Parallelization of DQMC Simulations for Strongly Correlated Electron Systems

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joint work with
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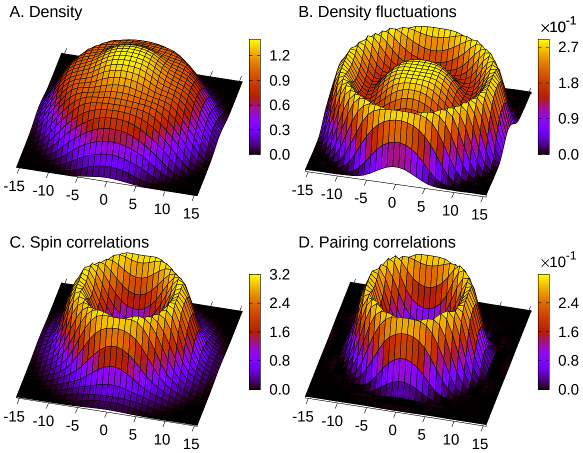
IEEE International Parallel and Distributed Processing Symposium 2010

Outline

1. DQMC simulations
2. DQMC parallelization
    - Algorithmic approaches
    - System approaches
3. Experiment results
4. Conclusion

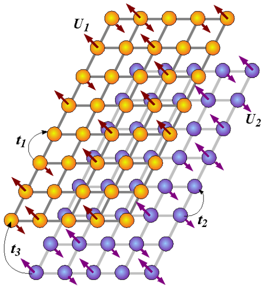
Computational Material Science

Understanding and exploiting the properties of solid-state materials: magnetism, metal-insulator transition, high temperature superconductivity, ...



Hubbard Model and DQMC Simulations

Many body simulation on multi-layer lattices using Hubbard model and quantum monte carlo method.



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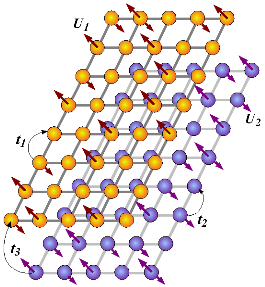
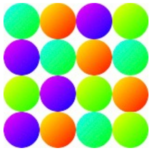




QUEST (QUantum Electron Simulation Toolbox): Fortran 90 package for Determinant Quantum Monte Carlo (DQMC) simulations.

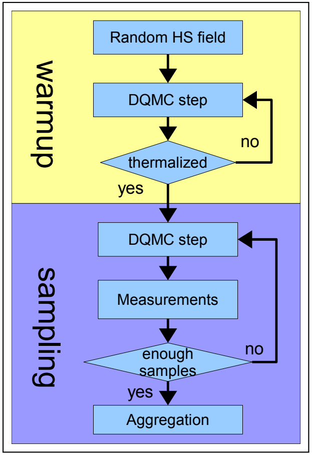
DQMC Algorithm

Two stages:

- Warmup stage
- Sampling stage

A DQMC step

1. Propose a local change: $h \to h'$.
2. Throw a random number $0 < r < 1$.
3. Accept the change if $r < \frac{\det(e^{-\beta H(h')})}{\det(e^{-\beta H(h)})}$.



Computational Kernels

The equal time Green's function

$$G_k = (I + B_k B_{k+1} \cdots B_1 B_L \cdots B_{k-1})^{-1}$$

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Physical measurements

Operations on G_k and G^τ, Fourier Transform, etc.

Computational Challenges

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- For simulating strongly correlated electron systems
  - The size of lattices need be large.
  - A longer warmup stage is required.
- Numerical stability issues.
  - Additional stabilizing steps are required.
  - Most calculations need double precision.
  - Many fast updating methods and parallel algorithms cannot be used.

DQMC Parallelization

Algorithmic approaches

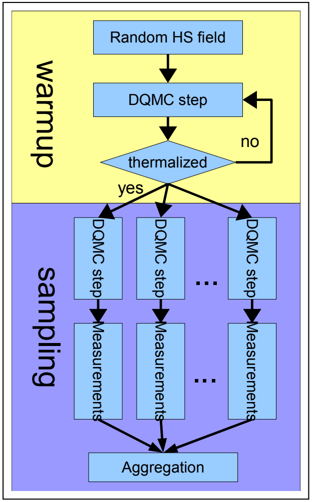
- Parallel Markov chain
- Rolling feeder algorithm
- Parallel matrix computations

System approaches

- Task decomposition
- Communication and computation overlapping
- Message compression
- Load balance

Parallel Markov Chain

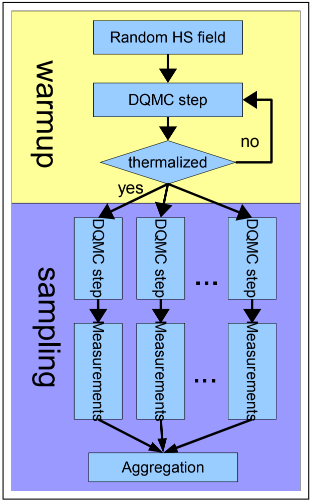
- The sampling stage can be parallelized embarrassingly.



Parallel Markov Chain

- The sampling stage can be parallelized embarrassingly.
- The speedup of parallelization is limited by the time of the warmup stage. (Amdahl's law)

$$\rho_{\text{speedup}} = \frac{T_{\text{warmup}} + T_{\text{sampling}}}{T_{\text{warmup}} + T_{\text{sampling}}/N_p} < \frac{T_{\text{warmup}} + T_{\text{sampling}}}{T_{\text{warmup}}}$$



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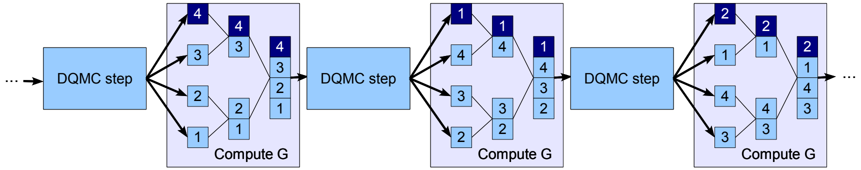
Parallel reduction (takes $O(N^3 \log L)$ time.)



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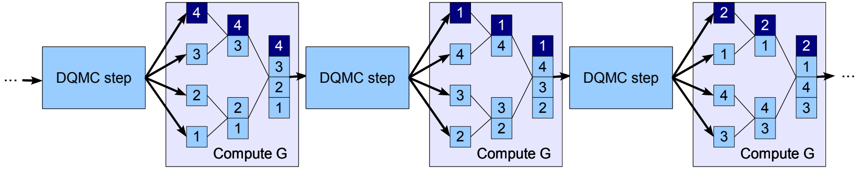

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Rolling Feeder Algorithm

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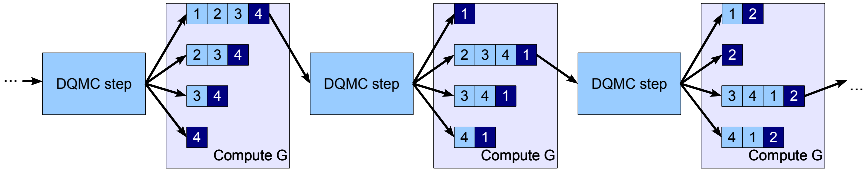

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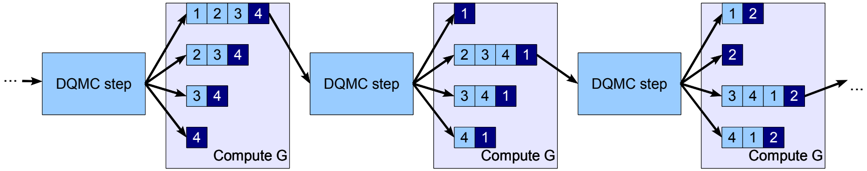

Tasks to get one G_k	Sequential	Parallel reduction	Rolling feeder
1. Matrix multiplication	L	$\log L$	1
2. Stabilization step	$O(L)$	$O(\log L)$	1
3. Inverting $(I + B_1 \dots B_L)$	1	1	1
4. Data transmission	N^2	$O(LN^2)$	N^2

Comparisons on resources and stability

Processor	$O(1)$	$O(L)$	$O(L)$
Numerically stable	Y	N	Y

Parallel Matrix Computations

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1. The unequal time Green's function is computed by blocks in parallel

$$G^{\tau}_{k,\ell} = \begin{cases} (I + B_k \cdots B_1 B_L \cdots B_{k+1})^{-1} B_k \cdots B_{\ell+1} & k > \ell \\ (I + B_k \cdots B_1 B_L \cdots B_{k+1})^{-1} & k = \ell \\ -(I + B_k \cdots B_{k+1})^{-1} B_k \cdots B_1 B_L \cdots B_{\ell+1} & k < \ell \end{cases}$$

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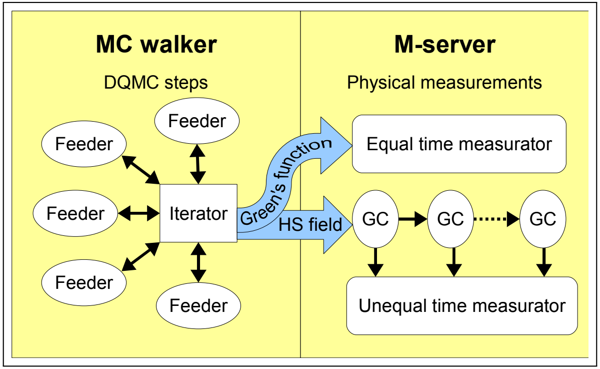
2. The matrix-matrix multiplication of G_k and each block matrix of G^{τ} is speeded up using multicore.
   - The matrix size of G_k, 100-1000, is too small such that the matrix computation cannot be benefited by using MPI-style parallelization.

System Design

- The system contains several “simulators” for parallel Markov chain.
- Each simulator consists of a “walker” and a “M-server”.

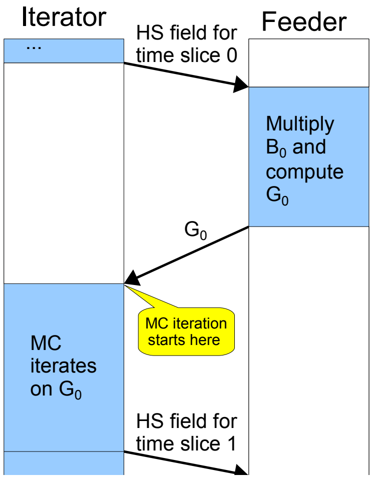


Implementation Techniques

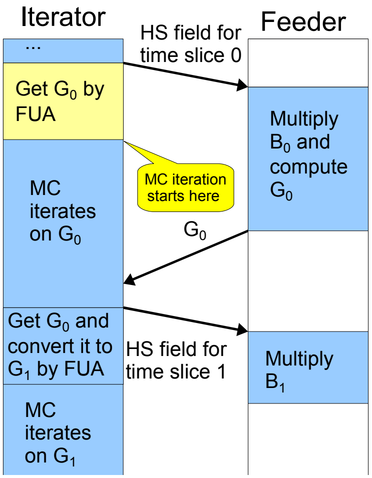
System is implemented for hybrid systems (cluster+multicore)

Task	MPI	OpenMP	Comm/comp overlapping	Message compression	Load balance
Parallel Markov chain	✓				
Rolling feeder algorithm	✓	✓	✓	✓	✓
Unequal time Green's fn	✓	✓		✓	✓
Physical measurement	✓			✓	✓

Communication/Computation Overlapping


Iterator
Feeder
...
HS field for time slice 0
Multiply B_0 and compute G_0
G_0
MC iteration starts here
MC iterates on G_0
HS field for time slice 1

Without overlapping


Iterator
Feeder
...
HS field for time slice 0
Get G_0 by FUA
Multiply B_0 and compute G_0
MC iteration starts here
MC iterates on G_0
G_0
Get G_0 and convert it to G_1 by FUA
HS field for time slice 1
Multiply B_1
MC iterates on G_1

Using fast update algorithm (FUA) to reduce waiting time

Load Balance

- Iterators are fully occupied $\rightarrow$ the bottleneck of speedup.

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  - For example, when computing unequal time Green's function, each processor can take care of more than one block submatrix.
- The load balance problem: how many block submatrices should one processor compute?
- Using the queueing theory (Little's law) to estimate.

$$n_C = \max_{P \leq 1} \left\lfloor \frac{P}{\lambda T} \right\rfloor \leq \left\lfloor \frac{1}{\lambda T} \right\rfloor .$$

  - λ: arrival rate; T: processing time; P: processor utilization.

System and Benchmark

System

- Run on the IBM Blue Gene/P
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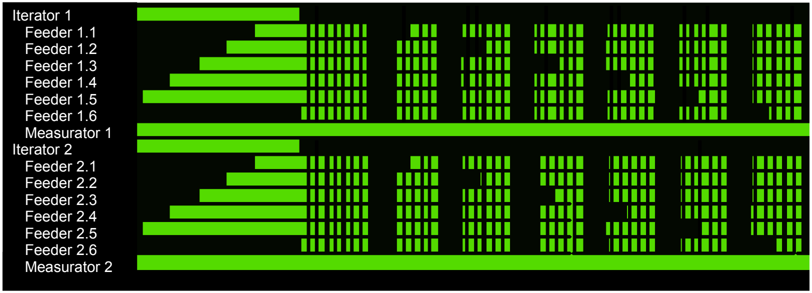
Benchmark

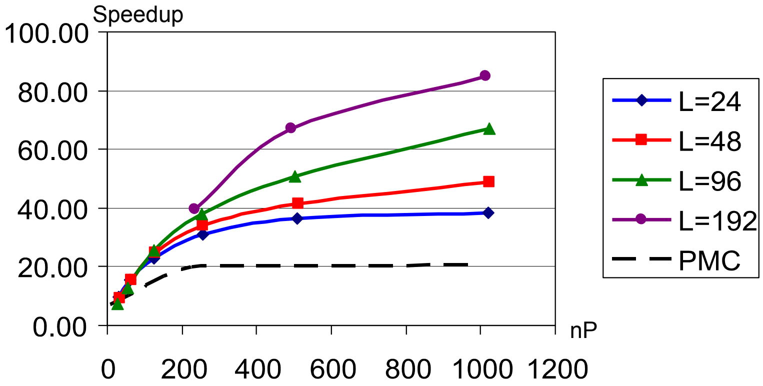
- DQMC simulation on a two-dimensional periodic lattice.
- The lattice size is $N = 16 \times 16 = 256$.
- The ratio of DQMC steps for the warmup stage and the sampling stages is $1 : 20$.

Communication Pattern

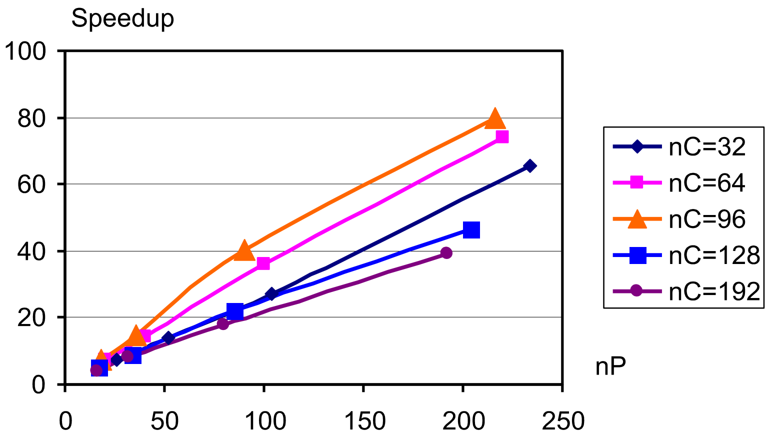


- Green bands show the waiting time of MPI_RECV.
- Iterators are fully occupied after started.

Speedup for Different *L*



Effect of Load Balance ($L = 96$)



- nC: number of block submatrices computed per processor.

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- DQMC simulation for strongly correlated materials is a computationally intensive task, which is eager for parallelization.
- We targeted the hybrid massive parallel systems, and explored the parallelism of DQMC simulations on different levels of granularity.
- Our implementation shows over 80x speedup on thousand processors, which is much better than embarrassing parallelization (speedup < 21).

Future Works

- More fine-grain parallel matrix computation kernels (pivoted QR, QR, matrix inversion) to fully utilize the computational power of multicores.

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- Better system design to enhance the processor utilization.
- Different physics models and methods.
- Code is still in the experimental stage. Further development is required for practical use.