbard Model: studies with DMFT and exact diagonalization*
4:15-4:30	Discussion
4:30-5:15	**Luca de' Medici** (ESRF Grenoble), *Slave-spin mean-field calculations, an essential dynamical multi-orbital mean-field: application to Iron superconductors*
5:15-5:30	Discussion
6:00-8:00	Conference Dinner

	Saturday, February 14th, 2015
8:30	Registration & Coffee

Session 5	**Chair: Randy Fishman** (Oak Ridge National Lab)
9:00-9:45	**André-Marie Tremblay** (Université de Sherbrooke), *Strongly correlated superconductivity in cuprates and layered organics: results & some algorithmic details*
9:45-10:00	Discussion
10:00-10:45	**Václav Janiš** (Acad. Sciences, Czech Republic & Louisiana State Univ.), *Parquet equations for disordered and interacting electron systems: Self-energy and the role of the Ward identity*
10:45-11:00	Discussion
11:00-11:45	**Hartmut Hafermann** (Inst. Physique Théorique, CEA Saclay), *Collective charge excitations of strongly correlated electrons, vertex corrections and gauge invariance*
11:45-12:00	Discussion
12:00	Closing remarks
12:15	Leaving to the Krewe of Endymion parade in New Orleans

Mardi Gras Workshop

Petascale Many Body Methods for Complex Correlated Systems
Louisiana State University, Center for Computation & Technology
Baton Rouge, U.S.A., February 15^{th} to 16^{th}, 2015

Sunday, February 15^{th}, 2015

8:30	Registration & Coffee
9:00-9:05	Opening remarks

Session 1	**Chair: Rudolf Roemer** (University of Warwick)
9:05-10:35	Pedagogical lecture: **Václav Janiš** (Acad. Sciences, Czech Republic & Louisiana State Univ.), *Ergodicity in statistical mechanics of interacting and disordered systems: Destroying and restoring equilibrium ergodic states*
10:35-10:50	Discussion
10:50-11:20	**Valéry Rousseau** (Louisiana State University), *The superfluid density in systems with complex interactions*
11:20-11:30	Discussion
11:30-12:00	**Kalani Hettiarachchilage** (Louisiana State University), *Ferromagnetism in a two-dimensional two species bosonic Hubbard model.*
12:00-12:10	Discussion
12:10-1:30	Lunch break

Session 2	**Chair: Erik Koch** (German Research School for Simulation Sciences)
1:30-3:00	Pedagogical lecture: **Rudolf Roemer** (University of Warwick), *Sparse matrix diagonalization, what it is, why and when it works.*
3:00-3:15	Discussion
3:15-3:45	**Herbert Fotso** (Ames National Lab), *Field-driven quantum systems, From transient to steady state.*
3:45-3:55	Discussion
3:55-4:25	**Peng Zhang** (Carnegie Institution of Washington), *DFT+DMFT study of magnetic properties in FeO at high pressure.*
4:25-4:35	Discussion
4:35-5:05	**Shuxiang Yang** (Louisiana State University), *Numerical study of the periodic Anderson model with a quarter-filled conduction band.*
5:05-5:15	Discussion

	Monday, February 16th, 2015
8:30	Registration & Coffee

Session 3	**Chair: Frank Marsiglio** (University of Alberta)
9:00-10:30	Pedagogical lecture: **Erik Koch** (German Research School for Simulation Sciences, Jülich), *The Lanczos Method*
10:30-10:45	Discussion
10:45-11:15	**Shi-Quan Su** (University of Tennessee), *A Distributive Linear Algebra Approach for Scalable Computing Platform with Accelerator*
11:15-11:25	Discussion
11:25-11:55	**Yi Zhang** (Louisiana State University), *Study of multiband disordered systems using the typical medium dynamical cluster approximation.*
11:55-12:05	Discussion
12:05-1:30	Lunch

Session 4	**Chair: Juana Moreno** (Louisiana State University)
1:30-3:00	Pedagogical lecture: **Wei Ku** (Brookhaven National Lab), *How to construct symmetry-respecting Wannier functions*
3:00-3:15	Discussion
3:15-3:30	Coffee Break
3:30-5:30	**Panel: What I did with my Physics degree:** **Alex Brandt** (Rackspace), *Physics B.S.: How I learned to stop worrying and live in business* **Sean Hall** (Carver Scientific), *Some surprising thoughts and realizations from a would be research scientist about employment in the 'Real World'* **Peter Reis** (PosiTech Corp.), *Using Physics and Computation in Industry*

20th Mardi Gras Conference
Petascale Many Body Methods for Complex Correlated Systems
Invited Talks

Philip Adams (Louisiana State University, USA), *Hysteresis, Avalanches, and Slow Relaxation: Complex non-equilibrium spin dynamics in a Zeeman-limited superconductor.* We have recently been studying non-equilibrium spin dynamics of BCS superconductivity in a high Zeeman field. Thin aluminum films are driven from the superconducting phase to the normal phase by the application of a magnetic field that is oriented parallel to the film surface. Near the first-order parallel critical field transition, we observe avalanches in both transport and density of states measurements. These avalanches are not associated with flux jumps but are representative of the behavior of the condensate as the system tries to accommodate spin-singlet superconductivity in the presence of a large Zeeman field and disorder. I will argue that the presence of avalanches in the density of state spectra has important implications for the nature of the superconducting ground state near the Clogston-Chandrasekhar limit. Specifically, we believe that a non-trivial, spatially modulated, order parameter emerges in the critical regime.

Kieron Burke (University of California, Irvine, USA), *Why strong correlation is difficult in density functional theory.* This talk will summarize a variety of work on strongly correlated systems, testing and understanding failures of the density functional theory (DFT). I begin with an illustration of DFT on the simplest possible system, a two-site Hubbard problem [D. J. Carrascal, J. Ferrer, J. C. Smith, and K. Burke, in prep.]. This is used to show how DFT works and its differences from traditional many-body approaches. Then I will show the importance of moving from lattice Hamiltonians to real-space (i.e., continuum) descriptions [Phys. Rev. Lett. 109, 056402 (2012)]. I will describe a number of papers[Phys. Chem. Chem. Phys. 14, 8581 - 8590 (2012); Phys. Rev. Lett. 111, 093003 (2013); Phys. Rev. B 90, 045109 (2014)] in collaboration with Steve White in which DMRG calculations are used to solve one dimensional systems exactly, and compared to essentially exact DFT and to approximate DFT. I will discuss our latest results in this area, and ask for ideas on directions to go in.

Randy S. Fishman (Oak Ridge National Laboratory, USA), *Using inelastic scattering measurements to determine the complex spin states of multiferroic materials.* Because they couple magnetic and electric degrees of freedom, multiferroic materials hold tremendous technological promise and remain the subject of intense scrutiny. In practice, elastic neutron scattering alone is insufficient to determine the complex, non-collinear spin structures of these materials. But inelastic spectra provide dynamical "fingerprints" for the spin states and interactions of multiferroic materials. This is demonstrated for two materials that fall within different classes of multiferroics. Whereas $BiFeO_3$ is a type I multiferroic with the ferroelectric transition temperature Tc higher then the Néel transition temperature TN, $CuFeO_2$ is a type II multiferroic with Tc = TN. Although the spin states of these materials are distorted cycloids or spirals, there are important differences between the two due to the different origins of their multiferroic behavior. I also discuss the computational challenges posed by solving the inelastic spectra for materials with very large unit cells, such as the type II multiferroic $MnWO_4$. Research sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy under contract with UT-Battelle, LLC.

Hartmut Hafermann (Institut de Physique Théorique, CEA Saclay, France), *Collective charge excitations of strongly correlated electrons, vertex corrections and gauge invariance.* The collective,

long wavelength charge excitations in correlated media are considered in presence of short and long range forces. As an example for the case of a short range interaction, the two-dimensional Hubbard model is examined within dynamical mean-field theory (DMFT). It is shown that the DMFT susceptibility including vertex corrections respects the Ward identity and yields a manifestly gauge invariant response in finite dimensions [Phys. Rev. B 90, 235105 (2014)]. A zero-sound mode is found as expected for short range forces. The relation between the vertex corrections, gauge invariance and the appearance of the collective modes is discussed. Long range forces are treated within extended dynamical mean-field theory (EDMFT). In order to obtain a gauge invariant response and a proper description of the plasmons in this case, it is necessary to additionally incorporate some non-local vertex corrections into the polarization. This may be achieved by means of the dual boson approach. It is shown that correlations induce a spectral weight transfer and renormalization of the dispersion in the two-particle spectra [Phys. Rev. Lett. 113, 246407 (2014)]. These effects are reminiscent of interaction induced changes found in single-electron spectra in correlated media. Finally, the role of the polarization corrections for the charge-ordering transition in the extended Hubbard model is discussed [Phys. Rev. B 90, 235135 (2014)].

Václav Janiš (Academy of Sciences, Czech Republic & Louisiana State University), *Parquet equations for disordered and interacting electron systems: Self-energy and the role of the Ward identity.* I introduce a way how to choose the one-electron Green functions in the parquet equations for two-particle vertices so that to reach qualitative thermodynamic consistency. Parquet equations for disordered and interacting electron systems are discussed separately. In the former case I show how to use the parquet equations in the construction of the two-particle vertex being compatible with the Ward identity. In the latter case I use a linearized Ward identity in the external magnetic field to introduce a thermodynamic self-energy that is then used in the one-electron Green functions of the parquet equations. The role and significance of the Schwinger-Dyson equation in such a formulation of the parquet equations are explained.

Ehsan Khatami (San Jose State University, USA), *Numerical Linked-Cluster Expansion Approach for Strongly-Correlated Electronic Systems.* Recent advances in computational methods for strongly-correlated electronic systems have helped us not only with the ability to simulate more realistic models and achieve lower temperatures, but also in gaining a better control and even eliminating sources of error and approximations. In this talk, I will introduce the numerical linked-cluster expansion (NLCE), a novel and highly-parallelizable technique for quantum lattice models and discuss its advantages and disadvantages over some of the more popular methods that rely on quantum Monte Carlo algorithms. NLCEs combine two powerful techniques, namely, high-temperature series expansions and the exact diagonalization to provide highly-precise finite-temperature properties of the model directly in the thermodynamic limit. As an example, I will focus on the applications of NLCEs to the Fermi-Hubbard model and show results for the thermodynamic properties, including magnetic and superconducting correlations, of the model on several different geometries. Comparisons to results from the determinantal quantum Monte Carlo will be presented for select cases.

Erik Koch (German Research School for Simulation Sciences, Jülich, Germany), *Stochastic sampling for the analytic continuation of imaginary-time data.* Stochastic sampling methods solve an inverse problem, e.g., reconstructing the spectral function from imaginary-time data obtained in QMC simulations, by averaging all admissible solutions with a weight given by how well they reproduce the data. They are appealing, as they appear unbiased and thus have the potential to resolve sharp features in the spectral function. Discretizing the inverse problem to make numerical

calculations possible we have, however, to introduce a parametrization of the real-axis that acts like a default model, i.e., determining the result in the absence of data. We discuss how the effect of this default model depends on the number of points in the real-axis grid. To make this analysis possible, we (i) introduce an efficient stochastic sampling algorithm, blocked mode sampling, based on the singular-value decomposition of the discretized integral kernel, and (ii) derive how the stochastic processes for different discretizations are related. Finally we give a recipe for constructing real-axis grids for practical calculations.

Wei Ku (Brookhaven National Laboratory, USA), *Connecting real materials to low-energy effective Hamiltonian: applications of symmetry-respecting Wannier functions.* This talk will cover the basics of capturing the realistic aspects of materials by using symmetry-respecting Wannier functions. Specifically, low-energy effective Hamiltonian can be obtained (so-called down-folding) for various purposes, including further analysis of density functional theory and many-body treatment of one-particle and two-particle excitations. The talk will also include recent development in treating disordered impurities and propagation of excitations.

Salvatore R. Manmana (Universität Göttingen, Germany), *Matrix product state formulation of frequency-space dynamics at finite temperatures.* I will present a flexible density-matrix renormalization group approach to calculate finite-temperature spectral functions of one-dimensional strongly correlated quantum systems. The method combines the purification of the finite-temperature density operator with a moment expansion of the Greens function. Using this approach, we study finite-temperature properties of dynamical spectral functions of spin-1/2 XXZ chains with Dzyaloshinskii-Moriya interactions in magnetic fields and analyze the effect of these symmetry breaking interactions on the nature of the finite-temperature dynamic spin structure factor.

Frank Marsiglio (University of Alberta, Canada), *The Dynamic Hubbard Model: studies with DMFT and exact diagonalization.* Strong correlations play an important part of all superconductors. Many of these correlations are described through a competition between kinetic energy processes and potential energy considerations. In the Dynamic Hubbard model these two considerations become somewhat blurred. We describe various effective models where the role played by hole-like quasiparticles becomes very distinct from that of their electron-like counterparts.

Luca de' Medici (European Synchrotron Radiation Facility, Grenoble, France), *Slave-spin mean-field calculations, an essential dynamical multi-orbital mean-field: application to Iron superconductors.* Slave-variable mean fields have a long history in condensed matter theory, slave bosons being a most known example. They enable a non-perturbative treatment of interacting many-body fermions and, in their simplest mean-field for Hubbard-like models to minimally treat the local dynamical fluctuations generating the mass enhancement caused by electronic correlations, for instance. The slave-spin mean field is a very convenient implementation that allows to easily tackle multi-orbital systems at a very cheap computational cost. Successes of this method include realistic studies of the recently discovered iron superconductors, that will be illustrated.

Rudolf Roemer (University of Warwick, United Kingdom), *Self-assembling tensor networks and holography in disordered spin chains.* We show that the numerical strong disorder renormalization group algorithm of Hikihara et al. [Phys. Rev. B 60, 12116 (1999)] for the one-dimensional disordered Heisenberg model naturally describes a tree tensor network (TTN) with an irregular structure defined by the strength of the couplings. Employing the holographic interpretation of the

TTN in Hilbert space, we compute expectation values, correlation functions, and the entanglement entropy using the geometrical properties of the TTN. We find that the disorder-averaged spin-spin correlation scales with the average path length through the tensor network while the entanglement entropy scales with the minimal surface connecting two regions. Furthermore, the entanglement entropy increases with both disorder and system size, resulting in an area-law violation. Our results demonstrate the usefulness of a self-assembling TTN approach to disordered systems and quantitatively validate the connection between holography and quantum many-body systems [Phys. Rev. B 89, 214203 (2014)].

Alexey Rubtsov (Moscow State University & Russian Quantum Center, Russia), *Towards a numerically exact description of correlated open quantum systems.* A description of the dynamics of a correlated quantum system coupled to a bath remains a major challenge for the community. The most remarkable progress has been achieved for an equilibrium state, when continuous-time Quantum Monte Carlo schemes deliver a good accuracy for realistic multiorbital impurity problems. We will discuss state-of-art algorithms, as well as approximate schemes that allow to reduce the description of correlated media to a multiorbital impurity problem – in particular, Dynamical Mean Field theory and dual-fermion formalism. The calculation of real-time dynamics is much more complicated, primary because of a limited applicability of the stochastic schemes. Some understanding can be obtained operating with a simplified bath operators. An assumption that the bath is Markovian leads to Lindblad formalism and similar schemes. We will consider how the Lindblad term should be modified for a correlated system coupled to a non-vacuum bath, and present our results for a metastability of the decay dynamics of a frustrated correlated system. We believe that our theory can be used for a practical calculation of the metastability effects in nanodevices, catalysis etc. A special attention will be paid to the scalability of the algorithms, to check out where the use of petascale systems can result in a breakthrough.

Ka-Ming Tam (Louisiana State University, USA), *Simulations of Edwards-Anderson model using GPU.* Monte Carlo simulations of the Ising model and its variants play an important role in the computational physics, and they have helped the discovery of many important physics phenomena over the past few decades. Unfortunately, the existence and nature of spin glass due to random disorder still remains as open questions. A main obstacle in Monte Carlo simulations of random frustrated systems is the long relaxation time. Developing an efficient parallel implementation on state-of-the-art computation platforms is highly desirable. The Graphics Processing Unit (GPU) is such a platform that provides an opportunity to significantly enhance the computational performance. In this talk, we present optimization and tuning approaches for the CUDA implementation of the spin glass simulation on GPUs. We discuss the integration of various design alternatives, such as GPU kernel construction with minimal communication, memory tiling, and look-up tables. We present a binary data format, and introduce the Compact Asynchronous Multispin Coding (CAMSC), which provides an additional speedup compared with the traditionally used Asynchronous Multispin Coding. We employ the GPU code to calculate an indicator composed of the ratio of susceptibilities at finite wavenumbers, which has been recently proposed to avoid the difficulties in the finite size scaling of a zero momentum quantity. This new indicator is rather noisy, the GPU implementation facilitates the generation of a large pool of samples at low temperature to reduce the the noise.

Karen Tomko (Ohio Supercomputer Center, USA), *MPI+PGAS Hybrid Programming.* MPI has been a widely ported and dominant programming model in parallel computing for the past few

decades. As a result, most scientific applications are written using MPI. System advances including large shared memory nodes and low latency direct memory access between nodes provided on modern networks provide support for a wider range of programming models. It is widely believed that a hybrid programming model (MPI+X, where X is a PGAS model) is optimal for many scientific computing problems, especially for exascale computing. MVAPICH2-X provides a unified high-performance runtime that supports both MPI plus PGAS programming models on InfiniBand clusters. This talk will provide an overview of PGAS programming model. Introduce the high-performance unified runtime in MVAPICH2-X and review some recent MPI+PGAS application studies from the OSU Network-Based Computing Laboratory.

André-Marie Tremblay (Université Sherbooke, Canada), *Strongly correlated superconductivity in cuprates and layered organics: results and some algorithmic details.* In cuprates, the Mott insulating state is reached by doping. Pressure, or bandwidth control, tunes the Mott transition in layered BEDT organics. Superconductivity can occur in the metallic phases of both types of compounds near the Mott insulator. This "strongly correlated superconductivity" exhibits special features, discussed in this talk, that distinguish it from BCS superconductivity. Comparisons with experiment and a few predictions will be presented. The results are obtained with cellular-dynamical mean-field theory using the continuous-time hybridization-expansion (CT-HYB) impurity solver. I will also explain how considerable speedup of CT-HYB can be obtained using skip-list concepts and how ergodicity can be implemented in the CT-HYB algorithm in the presence of broken symmetry.

Ilya Vekhter (Louisiana State University), *Quasiparticle Étouffée: unconventional superconductors probed by magnetic field.* In many materials superconductivity arises from the same strong electron-electron interactions that give rise to unconventional metallic properties, and present challenges for computational approaches. Superconducting state in such systems is anisotropic, strongly varying with the direction of motion of the electrons. Determining this anisotropy is a crucial step in identifying the origin of superconductivity and dominant interactions. In this talk I will introduce and review theoretical ideas and experimental methods for studying anisotropic superconductors. I will show how the dependence of the thermal properties on the direction of the applied magnetic field allows determination of the symmetry of the superconducting state. I will use examples from heavy fermion compounds, pnictides, and organic superconductors, and discuss the successes and challenges of this approach.

Martin Weigel (Coventry University, United Kingdom), *Simulating spin models on GPU: A tour.* Over the last couple of years it has been realized that the vast computational power of graphics processing units (GPUs) could be harvested for purposes other than the video game industry. This power, which at least nominally exceeds that of current CPUs by large factors, results from the relative simplicity of the GPU architectures as compared to CPUs, combined with a large number of parallel processing units on a single chip. To benefit from this setup for general computing purposes, the problems at hand need to be prepared in a way to profit from the inherent parallelism and hierarchical structure of memory accesses. In this overview lecture I discuss the performance potential for simulating spin models, such as the Ising or Heisenberg models as well as the Edwards-Anderson spin glass, on GPU as compared to conventional simulations on CPU. Different algorithms, including Metropolis and cluster updates, as well as computational tricks such as multi-spin coding are taken into account. A very recent development concerns simulations using population annealing, a new generalized ensemble heuristic that is particularly well suited for massively parallel architectures.

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Posters

Chinedu Ekuma (Louisiana State University), *A Typical Medium Dynamical Cluster Approximation for the Study of Anderson Localization.* We develop a systematic typical medium dynamical cluster approximation (TMDCA) to study localization in disordered electronic systems. The TMDCA utilizes the momentum resolved typical density of states and the non-local hybridization function to characterize the localization transitions. We apply the formalism to the Anderson model of localization in one (1D), two (2D), and three (3D) dimensions. In 1D, we find that the critical disorder strength W_c scales inversely with the linear cluster size with a power law, $W_c \sim (1/Lc)^{\nu}$; in 2D, W_c decreases logarithmically with L_c; whereas in 3D, our method successfully captures the localization phenomenon both in low and large disorder regimes. In 3D as a function of cluster size, our method systematically recovers the re-entrance behavior of the mobility edge, obtains the correct W_c, and the associated order parameter critical exponent for the Anderson localization. Once combined with electronic structure calculations and more sophisticated many-body techniques for electron interactions, it will open a new avenue for studying localization phenomenon in real materials as well as the competition between disorder and electron correlations.

Sheng Feng (Louisiana State University), *Study of the Three Dimensional Edwards-Anderson Spin Glass Model in an External Field.* We study the Edwards-Anderson model on a simple cubic lattice with a finite constant external field using a Monte Carlo simulation code, which employs graphics processing units to dramatically speedup the simulation. The parallel tempering method has been used to alleviate the long equilibration time. Conventional indicators, such as the Binder ratio and correlation length, do not show any signs of a phase transition. We also studied R_{12}, or the ratio of spin glass susceptibilities at finite wave numbers, and show it is quite noisy that a systematic analysis cannot come to clear conclusion. We argue that the typical value should be also studied in additional to conventional linear average value, to provide another perspective for the study of phase transition in spin glasses.

Herbert Fotso (Ames National Lab, USA), *Visualizing the non-trivial momentum distribution of a field-driven correlated light-heavy Fermi-Fermi mixture.* Time-of-flight images are a common tool in ultracold atomic experiments, employed to determine the quasimomentum distribution of the interacting particles. If one introduces a constant artificial electric field, then the quasimomentum distribution evolves in time as Bloch oscillations are generated in the system and then are damped, showing a complex series of patterns. In different-mass Fermi-Fermi mixtures, these patterns are formed from a frustrated phase separation in momentum space that is driven by Mott physics for large electric fields which stabilize them for long times.

Kalani Hettiarachchilage (Louisiana State University), *Ferromagnetism in a two-dimensional two species bosonic Hubbard model.* We study a doped two-dimensional bosonic Hubbard model with two hard-core species with different masses using quantum Monte Carlo simulations. With doping we find several distinct phases, including a novel phase separated ferromagnet with Mott insulating behavior for the heavy species and both Mott insulating and superfluid behaviors for the light species. Introducing an imbalance in the population between species, we find a fully phase-separated ferromagnet. By using finite size scaling of the susceptibility, we find the critical exponent

of the transition related to the two-dimensional Ising universality class. Since the global entropy of this phase is higher than that of the other magnetic phases and the effects of trapping potential in the different phases is crucial in identifying them experimentally, we investigate the existing of the ferromagnetic phase in the presence of a harmonic trapping potential. It is emphasized that such trapping effects can lead to have the ferromagnetic phase in both hard-core and soft-core bosons. This may provide a new avenue to realize magnetic phases in cold atom experiments. Work in collaboration with V. G. Rousseau, K.M. Tam, J. Moreno, and M. Jarrell (Louisiana State University).

Patrick Haase (Universität Göttingen, Germany), *A dual-fermion analysis of the Anderson-Hubbard model.* We apply the recently developed dual-fermion method for disordered interacting systems to the Anderson Hubbard model. This method treats both disorder and interactions on an equal footing, takes into account non-local correlations systematically, and thus represents a significant extension of the single-site mean-field description. We analyze the metal-insulator transition as well as the antiferromagnetic transition of the three-dimensional lattice, by looking at both one- and two-particle quantities, such as the local Green function and the conductivity. Work in collaboration with Thomas Pruschke (Univ. Göttingen), Shuxiang Yang, Juana Moreno, and Mark Jarrell (Louisiana State University).

Samuel Kellar (Louisiana State University), *Parquet Equations Implemented using HPX.* The study of correlated electron systems is an area gaining increased interest due to the increase of computational resources that have made solving such problems viable. An example of such a problem is solving the Hubbard Model using the Parquet Equations. As the temperature decreases and the system sizes increases, the solution requires a non-linear increase in system resources. The current solution to such an increase in computational requirements is to move the simulation to a parallel system. This requires storing the vertex functions across many different nodes. Communication across various nodes can inhibit the efficient completion of this algorithm. We use a new runtime system (HPX) which dynamically schedules the distribution of work across all processors. Utilizing the advantages of such a system will help the Parquet Equations to find a solution to the Hubbard Model more quickly. It does this through a combination of latency hiding and efficient distribution of the work across the computational resources. Work in collaboration with Bibek Wagle, Ka-Ming Tam and Shuxiang Yang (Louisiana State University).

Enzhi Li (Louisiana State University), *Periodic Anderson model with electron phonon interactions and its susceptibilities.* The periodic Anderson model(PAM) is used to study the heavy-fermion behavior of transition metal materials and the nature of Kondo Screening. Recently, PAM with electron-phonon interaction was introduced to explain the volume collapse of Cerium under high pressure. It has been known that PAM with electron-phonon interactions will give rise to two phases, local moment and Kondo singlet. They are separated by a first order phase transition line that terminates at a second order phase transition point. However, the local moment phase is destabilized by the residual entropy problem at low temperature. Here we show that the residual entropy can be eliminated through a phase transition to an ordered state at low temperature.

Zhou Li (Louisiana State University), *Typical medium dynamical cluster approximation applied to Migdal-Eliashberg theory.* We use the recently developed typical medium dynamical cluster approximation (TMDCA) to study Anderson localization and the superconductor-insulator transition. In our analysis both phonons and disorder are treated on equal footing. For phonons we use the Holstein model Hamiltonian and perform analysis for different types of disorder distributions, i.e.

binary or box distribution. It is of interest to see how phonons and disorder compete in fine-tuning of this phase transition by re-normalizing the gap parameter. For weak disorder we find that the size of the gap depends on the phonon frequency. Since for large phonon frequencies the Holstein model maps onto an attractive Hubbard model, we focus on the region where the phonon frequency is small and intermediate for both weak and strong disorders.

Conrad Moore (Louisiana State University), *GPU Accelerated Hirsch-Fye Quantum Monte Carlo.* In Dynamical Mean Field Theory and its cluster extensions, such as the Dynamic Cluster Algorithm, the bottleneck of the algorithm is solving the self-consistency equations with an impurity solver. The discretization of the imaginary time dimension in the Hirsch-Fye Quantum Monte Carlo algorithm makes it a suitable cluster solver for porting to the Graphics Processing Unit (GPU). This work implements optimizations of the algorithm, such as exploiting large data re-use to take even more advantage of the accelerator architecture. We discuss the application of the code for large scale strongly correlated calculations for electronic systems.

Ryky Nelson (Louisiana State University), *A Study of Disorder in Diluted Magnetic Semiconductor.* Motivated by experimental studies [A. Richardella et al., Science 327, 665 (2010); M. Dobrowolska et al., Nature Mater. 11, 444449 (2012); N. Samarth, Nature Mater. 11, 360-361 (2012); M. E. Flatté, Nature Phys. 7, 285-286 (2011)] addressing the role of impurity disorder in diluted magnetic semiconductors, we investigate the effects of disorder using a simple tight-binding Hamiltonian with random impurity potential and spin-fermion exchange which is self-consistently solved using the typical medium theory. Adopting the typical density of states (TDoS) as the order parameter, we find that the TDoS vanishes below critical values of impurity potential & exchange parameters, which indicates an Anderson localization transition in the system.

Valy G. Rousseau (Louisiana State University), *The superfluid density in systems with complex interactions.* In the last decade, the development and the improvement of quantum Monte Carlo algorithms combined with the increased power of computers has opened the way to the exact simulation of Hamiltonians that include various types of interactions, such as inter-species conversion terms or ring-exchange terms. Simultaneously, developments made in the field of optical lattices, laser cooling and magneto/optical trapping techniques have led to ideal realizations of such Hamiltonians. A wide variety of phases can be present, including Mott insulators and superfluids, as well as more exotic phases such as Haldane insulators, supersolids, counter-superfluids, or the recently proposed Feshbach insulator. These phases are characterized by a set of order parameters, one of which being the superfluid density. It is well known that the superfluid density can be related to the response of the free energy to a boundary phase twist, or to the fluctuations of the winding number. However, these relationships break down when complex interactions are involved. To address this problem, I will propose a general expression of the superfluid density, derived from real and thought experiments.

Elisha Siddiqui (Louisiana State University), *Typical Medium Dynamical Cluster Approximation For Disordered Superconductors.* Department of Physics & Astronomy, Louisiana State University,Baton Rouge, LA 70803, USA Center for Computation and Technology, Louisiana State University, Baton Rouge, LA 70803, USA We study the effect of disorder on a three-dimensional attractive Hubbard model using the typical medium dynamical cluster approximation with the Bogoliubov-de Gennes approach as a cluster solver. We explore the effects of disorder (W) for a fixed interaction strength (U) on the diagonal and off-diagonal typical density of states. As the

disorder strength is increased, the pairing parameter(ϕ) or the off-diagonal typical density of states decreases and vanishes at a critical disorder strength W_c while the spectral gap remains finite. This indicates the transition from a superconducting to a super-resistive phase. A further increase in the disorder strength causes the diagonal density of states to vanish at a critical $W_c^{'}$. This shows the transition from a super-resistive to the Anderson insulator phase. Work in collaboration with H. Terletska (Ames National Lab), N. S. Vidhyadhiraja (Nehru Center, Bangalore), C. E. Ekuma, J. Moreno, and M. Jarrell (Louisiana State University).

Shi-Quan Su (University of Tennessee, Knoxville, USA), *Non-traditional HPC Approach Simulating Acute Kidney Injury (AKI) Recovery Process on XSEDE Platform: Time-Dependent Cellular Automaton (TDCA) Simulation Using Workflow Engine.* Acute Kidney Injury (AKI) is a common and serious injury. Renal tubule epithelial cell (RTEC) injury is the main mechanism of AKI. It is possible that the cellular death which occurs with an RTECs injury can be regulated. The recovery process can be simulated on a high performance computer (HPC). The numerical model is the "Time-Dependent Cellular Automaton" (TDCA). We carry out the simulation in a Non-traditional HPC approach by managing the ensemble runs of the generic serial code on the Workflow engine, Unicore, provided on all the XSEDE platforms. The preliminary numerical result captures the features which qualitatively agree with the process observed in an actual experiment. Work in collaboration with Charles Collins (University of Tennessee).

Yu-Ting Tam (Sun Yat-Sen University, China & Brookhaven National Lab, USA), *Itinerancy enhanced quantum fluctuation of magnetic moments in iron-based superconductors.* We investigate the influence of itinerant carriers on dynamics and fluctuation of local moments in Fe-based superconductors, via linear spin-wave analysis of a spin-fermion model containing both itinerant and local degrees of freedom. Surprisingly against the common lore, instead of enhancing the (π,0) order, itinerant carriers with well nested Fermi surfaces is found to introduce significant amount of spatial and temporal quantum fluctuation that leads to the observed small ordered moment. Interestingly, the underlying mechanism is shown to be nesting-associated long-range coupling, rather than the previously believed ferromagnetic double-exchange effect. This challenges the validity of ferromagnetically compensated first-neighbor coupling reported from short-range fitting to the experimental dispersion, which turns out to result instead from the ferro-orbital order that is also found instrumental in stabilizing the magnetic order. Work in collaboration with Dao-Xin Yao (Sun Yat-Sen Univ. & Brookhaven National Lab), and Wei Ku (Brookhaven National Lab & Stony Brook Univ.).

Shuxiang Yang (Louisiana State University), *Numerical study of the periodic Anderson model with a quarter-filled conduction band.* Using the dynamical cluster approximation with continuous-time quantum Monte Carlo as the cluster solver and the recently introduced dual-fermion method, we study the underlying physics of the periodic Anderson model where the conduction band is near quarter-filling while the f-band electron band is half filled. For these parameters, the RKKY coupling changes its nature from ferromagnetic to anti-ferromagnetic, yielding an interesting phase-diagram. Especially, we find the charge ordering of the conduction band is strongly enhanced, which could be due to the proximity to a quantum critical point. Work in collaboration with Juana Moreno and Mark Jarrell (Louisiana State University).

Ge Yao (Louisiana State University), *Molecular dynamics in finding nonadiabatic coupling for β-$NaYF_4$: Ce^{3+} nanocrystals.* Optical and electronic properties of cerium ions doped into solid host matrices are explored by density functional theory (DFT). A spin-polarized (unrestricted) DFT + U

approach is applied to β-$NaYF_4$: Ce^{3+} nanocrystals, in which the Hubbard $U-J$ value is determined through experimental fitting to be 8.5 eV for yttrium, and 2.9 eV for cerium. Molecular dynamics simulations indicate that the energies of the localized f-like orbitals of the Ce^{3+} dopant exhibit strong thermal fluctuations compared to that of the p- and d-shaped orbitals due to charge-density localization. Our observation of mixing between the d and f orbitals of Ce^{3+} ion is consistent with experimental results. Combining time-dependent density matrix methodology, ab initio molecular dynamics, and on-the-fly nonadiabatic couplings simulates nonradiative transitions between electronic states at ambient temperature. Transition rates between individual orbitals decrease with their energy difference, which is similar to the format of the energy gap law. These transitions contribute to integrated rates of nonradiative thermalisation of different electronic excitations to the lowest excited state through multiple pathways. The integrated rates of thermalisation decrease with energy difference of the initial photoexcitation and the final excitation. Work in collaboration with Qingguo Meng (Laredo Community College), Mary T. Berry, P. Stanley May and Dmitri S. Kilin (University of South Dakota).

Peng Zhang (Carnegie Institution of Washington, USA), *DFT+DMFT study of magnetic properties in FeO at high pressure.* FeO is an insulator with anti-ferromagnetic (AFM) spin ordering at ambient pressure. As the external pressure is increased, the Néel temperature first increases when the pressure is below 20 GPa. It has been experimentally predicted that above 80 GPa the AFM ordering will collapse. The mechanism leading to such high pressure magnetic collapse is still under debate. We use the density functional theory plus dynamical mean-field theory (DFT+DMFT) to detect the nature of magnetic collapse in FeO at high pressure. Work in collaboration with R. E. Cohen (Carnegie Institution of Washington & University College London) and K. Haule (Rutgers University).

Yi Zhang (Louisiana State University), *Study of multiband disordered systems using the typical medium dynamical cluster approximation.* We generalize the typical medium dynamical cluster approximation to disordered systems with multiple bands. Using our extended formalism, we perform a systematic study of the non-local correlation effects induced by disorder on the density of states and the mobility edge of the Anderson localized states. We apply our method to the three dimensional multiband Anderson model with both inter- and intra-band hopping and disorder potential and find fast convergence with increasing cluster size. Our results are consistent with the ones obtained by the transfer matrix and the kernel polynomial methods. Our findings show that the typical medium dynamical cluster approximation method can be used to study the Anderson localization in real materials.

Yi-Fu Zhang (Louisiana State University), *Topological insulators in staggered flux systems.* Y. F. Zhang, Juana Moreno, Mark Jarrell Topological insulators are generally characterized by the Z_2 index, which requires time-reversal symmetry. On the other hand, the staggered flux states, known as orbital antiferromagnet or charge flux phases, break both time-reversal and translational symmetry. In this work, we investigate the behavior of topological insulators within staggered flux. Interestingly, gapless edge states consisting of counter-propagating states with opposite spins survive, and in some regions, a phase with two such pairs of edge states emerges. We exam the robustness of these phases in the presence of disorder and also show the topological phase transitions with varying the disorder strength. These systems demonstrate topological properties similar to but different from the well-known Z_2 topological theory. Work in collaboration with Wei Ku (Brookhaven National Lab), Juana Moreno and Mark Jarrell (Louisiana State University).

Mardi Gras Workshop
Petascale Many Body Methods for Complex Correlated Systems
Invited Talks

Alex Brandt (Rackspace, USA), *Physics B.S.: How I learned to stop worrying and live in business.* Physics B.S. – A degree that is used by many for any purpose the wielder chooses. This is the personal journey of one student's arrival in business after acquiring a degree in Physics. Alex's journey will explore what a Physics degree provides and how all Physics graduates use their degree daily. Alex is a Cloud Evangelist at Rackspace. Today he develops support and technology solutions to better Rackspace. Previously his work focused on training employees in Cloud, Python, Ruby, and Chef. He regularly consults with Rackspace customers to develop unique solutions while internally developing new approaches with evolving technologies. Alex holds a degree in Computer Science and Physics from Minnesota State University, Moorhead.

Herbert Fotso (Ames National Lab, USA), *Field-driven quantum systems, From transient to steady state.* Nonequilibrium dynamical mean field theory and nonequilibrium self-consistent strong coupling expansion are used to study the relaxation of correlated quantum systems driven out of equilibrium by DC electric fields. Both the Falicov-Kimball and the Hubbard model are found to exhibit different relaxation scenarios suggesting that driven quantum systems have a richer behavior than their quenched counterparts and that integrability does not play as critical a role. In the monotonic thermalization scenario, the system evolves through successive quasi-thermal states and it is possible to extrapolate its long time properties from its transient; bridging the gap between the transient and the steady state with very little computational cost. Furthermore, regardless of the relaxation scenario, it is interesting to ask how the particles are distributed as the system evolves in time. We will show that non-trivial parameter-dependent patterns are formed when the system is visualized in momentum space. These features should be observable in current cold atom experiments.

Sean Hall (Carver Scientific, USA), *Some surprising thoughts and realizations from a would be research scientist about employment in the 'Real World'.* Sean will talk about his experiences looking for employment and working at Carver Scientific, a small energy storage company specializing in capacitors and coatings. Sean holds a B.S. Degree in Computer Science and a M.S. Degree in Physics from Southern University in Baton Rouge. He has been recently awarded of a patent for a novel energy storage device.

Kalani Hettiarachchilage (Louisiana State University), *Ferromagnetism in a two-dimensional two species bosonic Hubbard model.* See list of posters for the abstract.

Václav Janiš (Academy of Sciences, Czech Republic & Louisiana State University), *Ergodicity in statistical mechanics of interacting and disordered systems: Destroying and restoring equilibrium ergodic states.* Statistical mechanics was introduced as a microscopic description of macroscopic thermodynamic phenomena. Laws of statistical mechanics become relevant for the thermodynamics only for infinite volumes, called thermodynamic limit. Such a limit exists only under certain assumptions, the most important of which is ergodicity. We discuss the irreplaceable role of ergodicity in the statistical description of thermodynamic equilibrium. There are, however, equilibrium situations when ergodicity is broken. Typically, ergodicity is broken at phase transitions with a broken symmetry of the Hamiltonian. Phase transition in frustrated disordered systems cause,

however, ergodicity breaking without any apparent broken symmetry of the Hamiltonian. We discuss the way the ergodicity breaking is treated in lattice spin models. We introduce the concept of symmetry-breaking fields to restore ergodicity at symmetry-breaking phase transitions. Further on we introduce replicas and hierarchical replications of the phase space of spin variables to successively restore an ergodic state in the mean-field theory of spin glasses with phase transitions without any symmetry breaking. We exemplify restoration of ergodicity in the low-temperature phases of the Ising spin model for a ferromagnet and a spin glass.

Erik Koch (German Research School for Simulation Sciences, Jülich, Germany), *The Lanczos Method.* See lecture notes at http://www.cond-mat.de/events/correl11/manuscripts/koch.pdf.

Wei Ku (Brookhaven National Lab), *How to construct symmetry-respecting Wannier functions.*

Peter Reis (PosiTech Corp., USA), *Using Physics and Computation in Industry.* Peter will talk about how he uses Physics to design electric and hydraulic circuits in Industrial Automation and how he uses Computation to program modern electrical circuits using the Programmable Logic Controller (PLC). In particular he will briefly describe how he configure the PLC using ladder logic.

Rudolf Roemer (University of Warwick, United Kingdom), *Sparse matrix diagonalization, what it is, why and when it works.*

Valy G. Rousseau (Louisiana State University), *The superfluid density in systems with complex interactions.* See list of posters for the abstract.

Shi-Quan Su (University of Tennessee, Knoxville, USA), *A Distributive Linear Algebra Approach for Scalable Computing Platform with Accelerator.* The heterogeneous architecture on supercomputers evolves in a fast pace, many of the top-ranked supercomputers take advantage of accelerators, such as the Intel Xeon Phi Many Integrate Core (MIC) or NVIDIA Graphics Processing Unit (GPU). But the software development lags behind in attaining high performance when dealing with heterogeneity. The large-scale dense matrix computation is a backbone of modern numerical simulations, such as thermal analysis, analysis using the boundary element method, and electromagnetic wave calculations in fusion application. Here we offer a solution, a high throughput parallel linear algebra package adapted to supercomputing platform with accelerator. On the front end, the users see the same library of functions as ScaLAPACK which they use everyday, plus they have the performance close to the theoretical peak of the accelerator device. Behind the scene, the algorithm is redesigned to conceptually embed the consideration of heterogeneity in every step, and implement with the latest architecture features. Work in collaboration with Eduardo D'Azevedo, Ki Sing Chan, and Kwai Wong (Oak Ridge National Lab.).

Shuxiang Yang (Louisiana State University), *Numerical study of the periodic Anderson model with a quarter-filled conduction band.* See list of posters for the abstract.

Peng Zhang (Carnegie Institution of Washington, USA), *DFT+DMFT study of magnetic properties in FeO at high pressure.* See list of posters for the abstract.

Yi Zhang (Louisiana State University), *Study of multiband disordered systems using the typical medium dynamical cluster approximation.* See list of posters for the abstract.