Computational Study of Colossal Magneto-resistive Manganites

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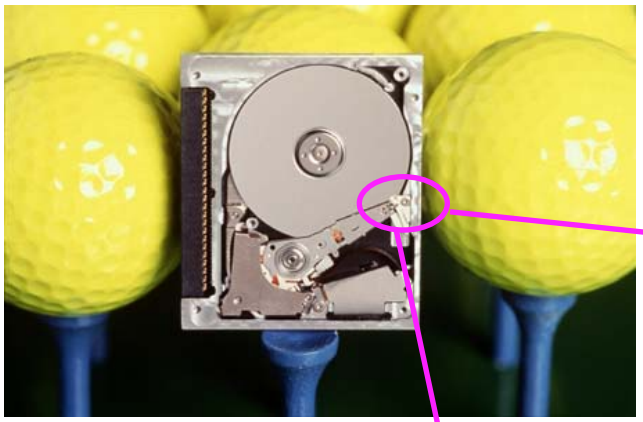
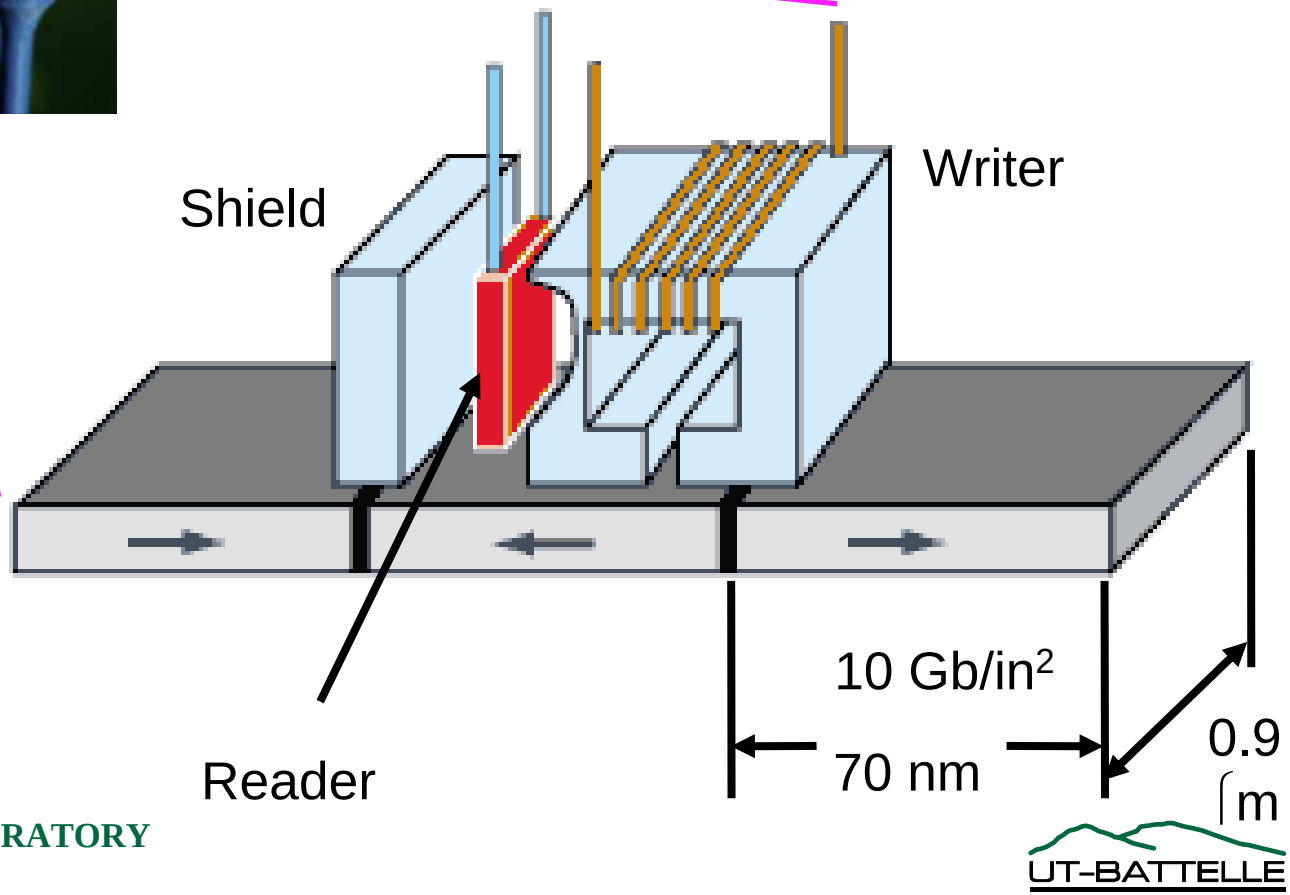
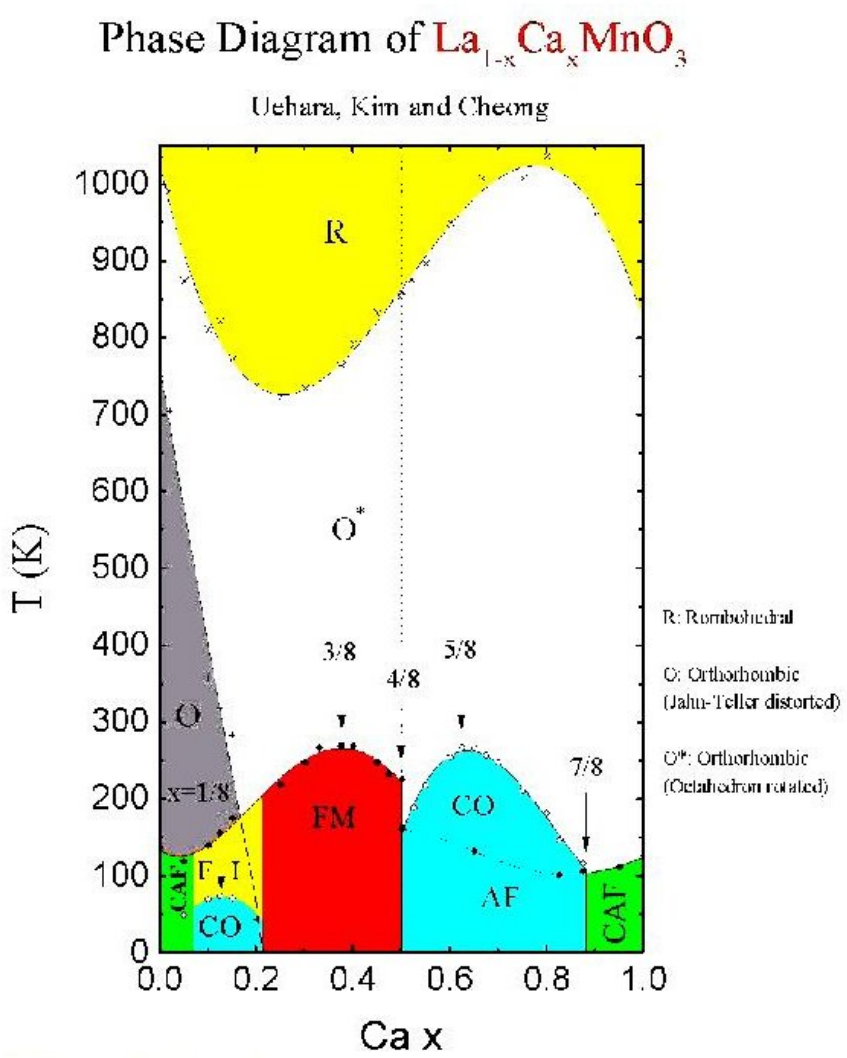
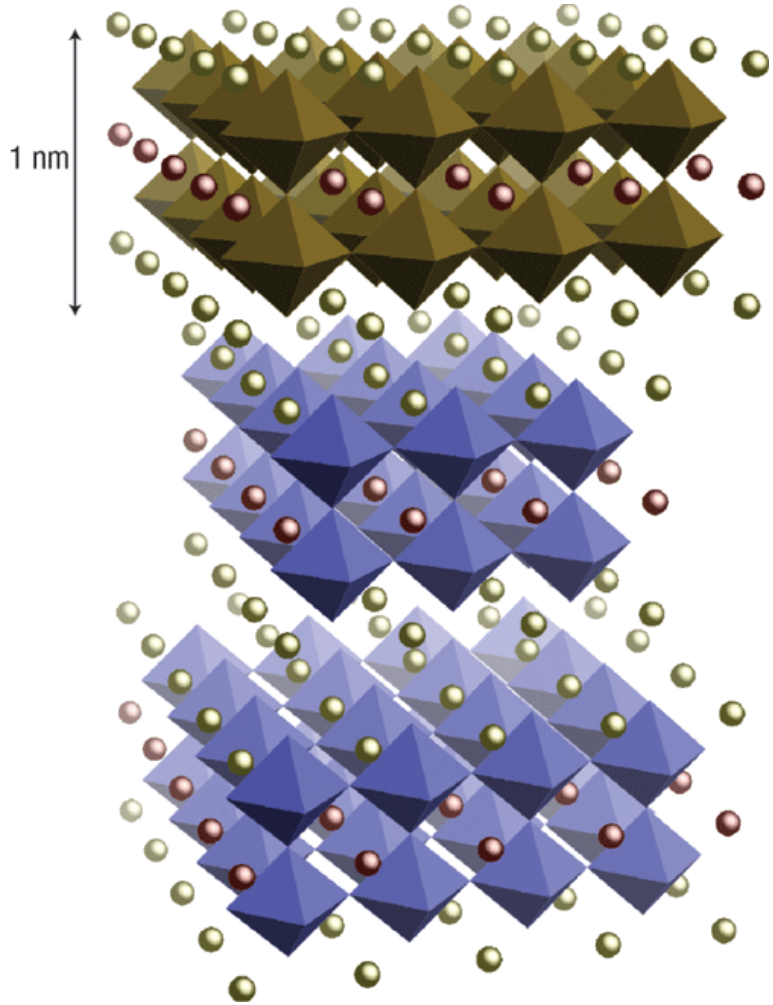
Recording Head





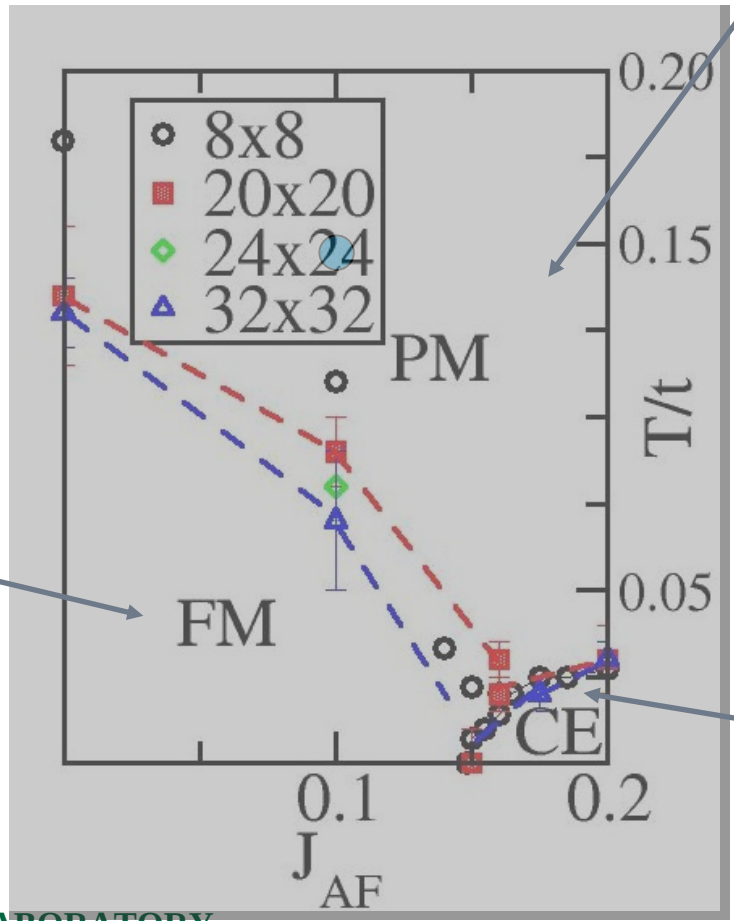
CMR Manganites: Phase Diagrams

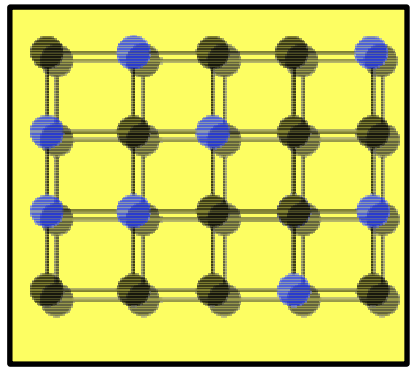


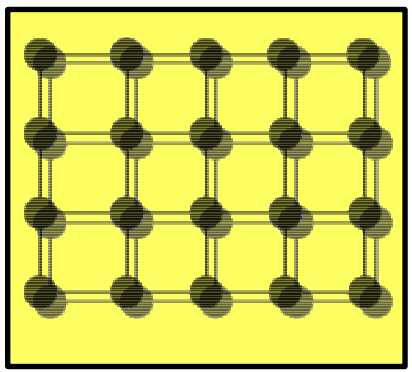


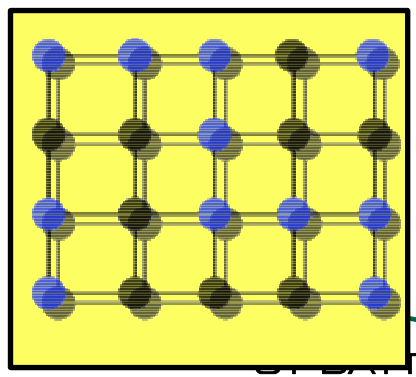
Model Phase Diagram Calculations

- http://arxiv.org/abs/cond-mat/0509418



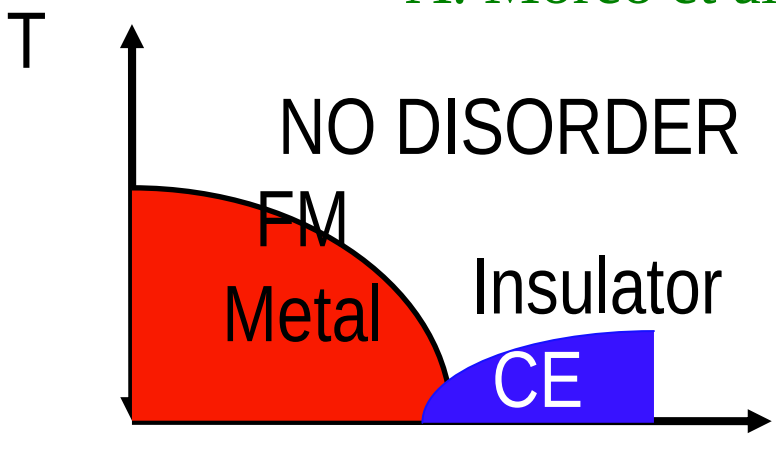




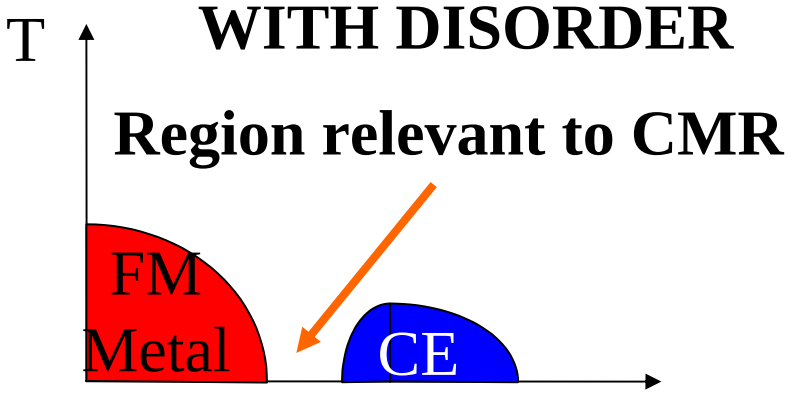


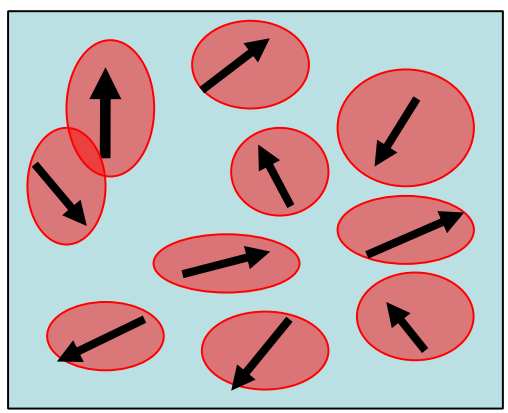
Understanding the CMR Effect

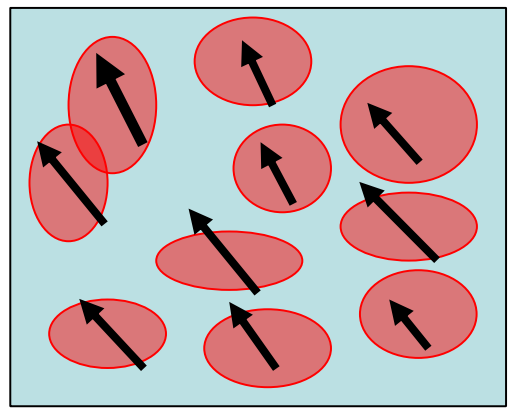
A. Moreo et al., Science 26, 283, (1999)



Recent review: E. Dagotto, Science 309, 257 (2005)







No Field

"Small" Applied Field

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 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.)

1st parallelization (trivial or not)

MONTE CARLO INTEGRATION (order N complexity)

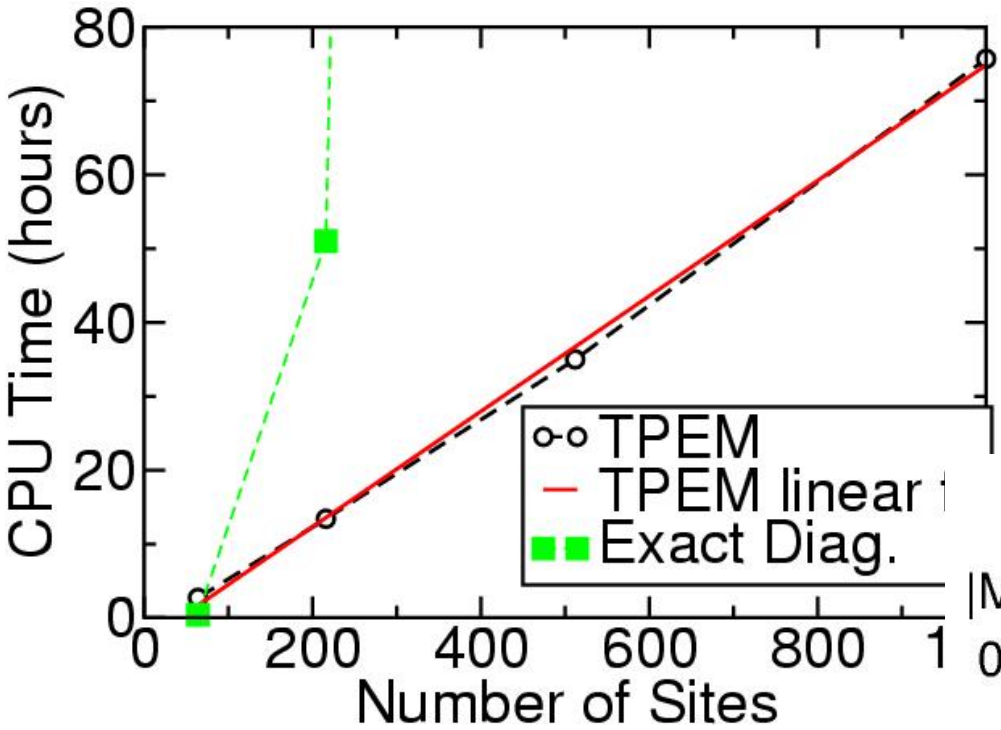
Polynomial expansion method for electrons. (scales up to 16 to 40 procs.)

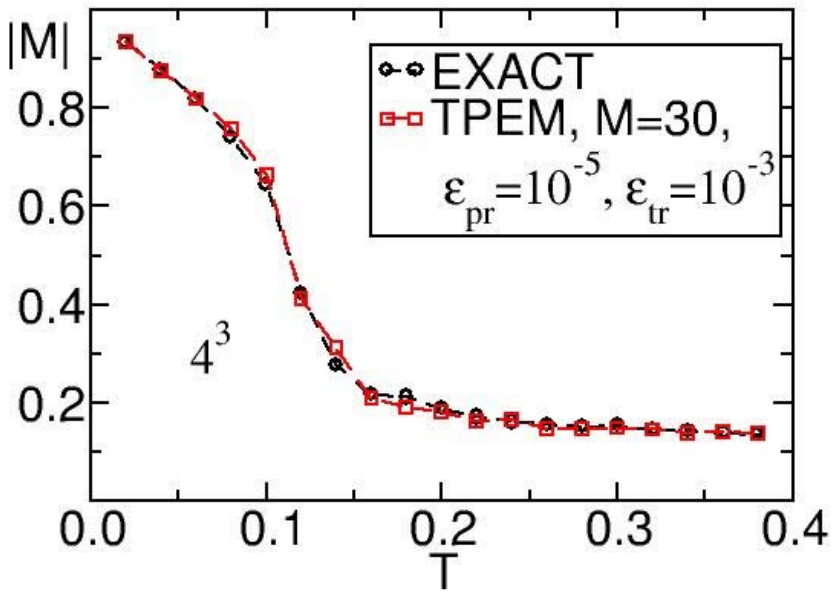
2nd parallelization (non-trivial)

Most time consuming function: Sparse matrix-vector multiplication

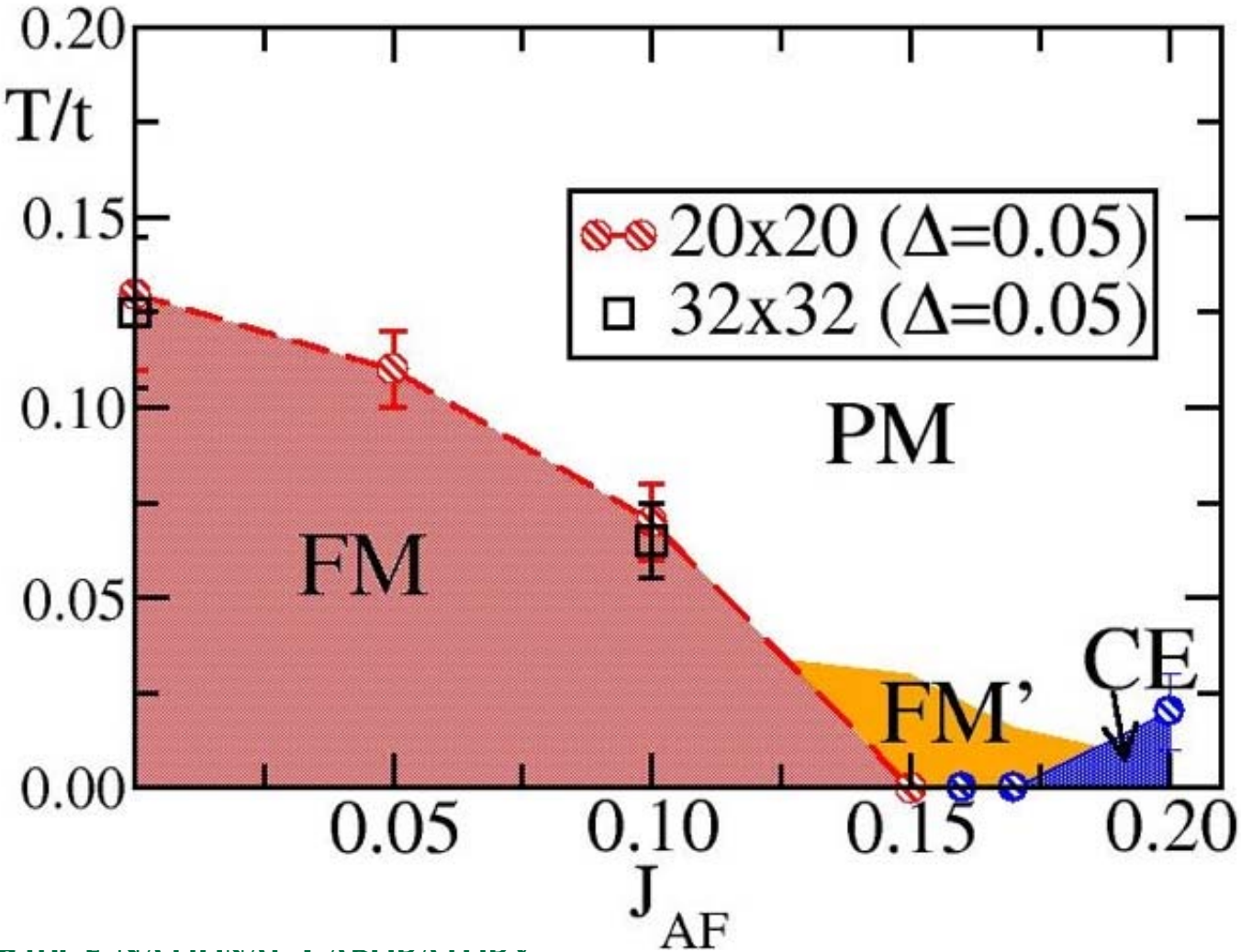
- Typical runs of 1600 to 4000 procs. For phase diagrams, etc.
- Runs usually take 12 to 20 hours to complete.

Scaling and Reliability of the Polynomial Expansion Method





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.**

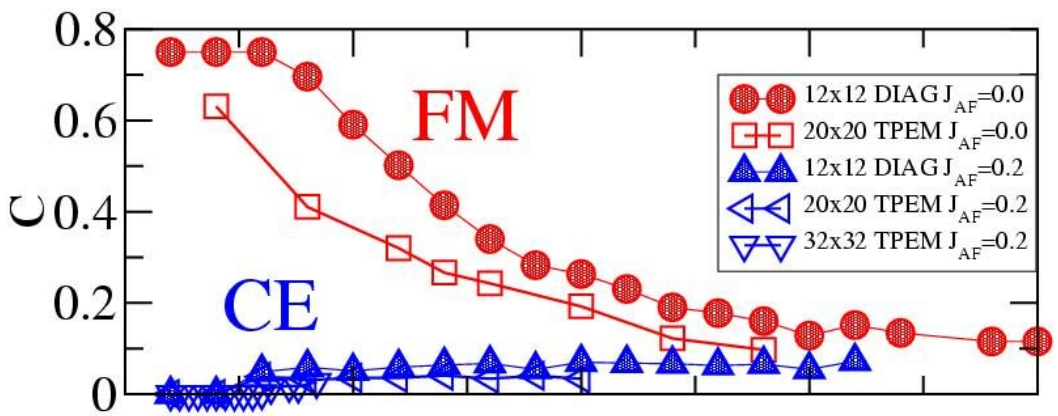
The End

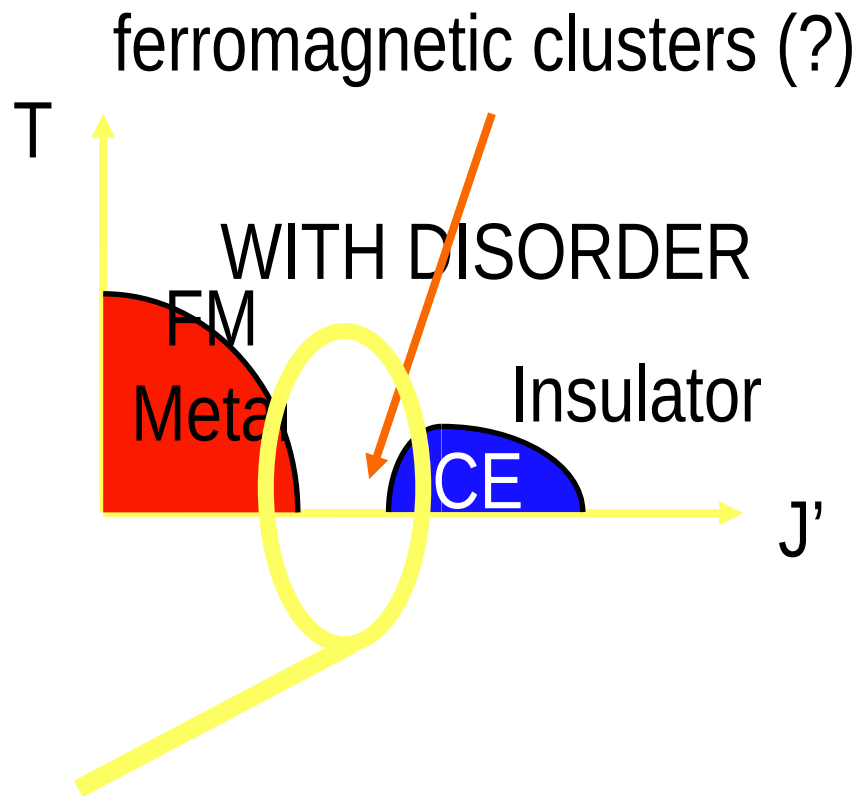
Conclusions

- **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.

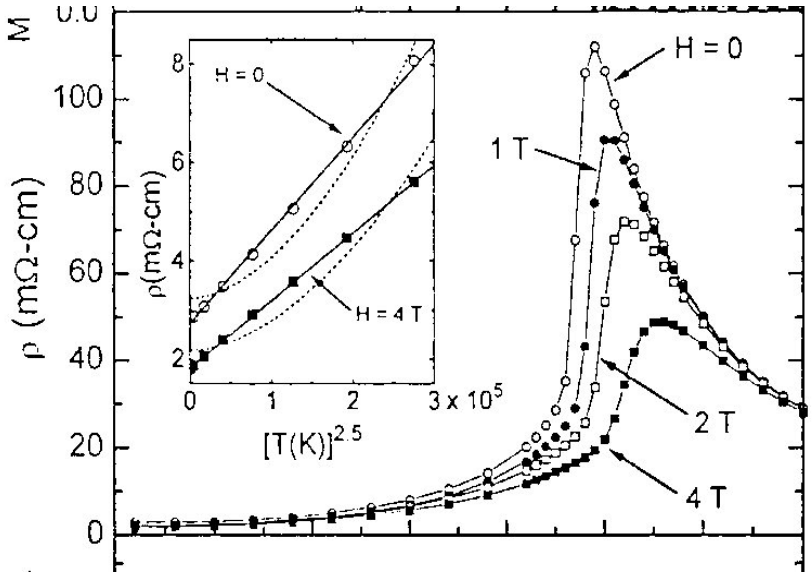




Interesting region where CMR effect happens!

[Schiffer et al., PRL 75, 3336 (1995)]

$La_{1-x}Ca_xMnO_3$



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.