Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials

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Abstract: Many technologically important materials display complex behavior due to strong electronic correlations. These include magnets, magnetoresistive materials, lanthanides and actinides and high temperature superconductors. Some of these materials display complex phase diagrams with multiple competing ground states, spin and charge ordering and complex excitations like those associated with spin and charge separation. An unbiased treatment of these phenomena requires a theory able to treat the correlations over all relevant length scales. In part, due to the minus sign problem, numerically exact methods employed to study these systems scale exponentially. Thus, despite great recent progress such as the development of the dynamical mean field approximation and its cluster extensions, there is as yet no unbiased study of these complex phenomena. The Multi-Scale Many-Body (MSMB) formalism and algorithms address these problems by separating the correlations into different length scales and treating each with an appropriate approximation: strong correlations at short length scales are treated by numerically exact Quantum Monte Carlo (QMC) simulations, those at intermediate length scales are treated by Feynman diagrammatic methods, while the weak correlations at long length scales are treated by a (dynamical) mean field approximation with a self-consistently determined effective medium.

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1.0 Introduction.
Many important classes of materials are strongly correlated, that is, the interactions between electrons are large. Most magnets and superconductors fall into this category, including the lanthanides and actinides, heavy Fermion materials, transition metal oxides, high-temperature superconductors, manganites, and high-density ferromagnets.

1.1 The multi-scale challenge to many-body theory. Although these are materials of great technological promise, they are poorly understood due to long-ranged spin and charge correlations, competing ground states, and their complex phase diagrams.

Some examples are illustrated in Fig 1.[1] In heavy Fermion systems, such as CeIn3, strong correlations on the f-orbitals cause the electronic mass, measured by transport, specific heat, and magnetic response, to be strongly enhanced, sometimes by several orders of magnitude.[2] Often, antiferromagnetism competes with this heavy Fermion state. In some of these materials, applied hydrostatic pressure drives the magnetic ordering temperature towards zero, and a region of superconductivity is found at the transition between the magnetic and heavy Fermion states. The cuprates[3] and single-layer Ruthenates[4,5] have richer phase diagrams, but the control parameter is now doping. Bilayer manganites[6] display even greater complexity, with as many as ten distinct states induced by doping. The situation in most of these materials is further complicated by the co-existence of different phases as seen in the superconducting phase of some heavy Fermion materials[7,8] and the charge and spin ordering in cuprates (c.f. Fig. 2)[9], as well as the existence of spin and charge separation seen in SrCuO2 ARPES spectra, and in the spectra of many other highly anisotropic systems. These are all materials at the forefront of current experimental and theoretical research in condensed matter physics. Furthermore, a correct description of all of the interesting physics requires a multi-scale approach. For example, In Fig. 1A, in heavy fermion superconductors such as CeIn3, the
superconductivity emerges at the crossover between regions of antiferromagnetism and normal metal. Both the normal metal and the antiferromagnet may be described with a local order parameter, but the superconductivity is believed to have a non-local order parameter. Therefore, both the normal metal and the antiferromagnet may be described with a mean-field or local approximation, whereas the superconductivity requires non-local corrections. Therefore a local or quasi-local approximation will bias the solution against the superconducting solution. A multi-scale approach, with an appropriate treatment of the correlation at each length scale is required for an unbiased approach. Of course, in systems with spin-charge separation, as illustrated in Fig. 3, a theory must be able to capture the correlations responsible for local moment formation, coupling of moments to its neighbors, as well as the repeat length of the ordering which may be several lattice spacing. Most perturbative approximations tend to unify the spin and charge, so that spin-charge separation is a phenomena that requires a non-perturbative description. It may only be captured by a theory capable of treating non-perturbative effects over the length scales that separate the spinon and holon.

1.2 Present Approach. The present generation of numerical and analytical methods has made considerable progress in studying these systems. Quantum Monte Carlo (QMC), combined with dynamical mean field theory and its cluster extensions, have for example lent qualitative understanding of the origins of antiferromagnetism, the suppressed magnetic susceptibility, and superconductivity in these systems. Yet these algorithms are fundamentally limited in their treatment of the different length scales, and therefore have often employed approximations which introduce systematic biases in order to make progress. Over the last several years, our group, and others, have developed the algorithms required for the next generation of codes which will be a significant step forward in treating the complete set of length and energy scales at a quantitative, material-specific level.

The Dynamical Mean Field Approximation (DMFA)[10] and its cluster extensions, including the Dynamical Cluster Approximation (DCA)[11,12] are at the heart of this approach. As illustrated in Fig. 4, these approaches map the lattice onto a cluster embedded in a self-consistently calculated effective medium. In a limited sense these approaches are multiscale methods, since the correlations within the cluster are treated explicitly while those at longer length scales are treated in a mean field approximation. The cluster solution and effective medium are calculated by iteration. Upon convergence, the irreducible quantities from the cluster (self energy and vertices) are used to approximate the corresponding lattice properties.

Figure 3: Cartoon illustrating spin-charge separation in one-dimensional nearly antiferromagnetic systems, as seen in SrCuO2 ARPES spectra. When an electron is ejected, a hole is left behind. As the system evolves in time, the vertical axis, the hole (holon) moves leaving behind a spin defect (spinon).

Figure 4: The mapping between the lattice and a self-consistently embedded cluster in the Dynamical Cluster Approximation. Correlations within the cluster are treated explicitly with a quantum Monte Carlo (QMC) simulation, longer ranged correlations are treated with a mean field approximation.
We solve the embedded cluster problem using a Quantum Monte Carlo (QMC) simulation. Either a perfectly parallel (MPI) or a hybrid parallel (MPI+OpenMP) calculation is used. The latter approach yields a parallel speedup and increases the memory associated with each Markov process allowing us to simulate larger clusters. Nevertheless, the calculation is limited by the amount of memory available on each shared-memory node.

A far more significant limitation of the technique is the minus sign problem. It emerges in quantum simulations, where the sampling weight, the exponential of the action, is not positive definite. To compensate for this, all measurements \( \langle m \rangle \), must be rewritten as a ratio \( \langle m \rangle = \langle mS \rangle / \langle m \rangle \), where now the absolute value of the exponential of the action is used as the sampling weight in the Markov process. The sign problem emerges when \( \langle S \rangle \) becomes much smaller than one so that this ratio is undetermined. This is illustrated in Fig. 5, where the sign is plotted for a Hubbard model simulation with interaction strength U and bandwidth W. For realistic values of U/W=1, the average sign becomes too small to allow accurate simulations when the temperature is about 1/100 of the bandwidth. For a system like the cuprates, where W is about 2eV, this would be a temperature of about 20K. Thus the minus sign problem restricts our ability to perform explicit simulations of length scales of extending over four sites to nearly room temperature. Worse, the minus sign problem for correlated electrons has recently been shown to be non-polynomial hard[14]. This means that apart from accidental cancellations of the sign problem, all simulations of correlated electrons will grow exponentially with the inverse temperature and cluster size. Consequently, it is generally very difficult or not possible to treat correlations on the length scales which characterize spin and charge order, or are responsible for spin-charge separation or complex phase diagrams with conventional QMC algorithms. Clearly a new approach is required.

2.0 MSMB Approach

The Multi-Scale Many-Body (MSMB) approach offers a way of circumventing many of these problems. It has several components, first we develop a way of separating length scales, so that only strong correlations at short length scales are treated with the expensive (NP hard) QMC simulation, while intermediate and long length scales are treated with appropriate approximations which grow algebraically with cluster size. Improved cluster solvers are being developed to increase the efficiency of the short-length scale problem, while new diagrammatic methods are used to treat the intermediate length scales. Finally to...
enable the approaches to study correlated systems from first principles, these approaches are being integrated with LDA.

2.1 Separation of length scales. The most important component of the MSMB approach is the separation of the many-body problem into different length scales. This is accomplished by a multiple embedding scheme, illustrated in Fig. 6, in which correlations over each length scale are treated with an appropriate approximation. Correlations at short length scales, which are responsible for moment formation and the interaction of adjacent moments, tend to be strong. They are captured by the small blue periodic lattice, referred to as a cluster, which is treated with an explicit (numerically exact) QMC simulation. The short-length scale (blue) cluster is embedded in the larger brown and orange cluster. Correlations at intermediate length scales tend to be weaker and are treated on the this intermediate size cluster using diagrammatic techniques. This cluster is in turn embedded in an effective medium which is used to treat correlations on the longest length scales. Here, each site has many such neighbors so that the fluctuations of one neighbor may be neglected. In the MSMB approach, correlations at the shortest and longest length scales are treated in the same fashion as illustrated in Fig. 4. The diagrammatic treatment of the correlations at intermediate length scales and the integration of the approaches is new.

2.2 Diagrammatic methods at intermediate length scales. To treat the intermediate length-scale correlations on the large cluster, we employ a diagrammatic single-particle and two-particle self-consistent field theory [15-16] defined by a set of highly non-linear equations for the single-particle and two-particle Green’s functions and its irreducible counterparts. As illustrated in Fig. 7, the large cluster diagrammatic calculation is parameterized with small cluster QMC results. The diagrammatic theory requires the self-consistent solution of Bethe-Salpeter and parquet equations which are represented diagrammatically in Figs. 8(a) and (b). The quantities entering these equations are rank-3 tensors. Typical sizes for the dimension of these tensors i.e. the number, \( N_t \), of momentum-frequency labels, are of order \( N_t > 1600 \). The momentum and frequency integrals implicit in these equations may be represented as matrix-vector and matrix-matrix multiplications. The resulting algorithm therefore scales algebraically in the size of the large cluster (number of momentum labels) and the number of frequencies. The two-particle fully irreducible vertex \( \Lambda \) is expected to be short-ranged and is therefore approximated by the QMC estimate on the small cluster. To speed up convergence, the set of equations is initialized with small cluster QMC estimates for the quantities entering the diagrams.

The solution of the parquet equations on large clusters is numerically very expensive, having restricted its application to one-dimensional systems [17]. Current supercomputer architectures however allow us to solve these equations on large clusters in higher dimension. The computational bottleneck of our implementation of this algorithm is given by the solution of the Bethe-Salpeter equations

\[
\Gamma(Q,K,K') = \Gamma_a(Q,K,K') + (\Gamma_a G G \Gamma)(Q,K,K')
\]

which require \( O(N_t^4) \) operations. By exploiting the locality in the index \( Q \), the code is easily parallelized by distributing the data and equations in the index \( Q \) reducing the CPU time to \( O(N_t^3) \).

The communication bottleneck is in the solution of the parquet equations which require the computation of terms like \( (\Gamma_a G G \Gamma)(K+K'+Q,-K',-K) \) which contribute to \( \Gamma_a(Q,K,K') \). These terms are pre-computed but the non-uniform access pattern in the momentum-frequency labels requires a

\[
\begin{align*}
F &= \Gamma_a + \Gamma_a \chi^0 F \\
\Gamma_a &= \Lambda + \frac{F}{\chi^0 \Gamma_b}
\end{align*}
\]

Figure 8: Feynman diagrams representing (a) the Bethe-Salpeter equations and (b) the parquet equations which are part of the diagrammatic approach for the large cluster.
rotation of the matrices (see also Fig. 8(b)) and therefore a complex and global message passing pattern which requires the exchange of $O(N_t^3)$ data values.

A performance estimate for the communication required to solve the parquet equations was performed based on data from a recent run of the Intel MPI Benchmark Suite V2.3 on the ORNL XT3 Jaguar system for message sizes up to 4096 Bytes. An extrapolation of these estimates to the message sizes required for typical numbers of momentum-frequency labels $N_t = 1600$ (25,600 Bytes) and $N_t = 6400$ (102,400 Bytes) results in MPI_AlltoAll times of 1.6 and 6.1 seconds on 4096 processors respectively.

2.3 Improved Cluster Solvers at short lengths. In addition to developing new methods to treat intermediate length scales, we have also been active in the development of improved QMC methods to increase the length scales that can be treated explicitly. These include the development of hybrid (Scalapack) QMC, order $N$, and continuous time QMC methods.

2.3.1 Hybrid DCA QMC Simulation based on Scalapack/Blacs. A massively parallel QMC algorithm[18,19] is used to solve the DCA cluster problem defined by the initial green function $G_0(K,z)$ and an interaction potential. The cluster problem is recast into a path integral on a space-time lattice of size $N_t$. A field $s_i$ is introduced at each point in space-time to decouple the interaction. A Markov process is used to integrate over the field configurations. Starting with $G_c = G_0$, the cluster Green function matrix $G_c({s_i})$ (sized $N_t \times N_t$) is updated with a Dyson equation every time a change in the fields is accepted. This Green function update is one of two inner loops which dominate the CPU time consumed by the code. The other dominant loop involves the two-particle measurements such as susceptibilities. Both the Green function update and the two-particle measurement calculation are composed of GEMM BLAS calls and therefore run at speeds near the theoretical optimal FLOPS rate on each node [20].

As the problem size is scaled, there are two primary limitations which hinder performance. (1) Memory Limitations. As the cluster size increases, the memory requirements, which increase like $N_t^2$ can become quite large. (2) The warmup problem. QMC is inherently parallel because it consists of a stochastic Markov-chain walk, which may be split into several parallel, shorter walks, thereby reducing the number of measurements on each processor. However, each parallel walk must begin with a finite number of warmups to ensure equilibrium and its independence from the other walks. During the warmup, no measurements are made. Therefore, as the number of processors increases, the calculations become dominated by warmup. For this SciDAC project we utilize two different types of codes which take advantage of the parallelism of the Markov process inherent to Quantum Monte Carlo (QMC) simulation. The first, perfectly parallel,
code splits the Markov process into a separate Markov chain on each processor as shown on the left in Fig 9. When the problem of each Markov process is too large to fit within the memory associated with each processor, or too much of the total CPU time is consumed by the warm-up sweeps needed to achieve independence of the different Markov chains, a hybrid parallel code is used as diagrammed on the right. It employs MPI for communication between Markov processes and ScaLAPACK [21] for parallel linear algebraic calculations. The ScaLAPACK implementation is not limited by the number of shared memory processors per node as a prior OpenMP implementation, but can scale parallelization of the linear algebra library calculations to a number of nodes enabling support for problems requiring significantly larger array sizes. Currently the computationally expensive GEMM calls in the update and measurement portions of the code utilize ScaLAPACK and other work is carried out redundantly on the processors assigned to each Markov chain. The required arrays are distributed in block-cyclic fashion with the blocksize and number of processors per Markov process, $lproc \times lproc$, as user-adjustable parameters. The parallelization approaches/advantages are summarized in Fig. 10.

2.3.2 Order-N methods. The computation time of Determinant Quantum Monte Carlo (DQMC) scales as the cube of the number of electrons $N$, limiting system size to $N \approx 200$. Here we exhibit linear scaling on systems up to an order of magnitude larger; $N = 4000$. $\beta$ is the inverse temperature, $U$ is the interaction strength, $t$ is the kinetic energy scale, and $\mu$ is the chemical potential.

![Figure 11: Scaling plot of the simulation time of a model of interacting electrons on a lattice. In the standard algorithm, the simulation time grows as the cube of the number of electrons $N$, limiting system size to $N \approx 200$. Here we exhibit linear scaling on systems up to an order of magnitude larger; $N = 4000$. $\beta$ is the inverse temperature, $U$ is the interaction strength, $t$ is the kinetic energy scale, and $\mu$ is the chemical potential.](image)

![Figure 12: Average sign versus inverse temperature for the one-dimensional Hubbard model calculated with CTQMC. The sign is found to increase with cluster size $N_c$, in contrast to what is found with HFQMC. Here, the unit of energy is set by the bandwidth, $W=1=U$, and the filling is 0.75 (3/8 filled).](image)
electron bandwidth. We are applying the technique to various interesting problems in this parameter regime, and working to extend the approach to stronger coupling.

2.3.4 Continuous time QMC. Recently, Rubtsov et al [22] proposed continuous time quantum Monte Carlo (CTQMC) as an alternative to Hirsch-Fye QMC (HFQMC). We have developed optimized massively parallel CTQMC codes to test for applicability to the DCA cluster problem. This code employs a matrix representation that may be easily adapted to include long ranged correlations, phonons (including phonon modes which couple to the hybridization and not the density), multiple orbitals, etc. The main challenge to all such QMC algorithms is the minus sign problem. As shown in Fig. 12 we compare the average sign of CTQMC versus HFQMC. Whereas the CTQMC sign is clearly worse than HFQMC for two-dimensional clusters, the average CTQMC sign actually increases with cluster size for one-dimensional clusters! Thus this code shows great promise for highly accurate MSMB treatments of highly anisotropic systems such as SrCuO$_2$.

2.4 Integration of approaches including LDA. The multi-scale many-body formalism, may be combined with the local density approximation to density functional theory to provide a first-principles treatment of correlated systems. To facilitate the integration of these codes, we employ a self-energy based electronic structure method. The relationship between these methods is illustrated in Fig. 13. The user will enter materials information into a windows interface, which will run a self-energy based electronic structure module which calculates the parameters entering the Quantum Monte Carlo module such as screened Coulomb parameters and hopping integrals. The different multiscale simulations produce the low energy physics, such as the phase diagrams, and correlation functions that tell us about the competing phases discussed in Sec. 2.0. They also yield the self energy needed to re-initialize the electronic structure calculation. The electronic structure module can also deliver sets of physical properties such as crystal structures, one-electron spectra, optical properties in a high energy interval. This process continues until convergence is reached.

The Parallel multi-scale many-body QMC solver is exploded on the right of the figure. Either DQMC or the Hirsch-Fye algorithm will be used to solve the small cluster problem. These QMC codes, on petascale machines, will allow us to describe correlations over tens of lattice spacings. Both algorithms provide the self energy needed to solve the large cluster problem, in which the mean field calculation is implicit. The parquet approach is used for the large cluster problem. These approaches will be used to treat correlations between tens to hundreds of lattice spacings. Correlations over longer length scales are treated at the mean field.

3.0 Summary, Outlook and Outreach

Complex materials present a significant challenge to computational many body theory. These materials show complex phase diagrams due to competing ground states, spin and charge order and complex excitations such as spinons and holons. An unbiased treatment of these phenomena requires a theory able to treat strong electronic correlations over many length scales.
The goal of our team is to develop the formalism, algorithms and codes for a complete multiscale many-body treatment of these materials from first principles. There are several aspects to this project. First, we have developed a formalism to separate correlations according to length scales. Each length scale is treated with an appropriate approximation. Strong correlations at short lengths are treated explicitly by solving a small cluster problem using numerically exact quantum Monte Carlo methods. Correlations at intermediate length scales are treated approximately using Feynman diagrammatic methods to solve a larger cluster problem. Weak correlations at long length scales are treated in a mean field approximation with a self consistently determined effective medium. The small cluster is embedded in the larger cluster which is embedded in the effective medium. Embedding is accomplished through the exchange of irreducible quantities like the self energy or fully irreducible vertex function. Second, we are developing greatly improved QMC cluster solvers for the short correlations treated explicitly. These include hybrid (MPI+ScaLapack) Hirsch-Fye and continuous time QMC methods which may employ an arbitrary number of processors to each Markov process; thereby obtaining a parallel acceleration of each while also accumulating the memory needed to calculate two-particle quantities like the fully irreducible vertex function. We are also developing order N cluster solvers which employ superior preconditioned conjugate gradient solvers. Third, we are developing massively parallel diagrammatic methods to solve the parquet equations for the intermediate length scale problem. Forth, this set of codes is being integrated with a self energy-based LDA, which allows us to complete first-principles simulations of correlated systems.

The different research teams at The University of Cincinnati, UC Davis and ORNL are closely collaborating on code development to ensure that the codes work seamlessly with each other. Monthly video/tele conferences and frequent email exchange facilitate this. Exchange of postdocs will have a more dramatic effect, with postdocs shared between the three locations and no postdoc spending more than one year at each site.

This suite of MSMB codes developed in this project will be released with a modified GPL license and will have a great impact on the condensed matter community. Starting this September, and each September of the project, we will release core elements of the suite. The impact of these codes will be significant due to the present lack of public massively parallel condensed matter many-body codes. Each MSMB code is massively parallel and highly optimized. For example, all inner loops of the present HFQMC code are level-3 BLAS Gemm calls, and execute at a significant fraction of peak efficiency on a variety of different machines. Together, the final suite of codes will have a graphical user interface and will be materials specific (LDA-based), making the code both accessible and useful broadly throughout Condensed Matter and Materials Physics.

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