Impact of Cray-X1 on Materials Science

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Computational Materials Science

- **A field of many "big-science" problems**
- **Push then envelope in high-performance computing**
  - **First to reach Gflop/s**
  - **First to reach sustained Tflop/s**
  - **At least two *real* problems lined up for peta-scale computing**
- **It pays off to bring scientists and HPC engineers together early on!**

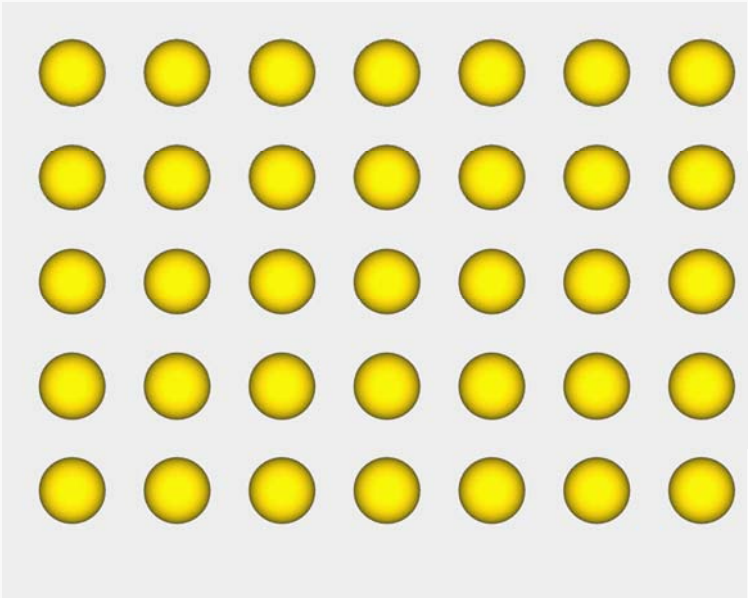
Decisive change in understanding of high temperature superconductivity

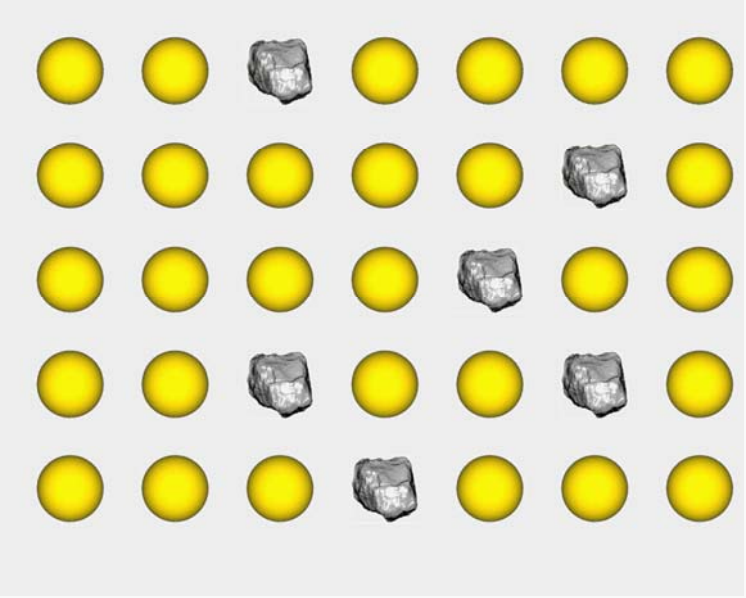
Thomas Maier, Trey White, and Thomas Schulthess (ORNL)
Mark Jarrell (University of Cincinnati)

Outline

- **Superconductivity: a short tutorial**
- **Single band 2-D Hubbard Model: Computational solution (!)**
- **Why Cray-X1 does well**
- **Summary / Conclusions / Outlook**

Conduction in metals





- **Perfect metal at T=0K, resistance is zero**
- **Real metal at finite temperature:**
  - **scattering from defects, lattice vibrations, …**
  - **this leads to fluctuation in current,**
  - **which leads to dissipation (fluctuation dissipation theorem),**
  - **which is equivalent to a non vanishing resistance.**

Superconductivity: what and what for

- **Zero resistance at finite (but low) temperatures**
  - **Discovered in 1911 by Kamerlingh-Onnes (Nobel Prize in 1913): Hg superconducting at 4.2 K**
  - **Later observed in other metals like Nb, Al, … but the critical temperature, T_c<23K**

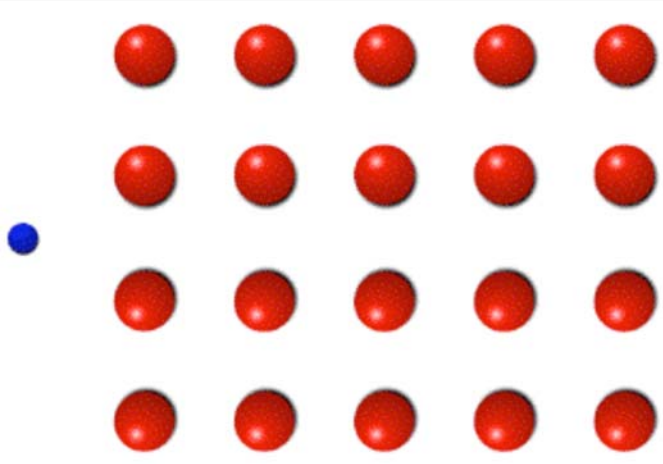
- **Applications (examples):**

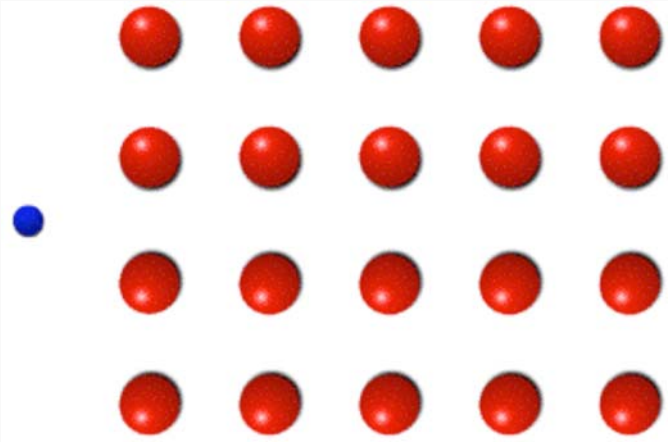
MRI (without need for liquid He cooling?)

Loss free power transmission (without cooling?)

BCS Pairing mechanism

- **When electrons form pairs, they behave like bosons and can condensed into a macroscopic quantum state**
- **Bardeen, Cooper, and Shriffer (BCS) develop rigorous description of pairing mechanism**
  - **Theory developed in the 1950s, Nobel Prize in 1973**

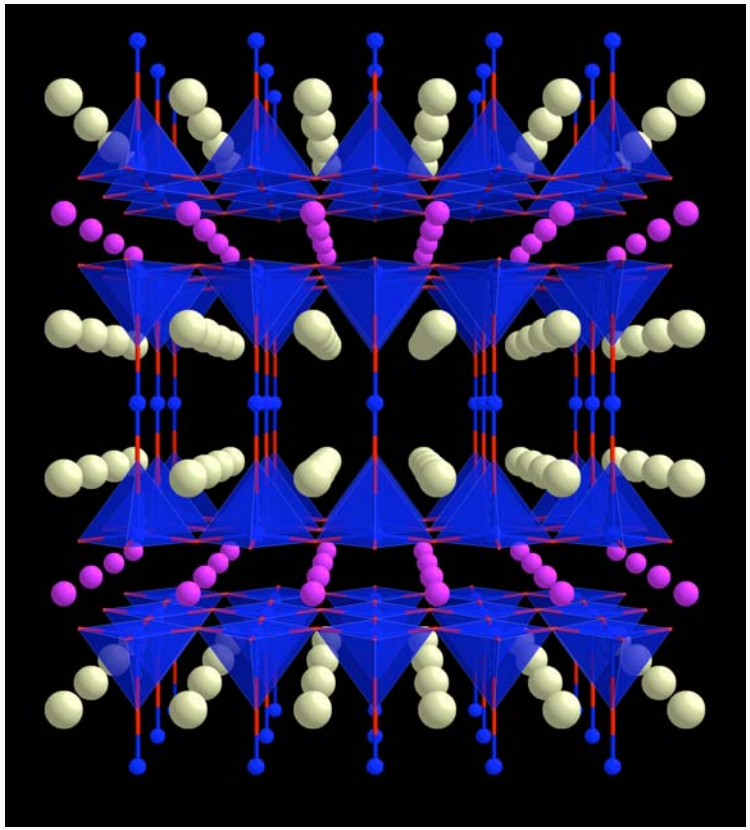




- **At T>20K, lattice vibration are strong and destroy pairs, superconductor becomes a normal metal.**

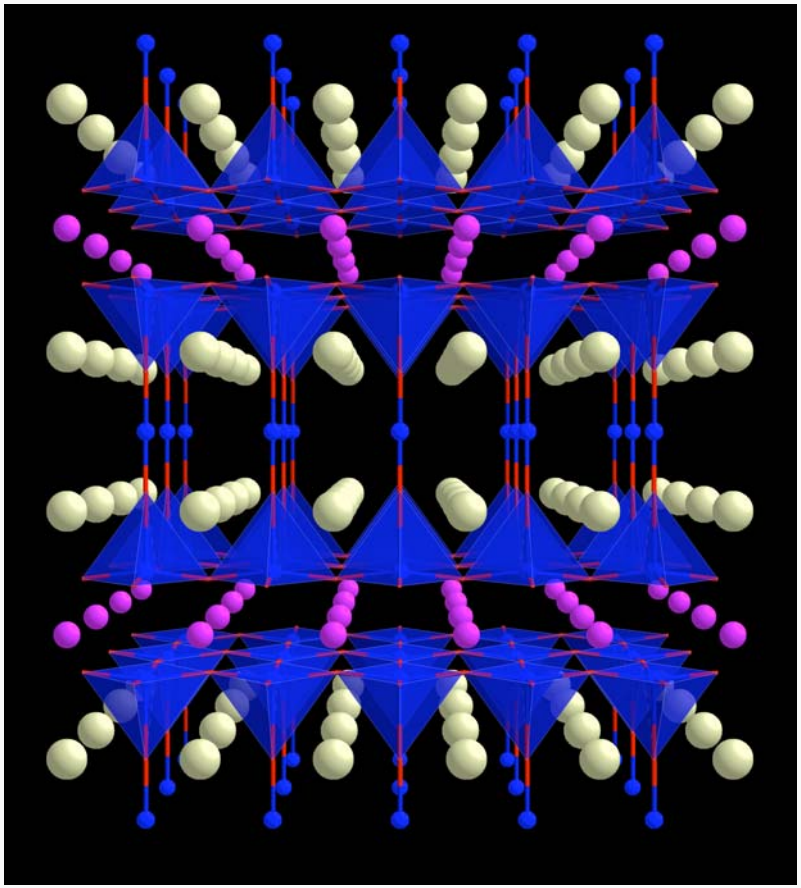
High Temperature Superconductivity

- **Doped $YBa_2Cu_3O_7$**
  - **Normal states is insulating / poor metal**
  - **Discovered to be a SC with T_c=30K in 1986 (75 years after Kamerlingh-Onnes)**
  - **1987 Nobel Prize for Bednorz and Muller**
  - **Within years, other transition metal oxides were discovered with T_c>100K (liquid Nitrogen cooled SC)**
- **There is general agreement that the pairing mechanism is not phonon mediated**

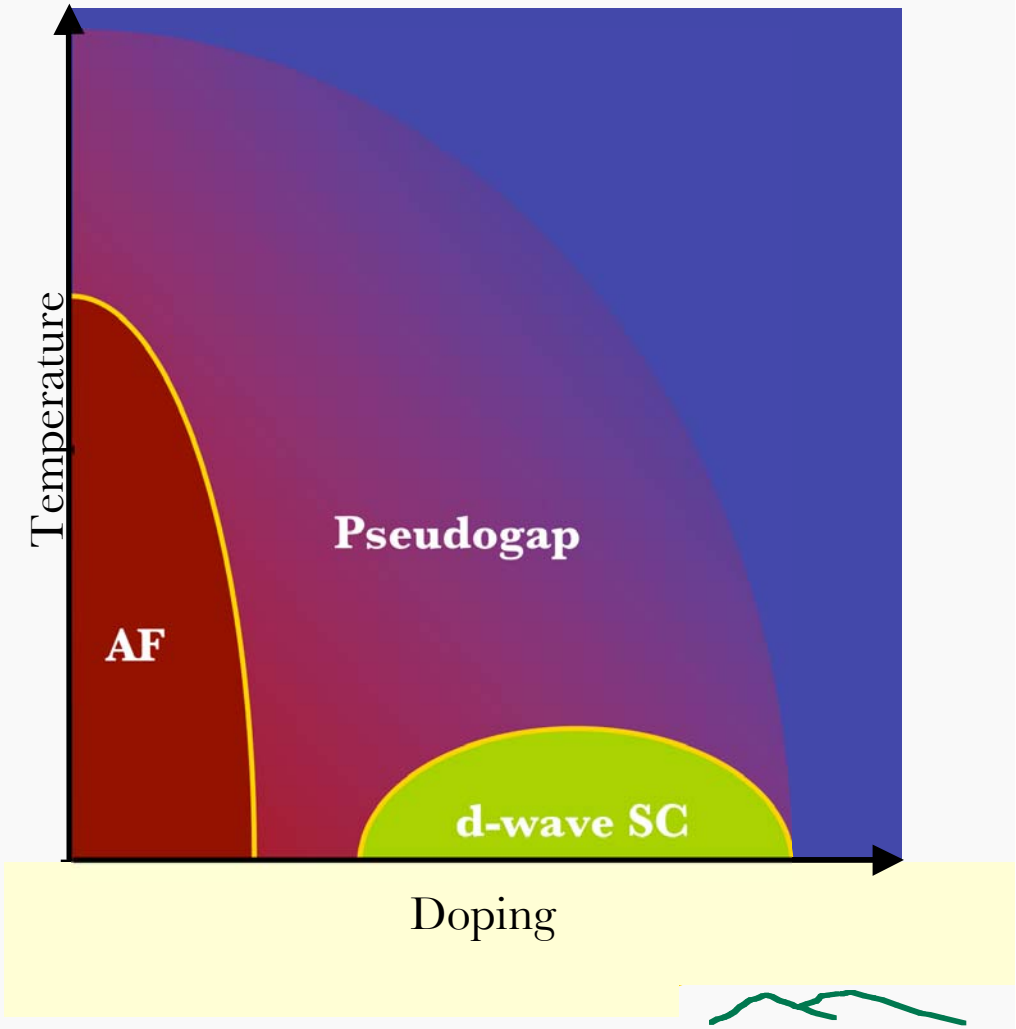


High-T_c cuprate superconductors

Layered structure

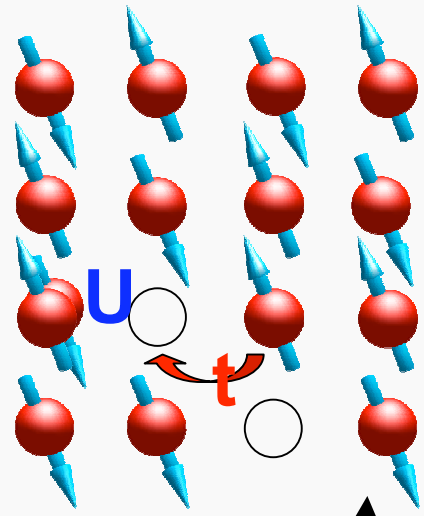


Generic HTSC Phase diagram

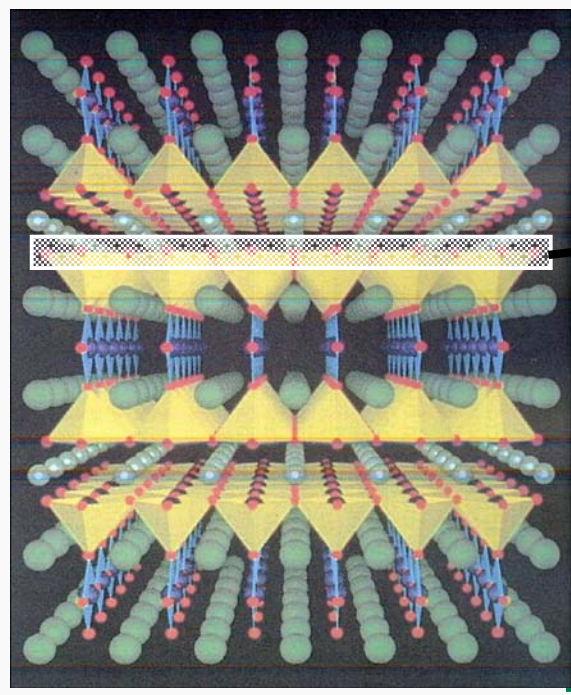


High Tc Superconductivity (conventional wisdom)

- **Model Copper oxide planes with single band 2D Hubbard models (Zhang & Rice, PRB 1989)**



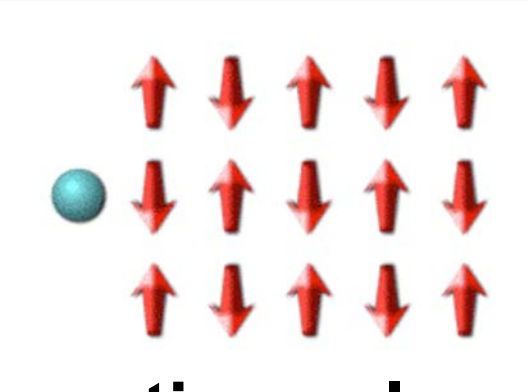
- **Solvable only in 1-D not in 2-D!**
  - **Computationally very challenging: *N* interacting electrons on a lattice, where N ≈ 10^{23}**

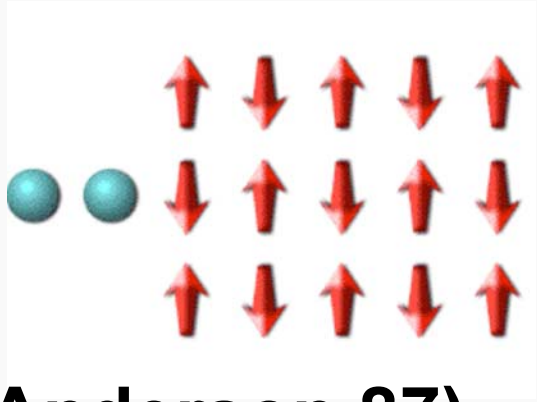


- **David Pines: "arguably the major problem in physics today"**

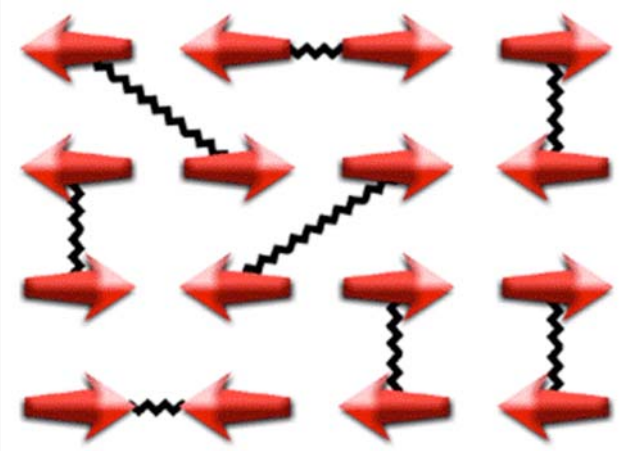
Many proposed paring mechanisms

- **Quasi particles in AF background (Hirsch 02)**





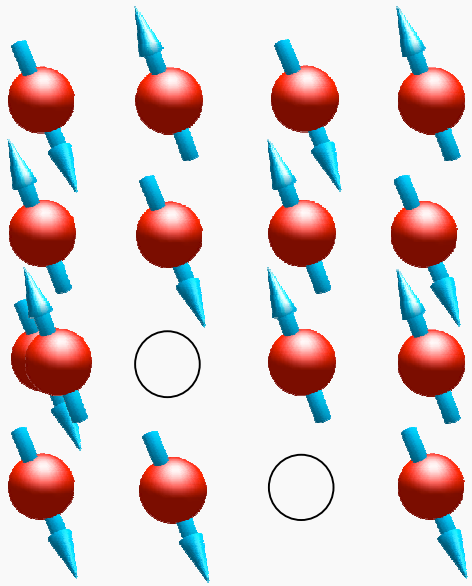
- **Resonating valence bond (Anderson 87)**



- **Computational solution ?**

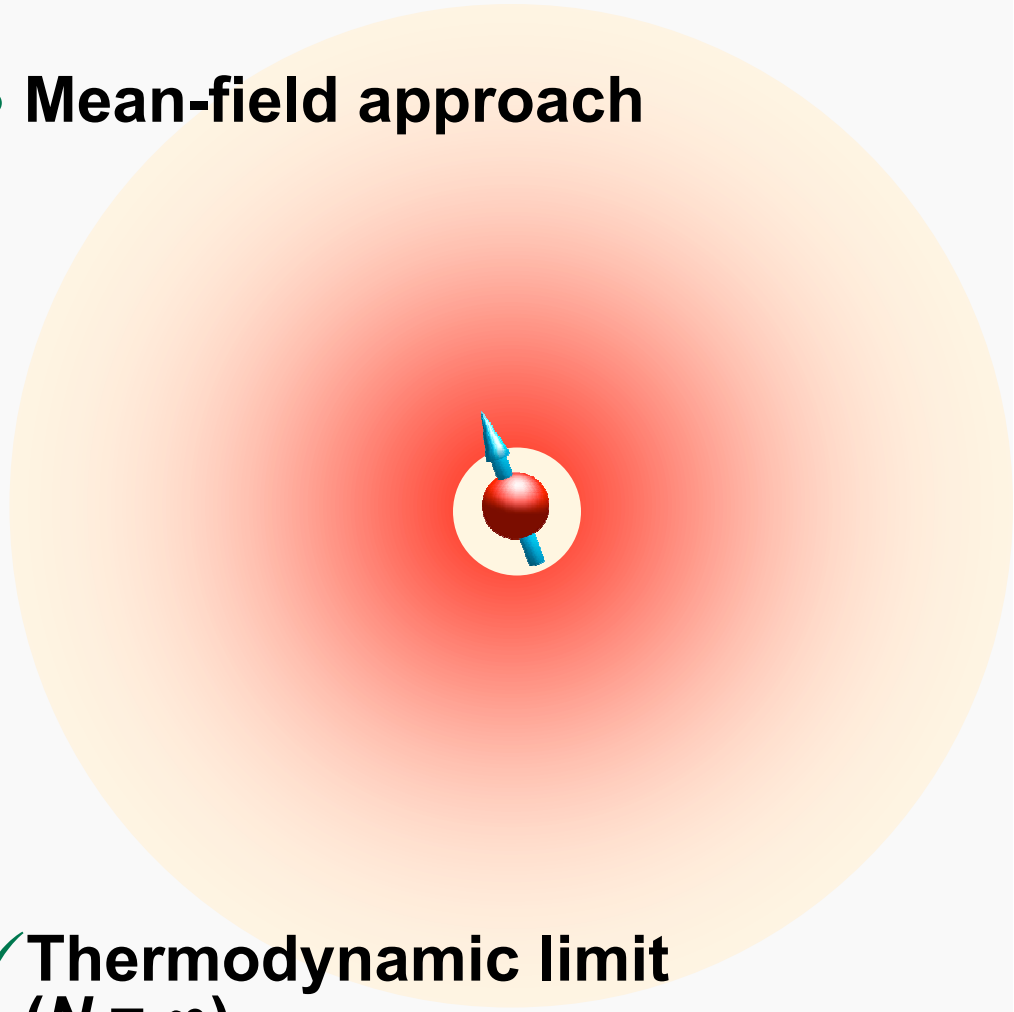
Computational Methods

- **Finite size simulations**



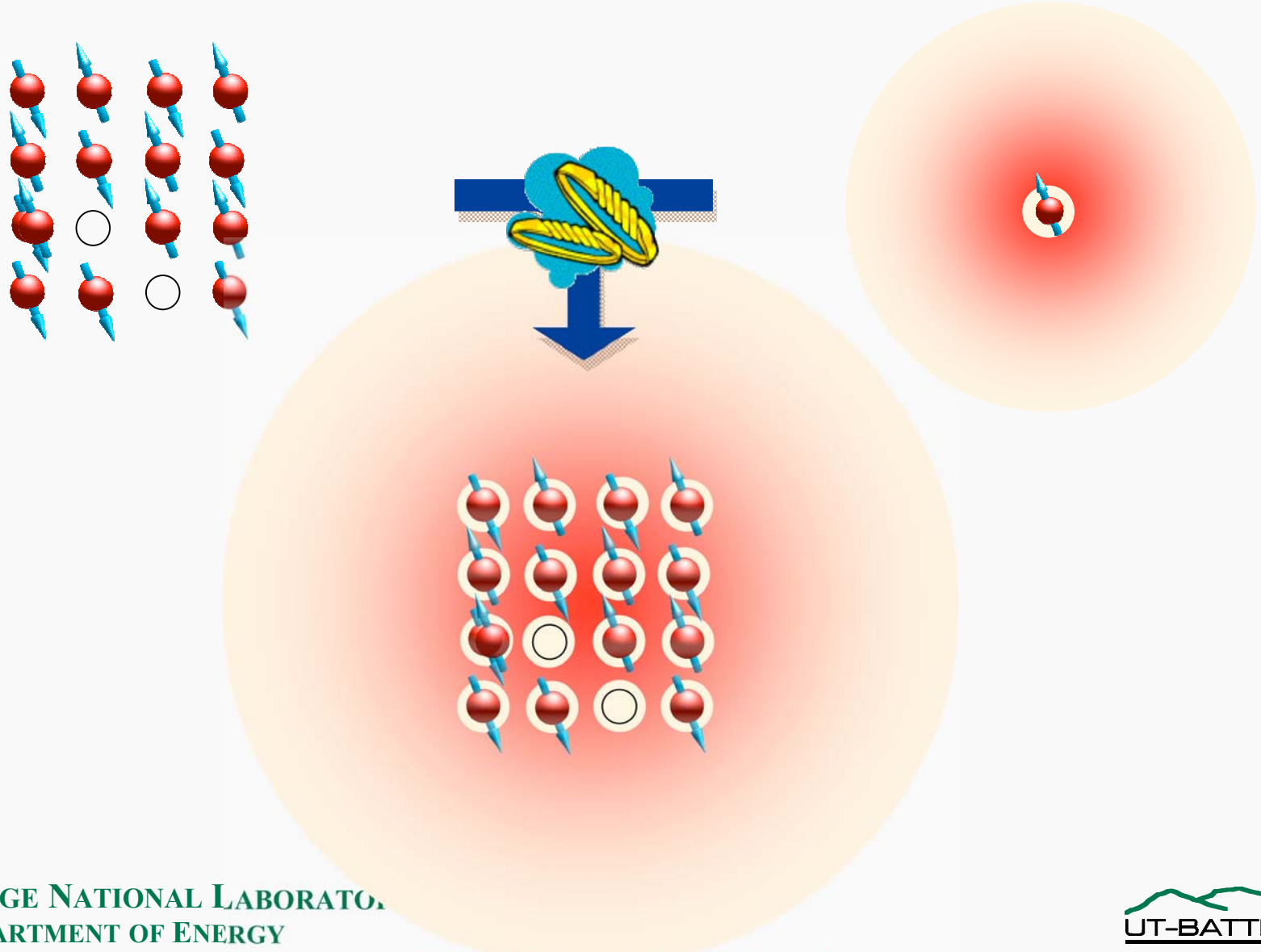
✓ **Exact solution for $N \approx 50$**

- **Mean-field approach**



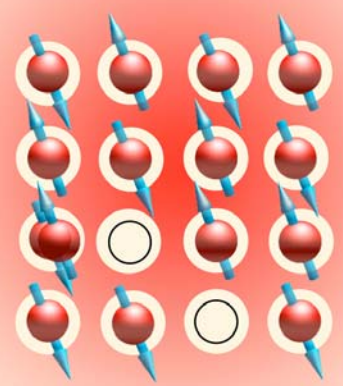
✓ **Thermodynamic limit ($N = \infty$)**

Dynamical Cluster Approximation



Dynamical Cluster Approximation

$$G_0(K,\omega) = \left[\left(\frac{N_c}{N} \sum_{\tilde{k}} \frac{1}{\omega + \mu - \varepsilon_{K+\tilde{k}} - \Sigma_c(K,\omega)} \right)^{-1} + \Sigma_c(K,\omega) \right]^{-1}$$



$$\text{QMC} \rightarrow \Sigma_c[G_0(K,\omega), U]$$

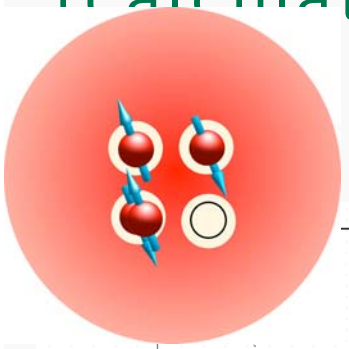
- ✓ **Thermodynamic limit**
- ✓ **Non-local correlations**

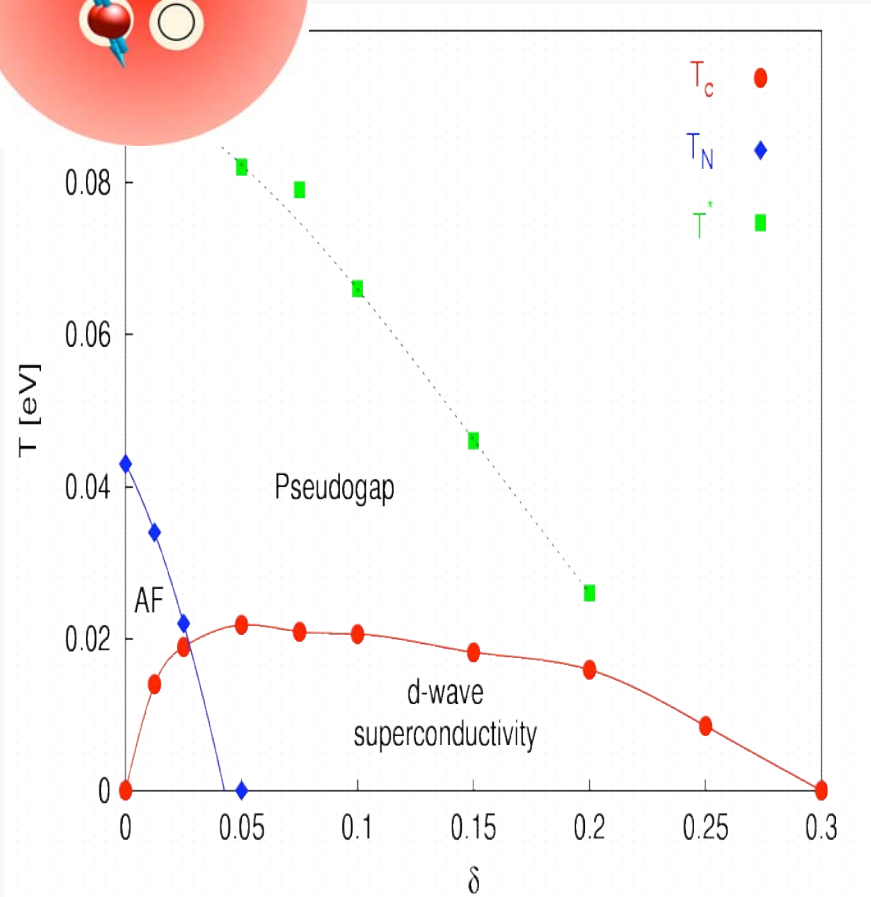
Cluster in reciprocal space

↓

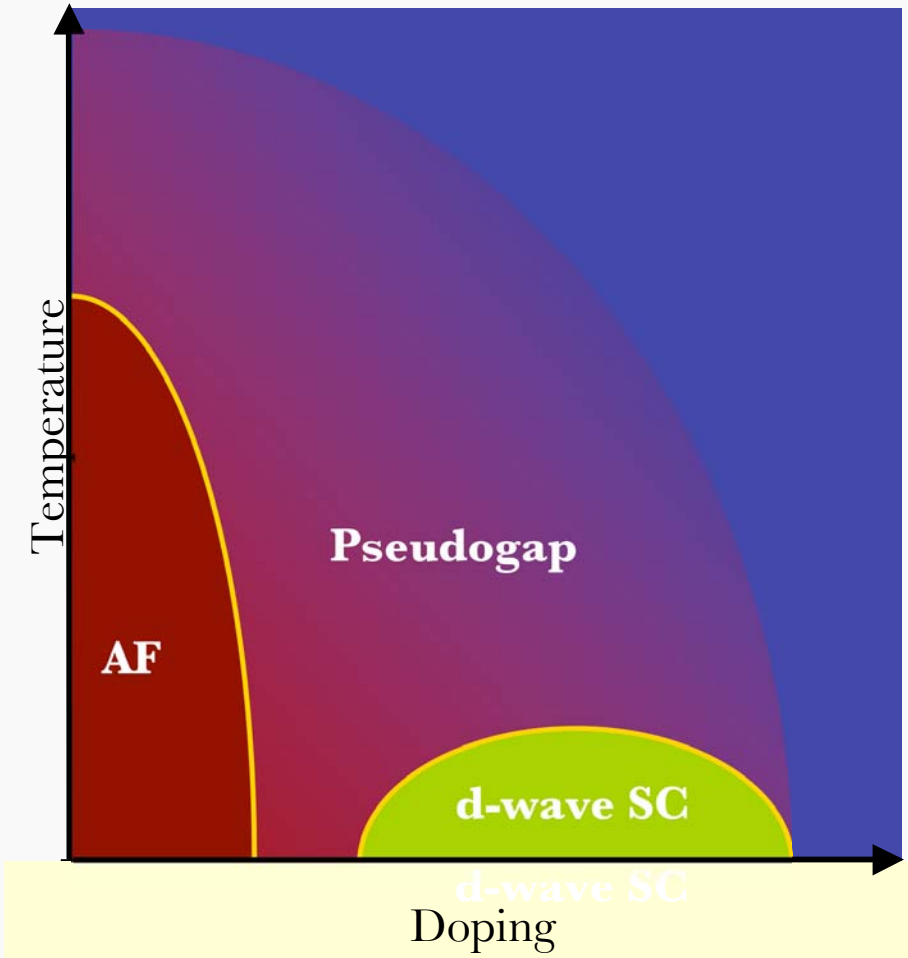
- ✓ **Translational symmetry**

4-site cluster
(calculations feasible on IBM or Compaq)





Generic HTSC Phase diagram



Problem ...

- **N_c=4 results in contradiction with Mermin-Wagner theorem:**
  - ***No finite temperature transition in 2D systems to state with broken continuous symmetry.***
- **Consequences:**
  - **$T_N = 0$**
  - **Superconductivity only possible as Kosterlitz-Thouless topological order**
- **Violation caused by small cluster**
- **Cure: Simulate larger clusters**
  - **Computational cost grows like ~N_c^3**
  - **Efficiency breaks down on IBM & Compaq**

Porting and tuning on Cray X1

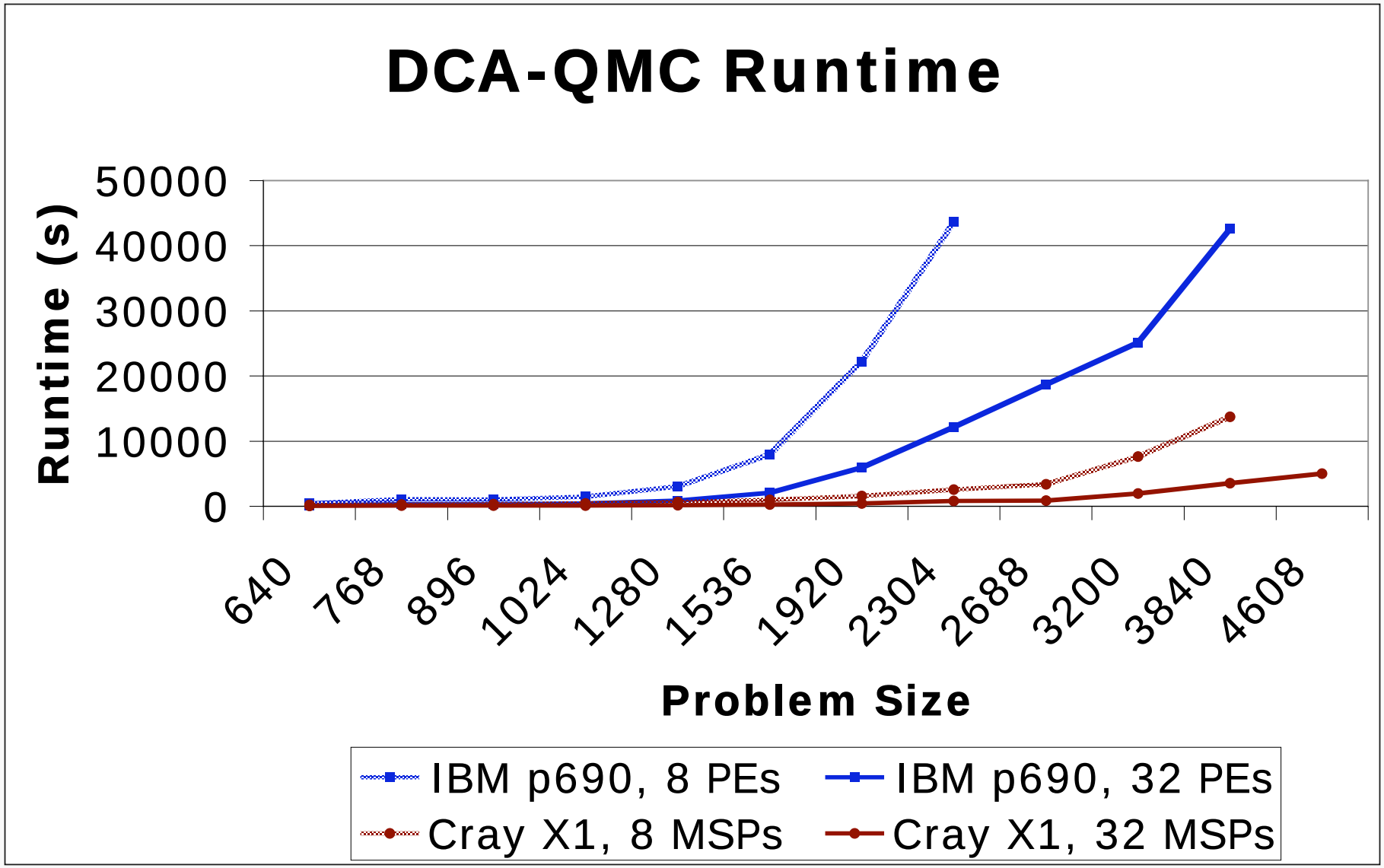
- **Easy port**
  - **Modifications to `Makefile`**
- **Tuning**
  - **Performance profile**
  - **Loopmarks**
  - **Unvectorized nested loops with indirect addressing (all in one file)**
  - **Figure out which loops are independent**
  - **`!dir$ concurrent`**

Performance

- **Quantum Monte Carlo**
  - **Highly parallel, easy to scale, right?**
  - **No, each process has a significant fixed startup**
  - **Favors fewer, faster processors**
- **Dominated by N^3 operations**
  - **CGEMM - level 3 BLAS, easy on memory**
  - **DGER - level 2 BLAS, needs memory bandwidth**
  - **O(1) CGEMMs and O(N) DGERs per step**
  - **DGERs dominate**

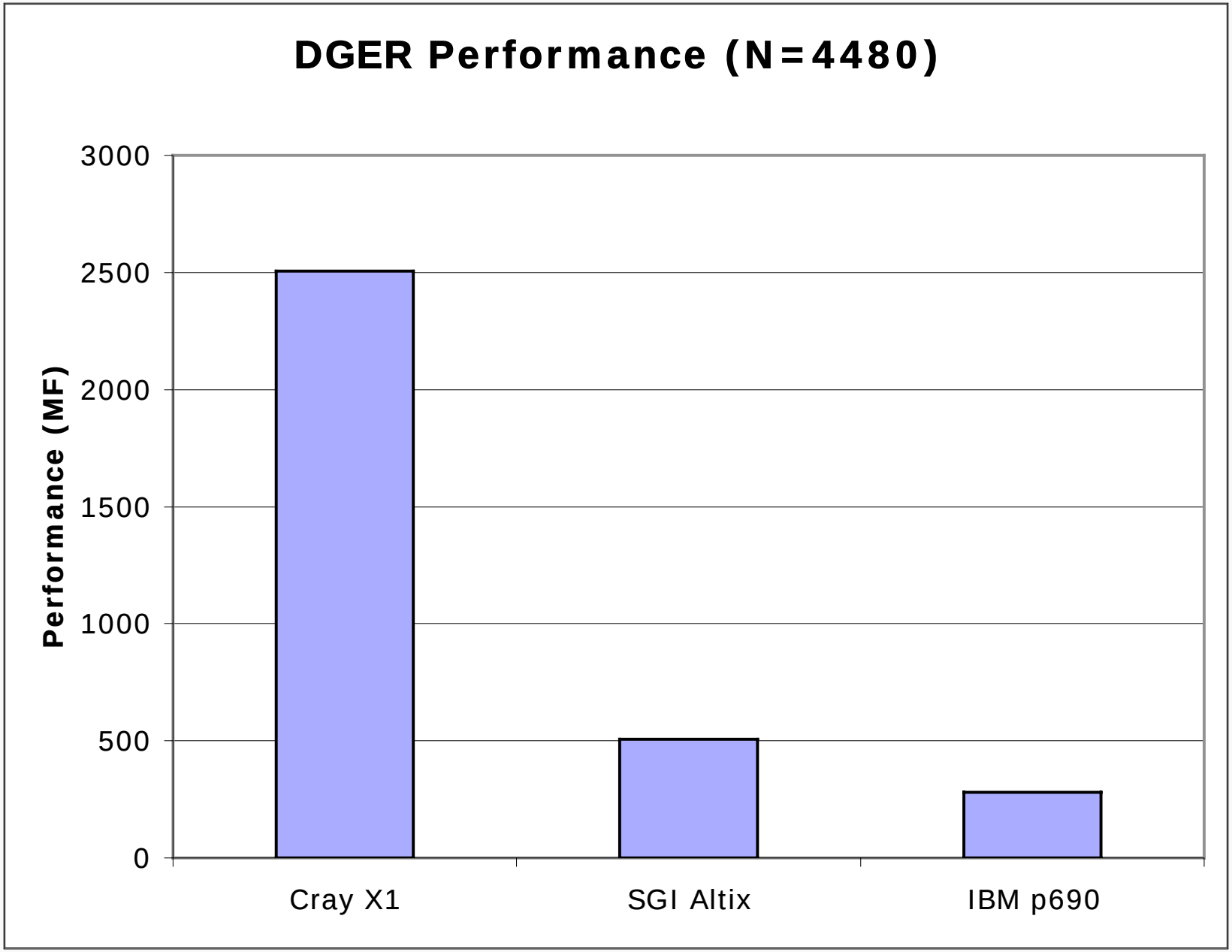
Performance experiment

- **Production simulation**
- **N = cluster size * time slices**
- **Cluster size of 64**
- **Series of runs**
  - **Increasing numbers of time slices (10-70)**
  - **Decreasing numbers of Monte-Carlo samples**
  - **Runs use different parameters but generally get more expensive**
  - **Lines connecting points are for clarity**


DCA-QMC Runtime
Runtime (s)
50000
40000
30000
20000
10000
0
640
768
896
1024
1280
1536
1920
2304
2688
3200
3840
4608
Problem Size
IBM p690, 8 PEs
IBM p690, 32 PEs
Cray X1, 8 MSPs
Cray X1, 32 MSPs

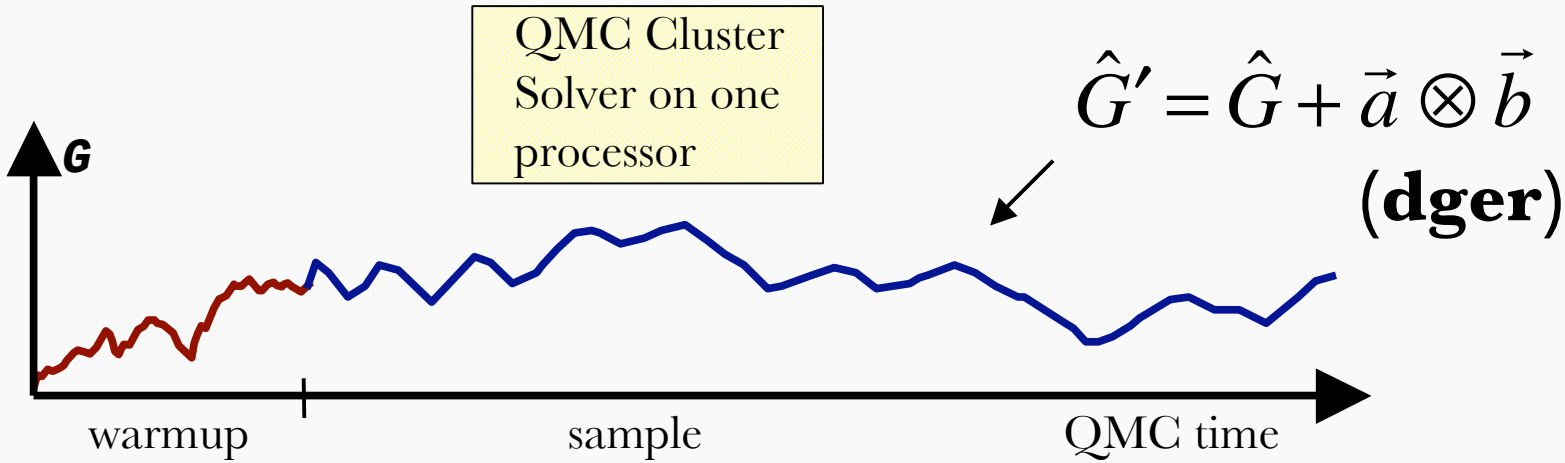
DGER experiment

- **Rank-1 matrix update**
  - **Few floating-point ops per memory op**
  - **Needs memory bandwidth**
- **N = 64 * 70 = 4480**
  - **Real application performs many moderate DGERs, not a few large ones**
  - **Cluster size of 64 with 70 time steps**
  - **Representative of current X1 runs**


DGER Performance (N=4480)
Performance (MF)
3000
2500
2000
1500
1000
500
0
Cray X1
SGI Altix
IBM p690

DCA/QMC Cluster solver

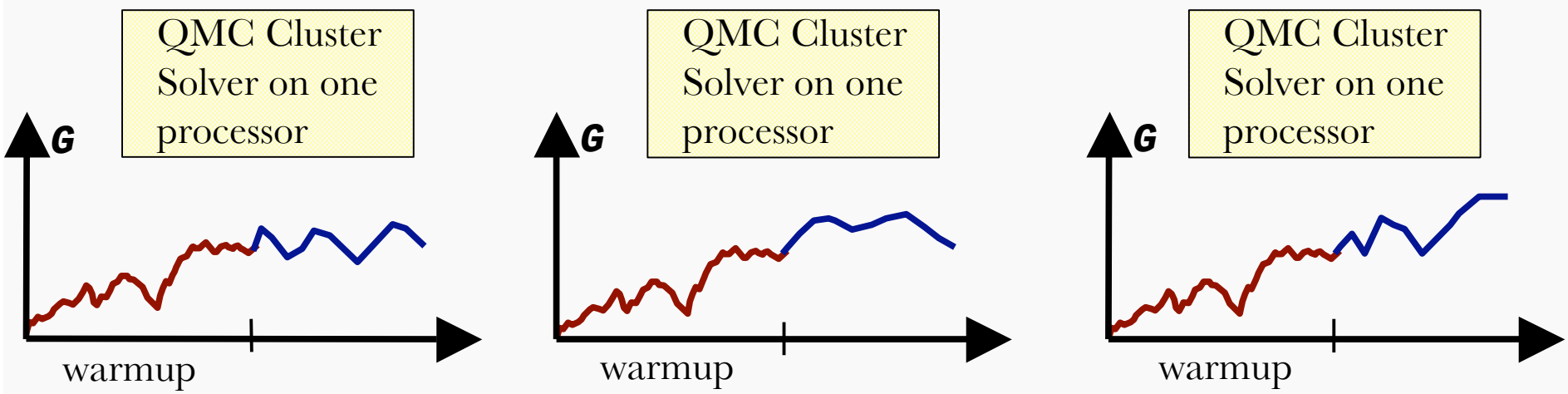
Serial:



$$\hat{G}' = \hat{G} + \vec{a} \otimes \vec{b}$$

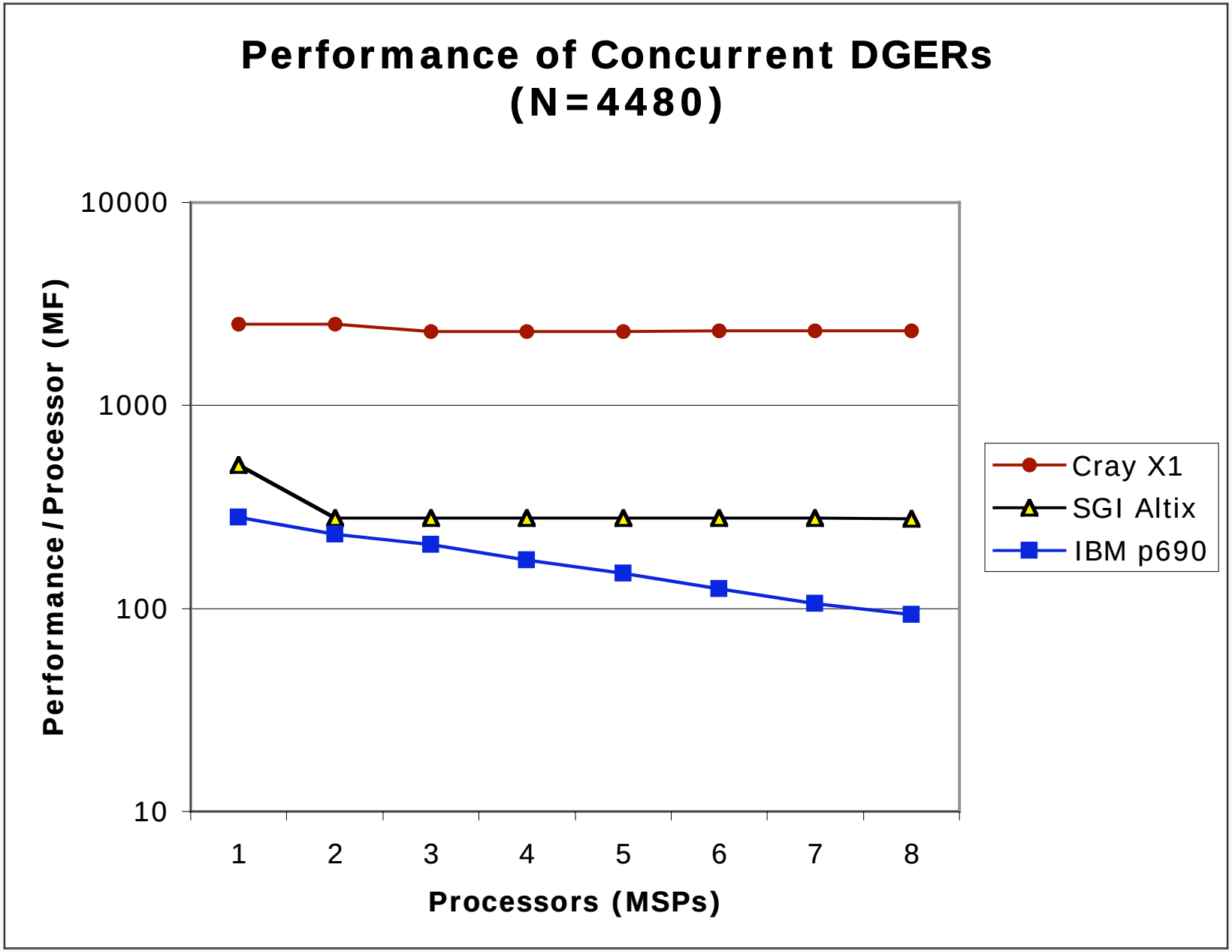
(dger)

Perfectly parallel:



Concurrent-DGERs Experiment

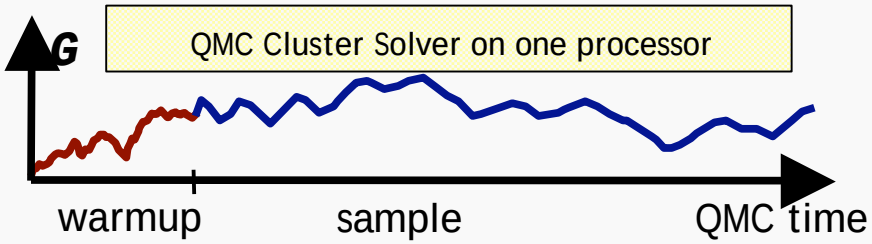
- **Real application loads processors with DGERs**
- **Perform concurrent DGERs, one per processor**
- **Does memory bandwidth scale?**
- **Does performance scale?**


Performance of Concurrent DGERs
(N=4480)
10000
1000
100
10
Performance/Processor (MF)
1
2
3
4
5
6
7
8
Processors (MSPs)
Cray X1
SGI Altix
IBM p690

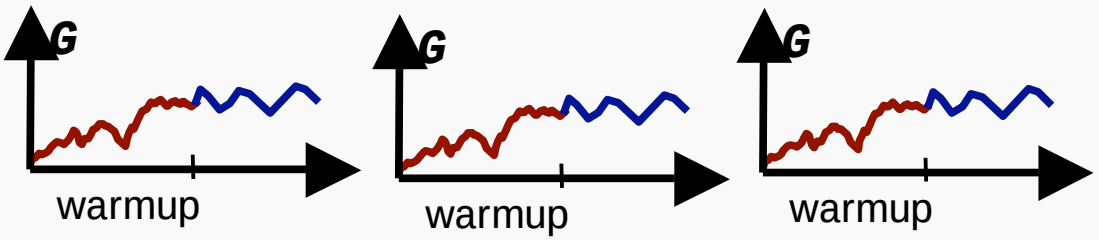
Parallelize (QMC) Cluster Solver

- **Monte Carlo is perfectly parallel**
- **But: warmup time does not scale**
- **Better to have fewer fast processors**

Serial:



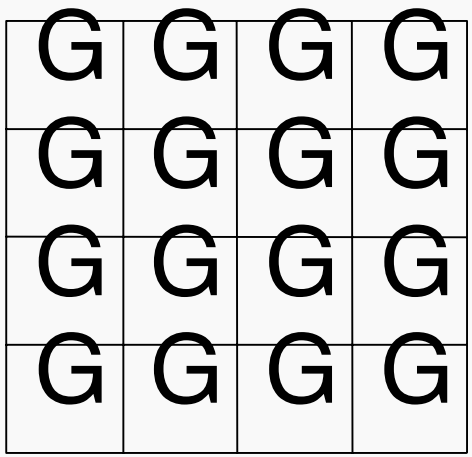
Perfectly parallel:



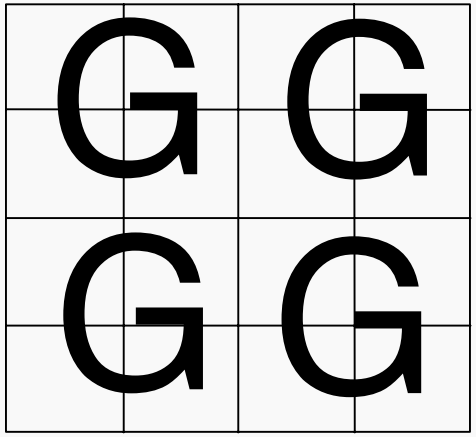
- **Runs on Cray X1 for present project:**
  - **Warmup on 256 CPUs is only a few percent of measurement time**
  - **We expect near perfect scaling for up to 1024 CPUs**
- **Alternatively: hybrid parallelization**
  - **Run one QMC cluster solver on one multiple CPUs**

Parallelize cluster solver (cont.)

Perfectly parallel array of cpu's



Hybrid parallel array of cpu's



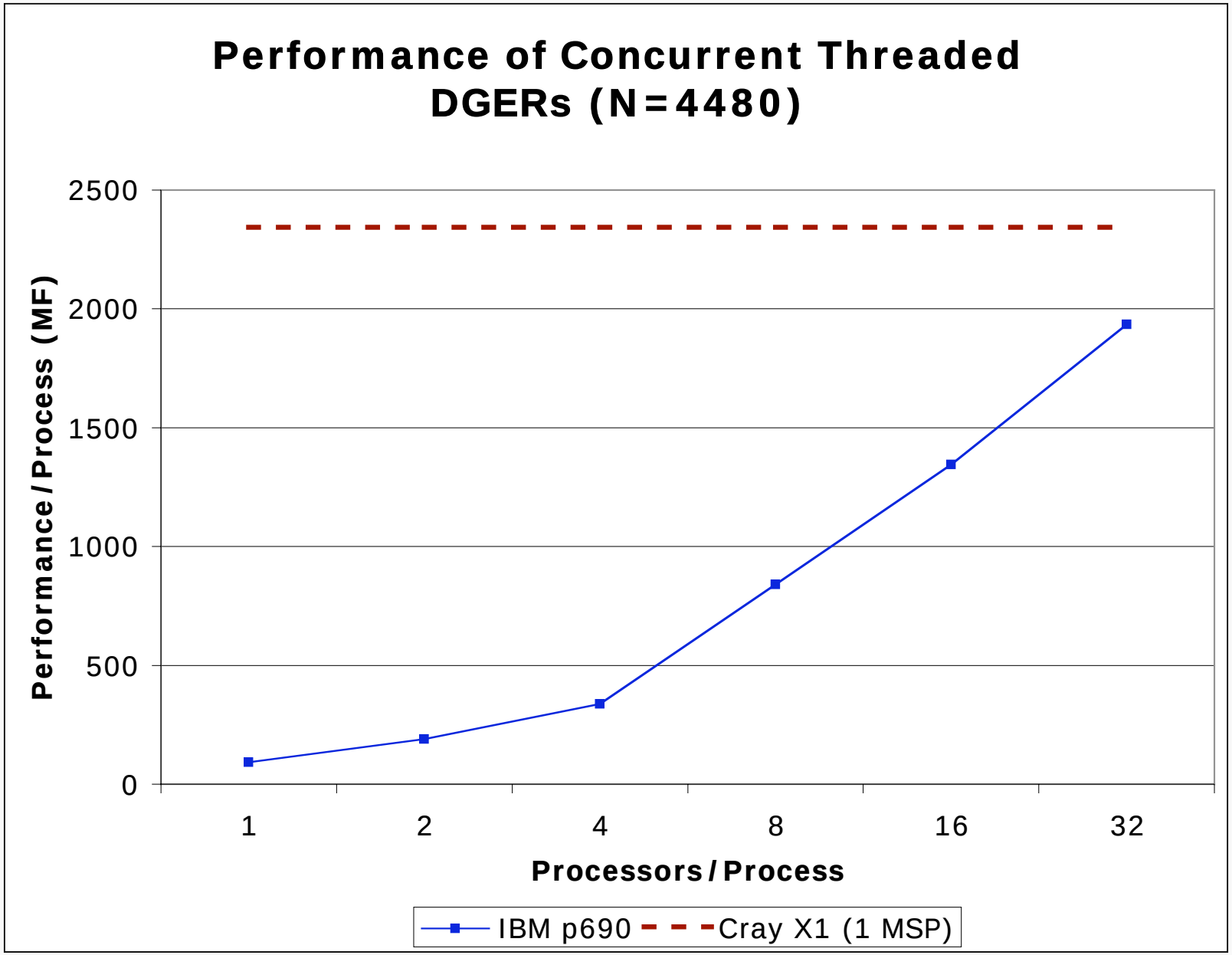
OpenMP

PBLAS

- **Hybrid parallelization implemented (needed on Compaq and IBM)**
- **Scalability depends on implementation of DGER and CGEMM**
  - **We anticipate that code should scale well for up to 8K processors on Black Widow (2K simulations at 4 CPUs)**
  - **Could scale even better with threaded DGER**

Threaded-DGER Experiment

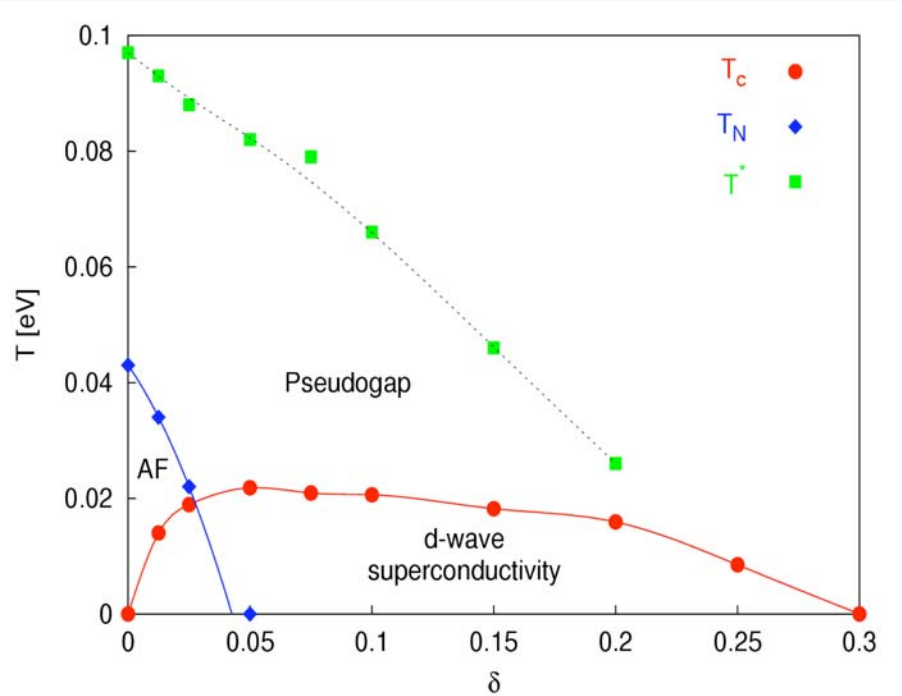
- **Developers could parallelize each Monte-Carlo process with OpenMP**
  - **Use SMPs to improve scaling**
- **Test possibilities using threaded DGER**
  - **Provided with IBM p690**
  - **Not yet available for SGI Altix, Cray X1**
- **Load 32-processor node with DGERs**
  - **Try different mixes of processes and threads**
  - **How fast can N=4480 DGER be?**


Performance of Concurrent Threaded DGERs (N=4480)
Performance/Process (MF)
2500
2000
1500
1000
500
0
1
2
4
8
16
32
Processors/Process
IBM p690
Cray X1 (1 MSP)

Runs with Nc=4 (on IBM Power 4)

- **Phase diagram of single-band 2D Hubbard model**
  - **In qualitatively agreement with experiment**
  - **Model captures physics of high T_c superconductors**
- **Mermin-Wagner Theorem**
  - **No phase transition at T>0K in less than 3D**
  - **Violated because N_c finite**
  - **Need N_c >>4 runs to verify**
- **Superconductivity due to coupling between planes or multi band?**

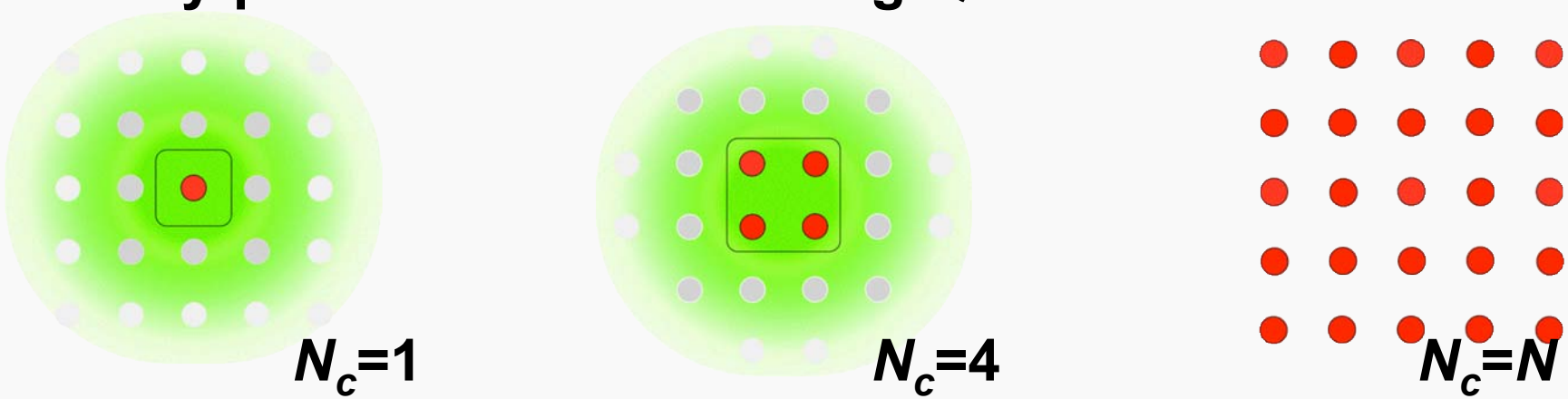
T. Maier & M. Jarrell



Dynamical Cluster Approximation (DCA)

- **The challenges:**
  - **Superconductivity is a macroscopic quantum effect (deal with N~10^{23} electrons)**
  - **Strong non-local quantum correlations**

- **Solution: DCA algorithm (Jarrell, et. al.)**
  - **Embed cluster into effective (mean field) medium**
  - **Many-problem in cluster using Quantum Monte Carlo**

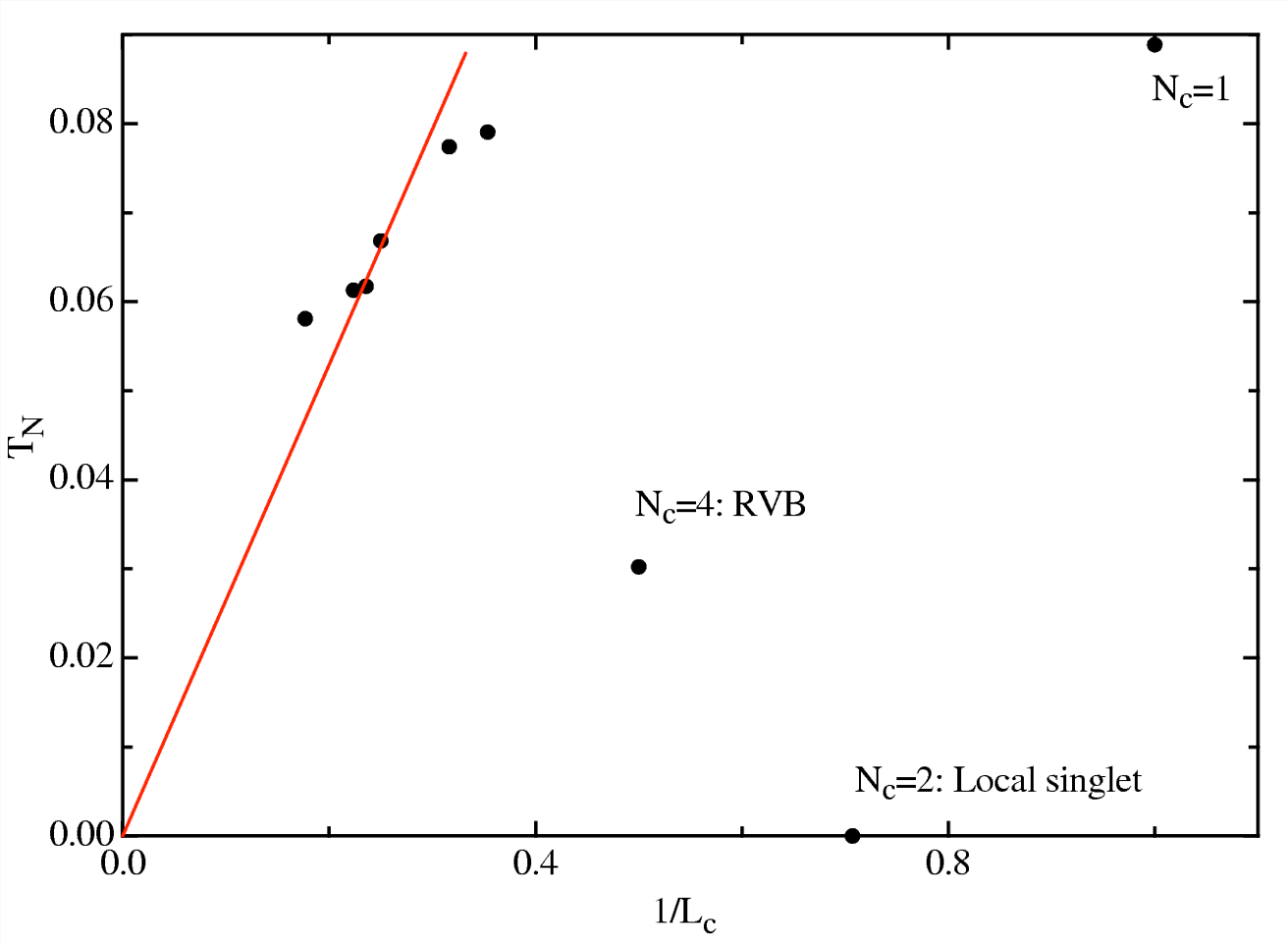


  - **Systematically recover exact solution as N_c=N**

Scalability = Capability

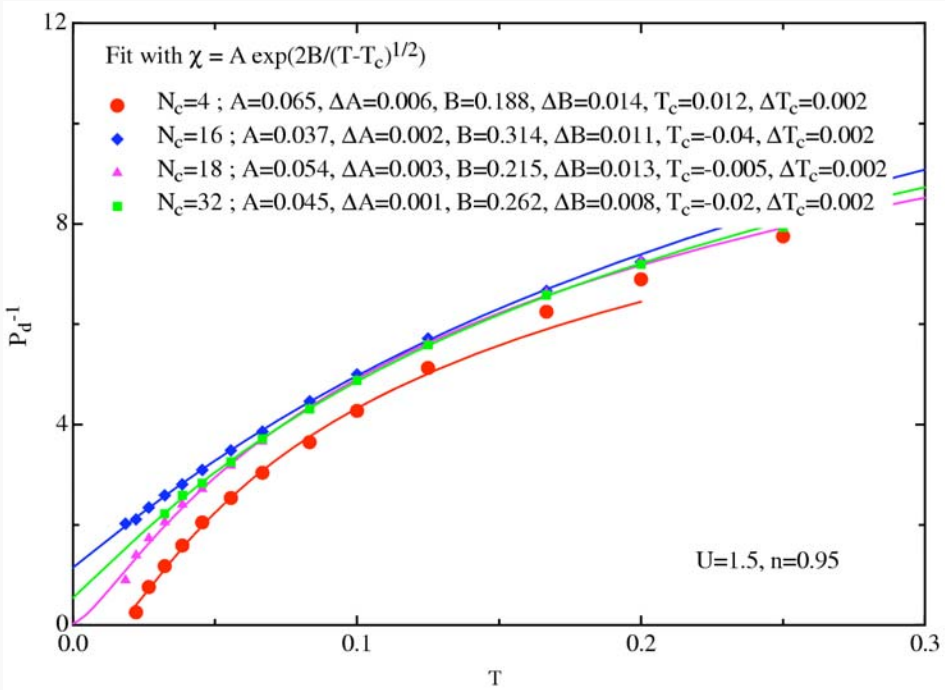
- **Cray X1 enables larger clusters (32-64)**
  - **Powerful processors**
  - **scalable memory bandwidth**
- **Provides capability**
  - **To check compliance with Mermin-Wagner theorem**
  - **To study possible Kosterlitz-Thouless transition to phase with superconducting topological order**

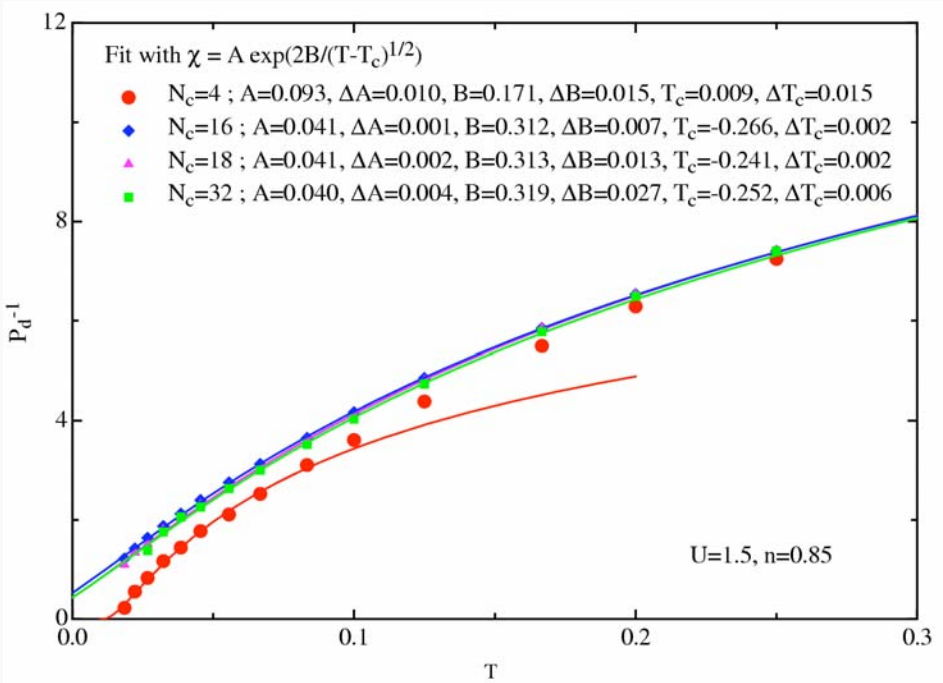
Larger clusters - Antiferromagnetism



✓ **Mermin-Wagner theorem recovered**

Larger clusters - Superconductivity



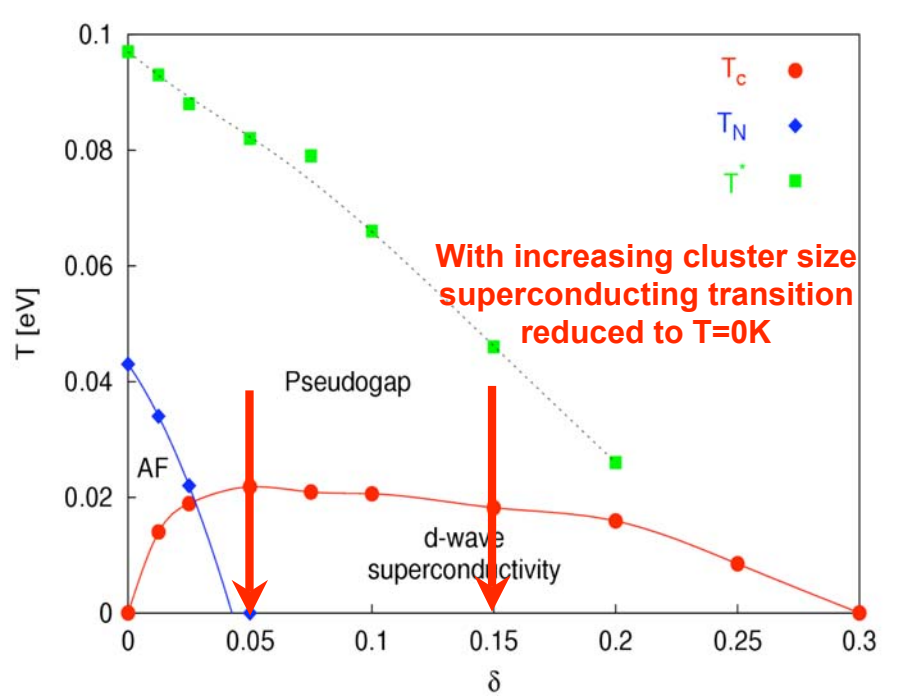


- **Superconductivity suppressed at larger clusters**
- **No Kosterlitz-Thouless transition**

Runs on Cray X1, N_c up to 64

- **Cray X1 allows us to run cluster sizes of up to 64 atoms**
- **Large enough to show that superconducting transition in 2D Hubbard model is suppressed at finite temperature**
- **Long standing problem solved: single band *2-D Hubbard model alone does not explain high T_c superconductors*.**
- **More than 10 years after Zhang & Rice, we are in a position to get to the bottom of the problem**

T. Maier, J. White, et. al.



Conclusions: Scalability = Capability

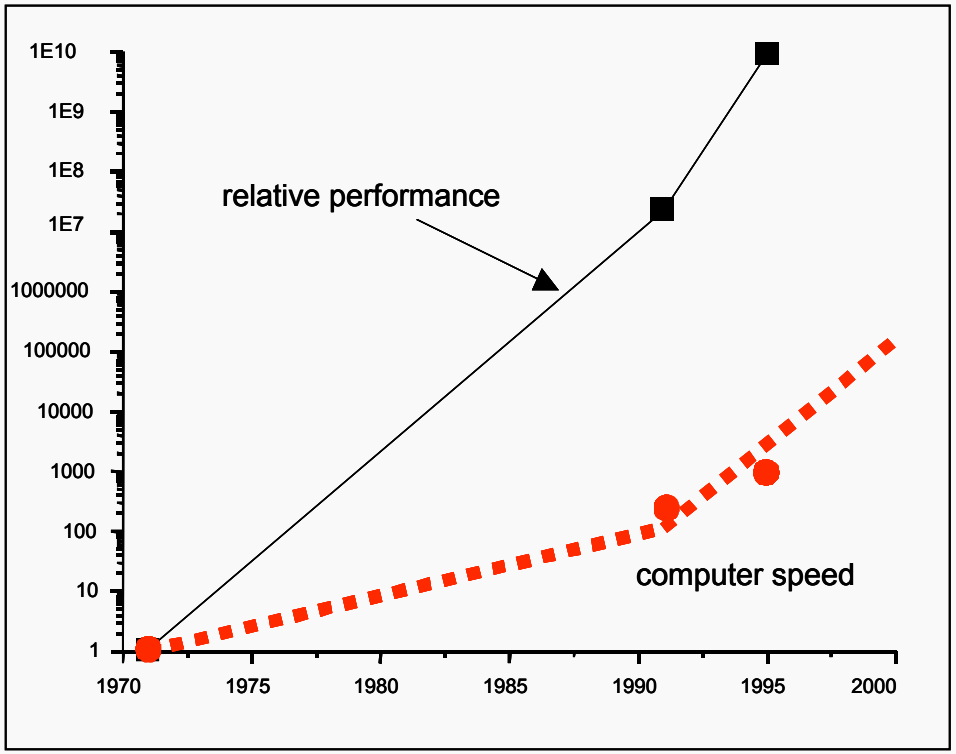
- **Previous runs used small clusters (2-4)**
  - **Violate fundamental theorem**
- **Cray X1 enables larger clusters (32-64)**
  - **Powerful processors, scalable memory bandwidth**
  - **Predicted physics has been restored**
- **Plans for full 3-D model (multi-band, coupled planes …)**
  - **Should validate or refute full theory**
- **Larger machines may enable prediction of new materials**

Peta-scale computing problems in materials science

- **QMC/DCA for strongly correlated electron systems**
  - **QMC: fewer faster processors**
  - **With threaded DGER: should scale to 30-60K processors on Cray Black Widow**
- **LSMS/W.-L. hybrid for magnetic free energy surfaces in nano particles**
  - **LSMS: limited by ZGEMM (BLAS-3), known to scale perfectly to ~10K processors**
  - **Hybrid with Wang-Landau sampling: should scale to many 100K processors**

The reality of "big-science" on big computers

(D. P. Landau, UGA)



- **The goal is the science and the computer is a tool**
- **Very high payoff from improvement in algorithms / methods**
- **Most algorithmic / methodological improvements happen in "small shops"**
- **Need a scalable architecture (!)**

Acknowledgements

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