Computational Study of Colossal Magneto-resistive Manganites

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Recording Head

[Diagram showing the components of a recording head: Shield, Writer, Reader. Dimensions: 10 Gb/in², 70 nm length, 0.9 µm width.]
**CMR Manganites: Phase Diagrams**

Phase Diagram of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$

Uehara, Kim and Cheong

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Model Phase Diagram Calculations

http://arxiv.org/abs/cond-mat/0509418
Understanding the CMR Effect


NO DISORDER

FM Metal Insulator

WITH DISORDER

Region relevant to CMR

FM Metal CE

No Field “Small” Applied Field

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Diagonalizing the fermion matrix

- Hamiltonian is *quadratic* in fermion operators (matrix): $4^N$ dimensional Hilbert space but problem is reduced to solving the “one-particle Hilbert space” (2N states) and filling levels.
- Integration of classical spins with Monte Carlo
- **Complexity:**
  - Previous method: Matrix diagonalization is $O(N^3)$, executed $O(N)$ times in the Monte Carlo integration: $O(N^4)$
  - More efficient diagonalization: truncated polynomial expansion of density of states (Motome and Furukawa): complexity $O(N)$ and it can be parallelized.
Computational Simulation on XT3

Microscopic phenomenological model

DISORDER (~100 procs.)

MONTE CARLO INTEGRATION
(order N complexity)

Polynomial expansion method
for electrons.
(scales up to 16 to 40 procs.)

Most time consuming function:
Sparse matrix-vector multiplication

1st parallelization (trivial or not)
2nd parallelization (non-trivial)

➢ Typical runs of 1600 to 4000 procs. For phase diagrams, etc.
➢ Runs usually take 12 to 20 hours to complete.
Scaling and Reliability of the Polynomial Expansion Method

![Graph showing CPU Time vs. Number of Sites]
Phase Diagram with Disorder on the XT3
Spin-Phonon-Fermion (SPF) Code

- Http: //mri-fre.ornl.gov/spf
- Integration into psimag toolkit in progress (http: //mri-fre.ornl.gov/psimag)
- MPI with two group communicators: one for the inner integration (PEM) and another to parallelize chemical disorder.
- Code profiled so that most time consuming function is the **sparse matrix-vector multiplier** as expected.
- SPF code also allows us to simulate other magnetic materials: e.g. Diluted magnetic semiconductors (have interest in spintronics).
Conclusions

- Get inspiration for future technologies by studying CMR in manganites.
- New $O(N)$ algorithm and scalable implementation on XT3 allows us to solve a realistic model.
- Chemical disorder creates a region in the phase diagram relevant to understand the CMR effect.
The End
Conclusions

- Calculation of phase diagrams with the polynomial expansion (PEM) are now possible using ~1600 procs. on the Cray XT3.
- By including chemical disorder into the model we will be able to test a hypothesis to explain the CMR effect and more generally to study phase separation and inhomogeneities.
- The PEM will be used on the Cray XT3 to study material-specific spin-fermion models with unbiased techniques.
Complex Observables

- Spectral functions and dynamical observables require more moments for the expansion.
- This implies that the inner parallelization scales up to a larger number of procs. (from 50-100 procs).
- Similar trends for the calculation of conductances or resistivities.
- These “complex” observables are calculated in selected regions of the phase diagram.
Interesting region where CMR effect happens!
La$_{1-x}$Ca$_x$MnO$_3$

[Schiffer et al., PRL 75, 3336 (1995)]
Colossal Magneto-resistive manganites

- Certain manganites (Mn oxides) show the so-called CMR effect.
- Applied magnetic fields produce colossal variations of resistivity.
- Theoretical interest in manganites: they are correlated electron systems.
- Possible technological applications in the future.
Main goals remove

➢ Study the magnetic phase diagram of the model.
➢ Include disorder to search for explanations to the CMR effect.
➢ Include even more realistic band structure and build material-specific models.