ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

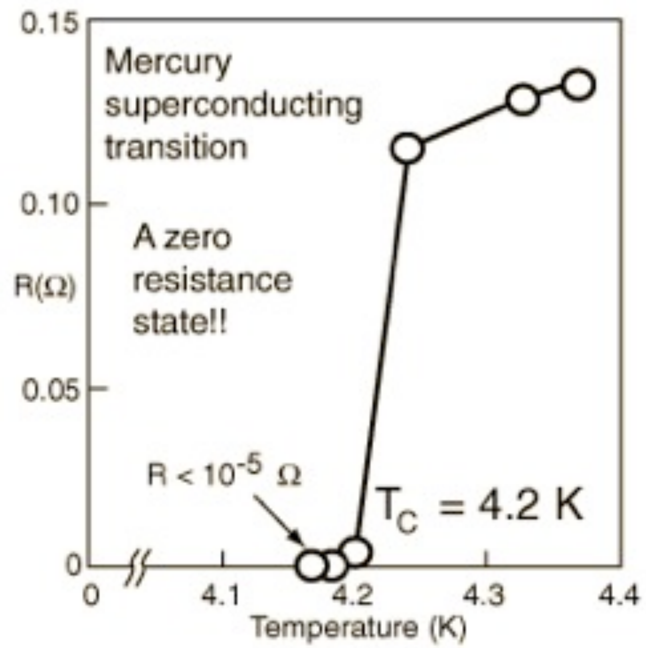
CSCS
Swiss National Supercomputing Centre

Extreme scale simulations of high-temperature superconductivity

Thomas C. Schulthess

Superconductivity: a state of matter with zero electrical resistivity

Heike Kamerlingh Onnes (1853-1926) Discovery 1911



Microscopic Theory 1957

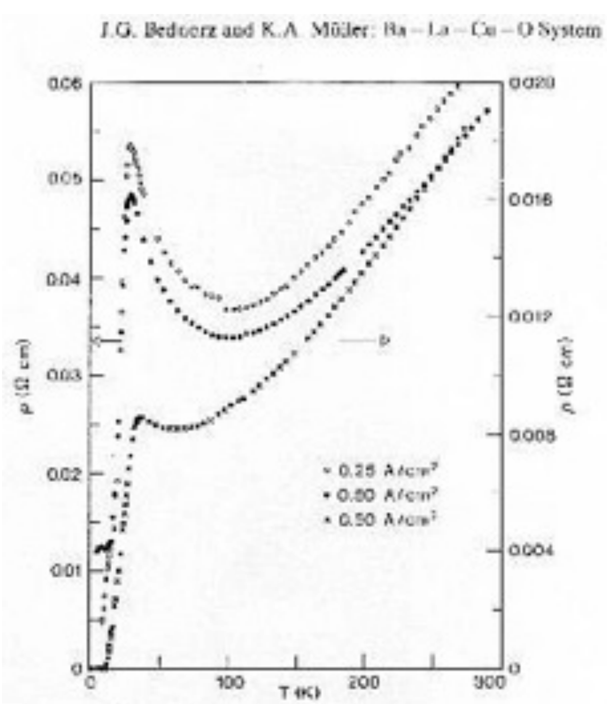
PHYSICAL REVIEW VOLUME 108, NUMBER 5 DECEMBER 1, 1957

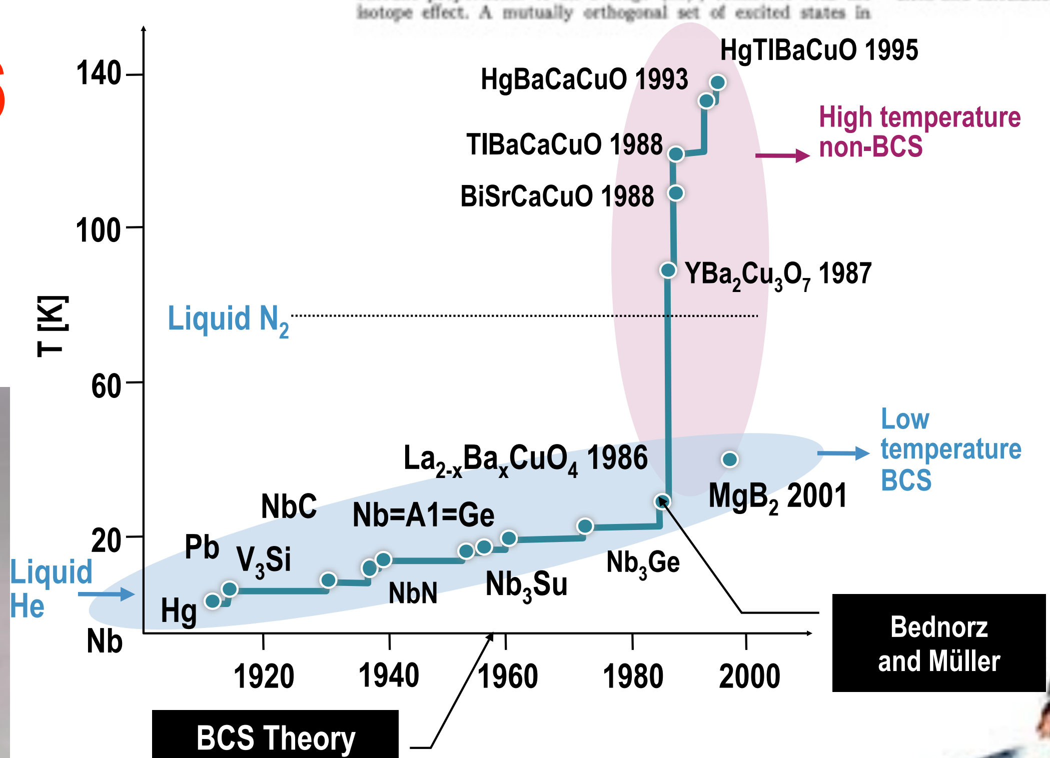
Theory of Superconductivity*

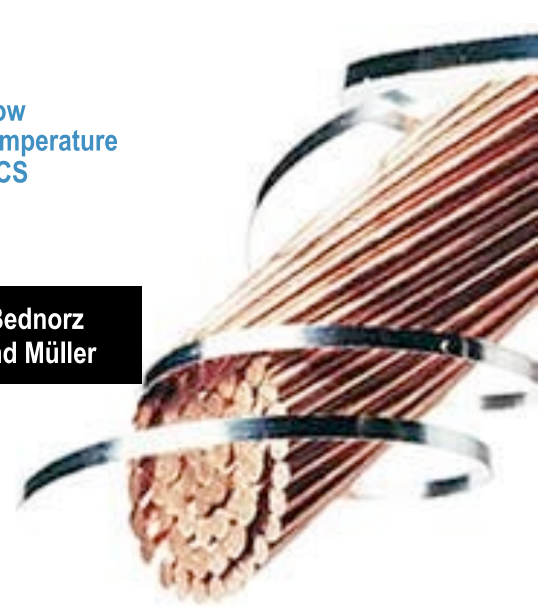
J. Bardeen, L. N. Cooper,† and J. R. Schrieffer‡
Department of Physics, University of Illinois, Urbana, Illinois
(Received July 8, 1957)

A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy, $\hbar\omega$. It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by amount proportional to an average $(\hbar\omega)^2$, consistent with the isotope effect. A mutually orthogonal set of excited states in one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about $3.5kT_c$ at $T=0°K$ to zero at T_c. Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.

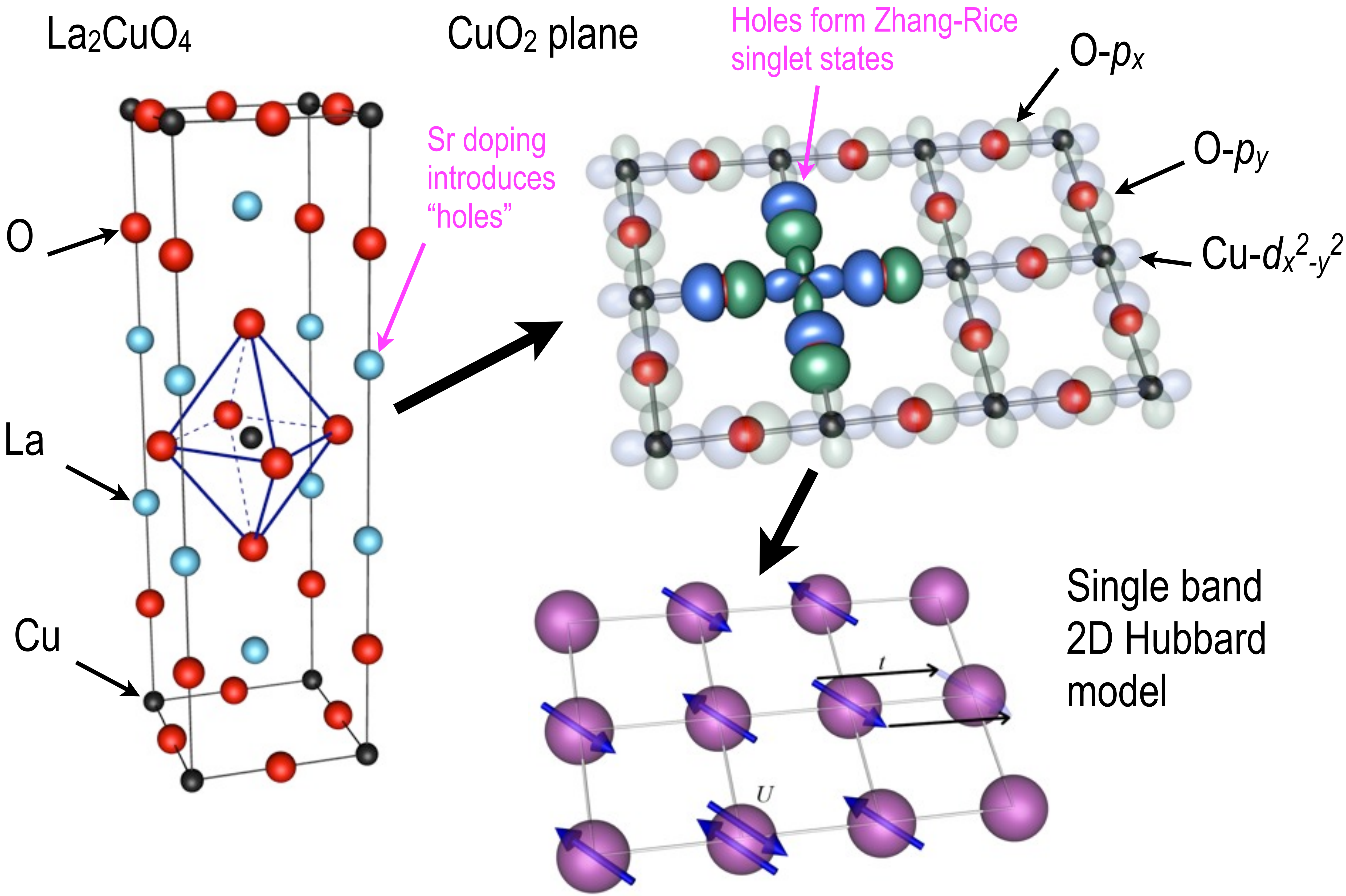
Superconductivity in the cuprates 1986



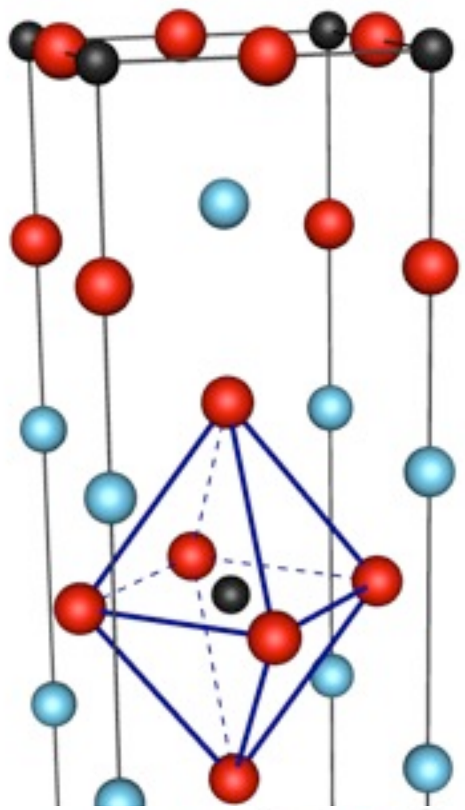


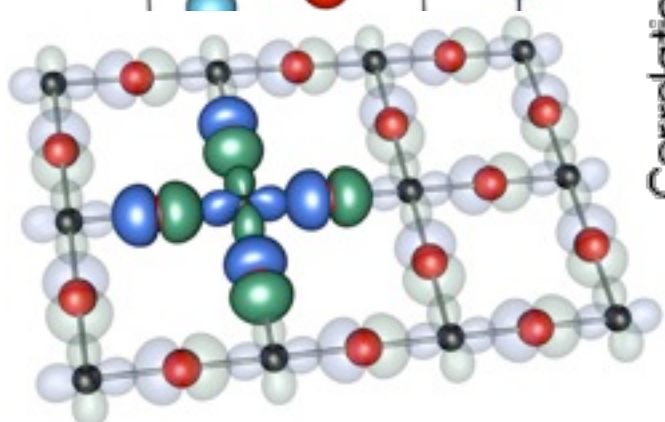


From cuprate materials to the Hubbard model



The challenge: a (quantum) multi-scale problem

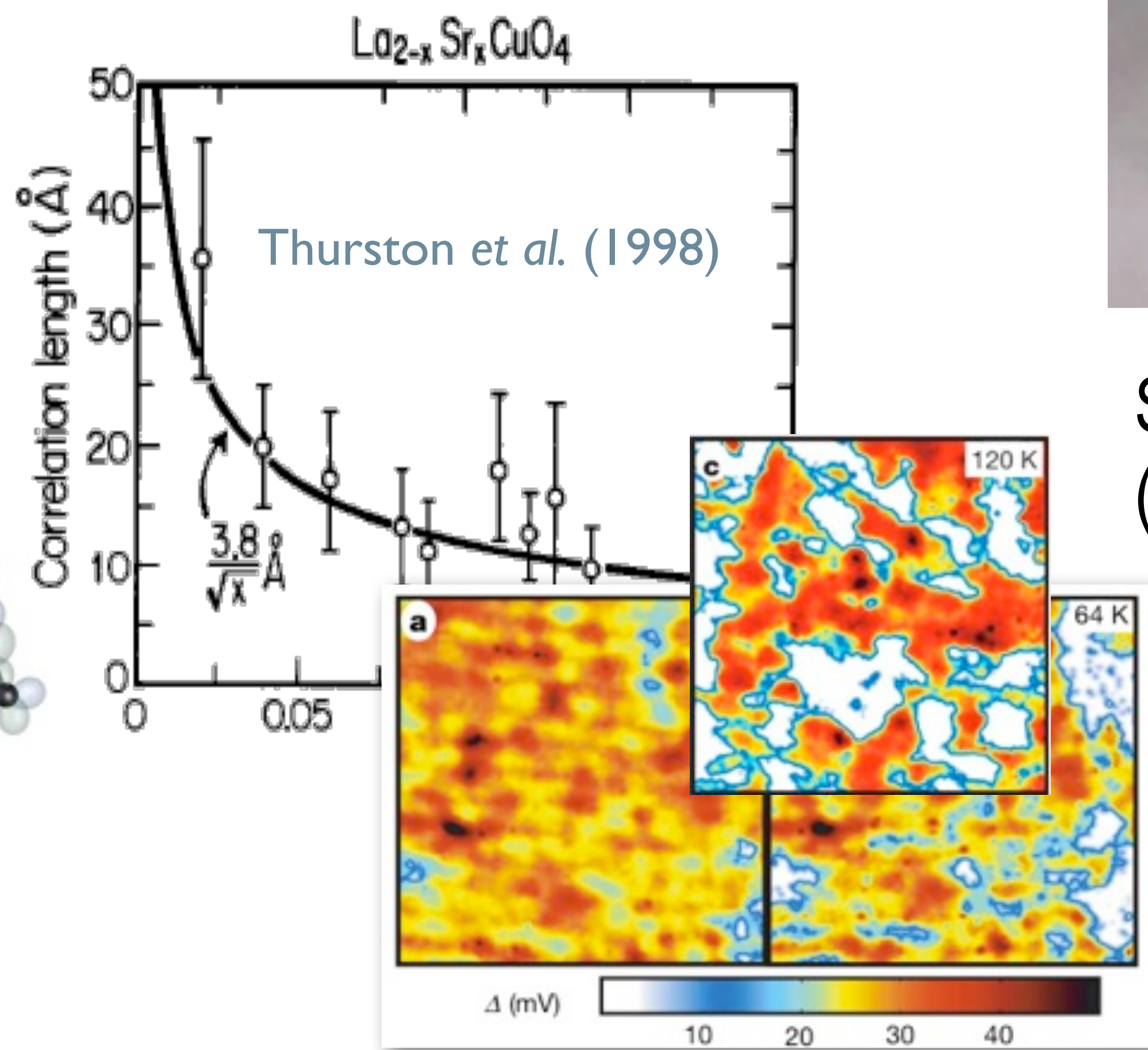




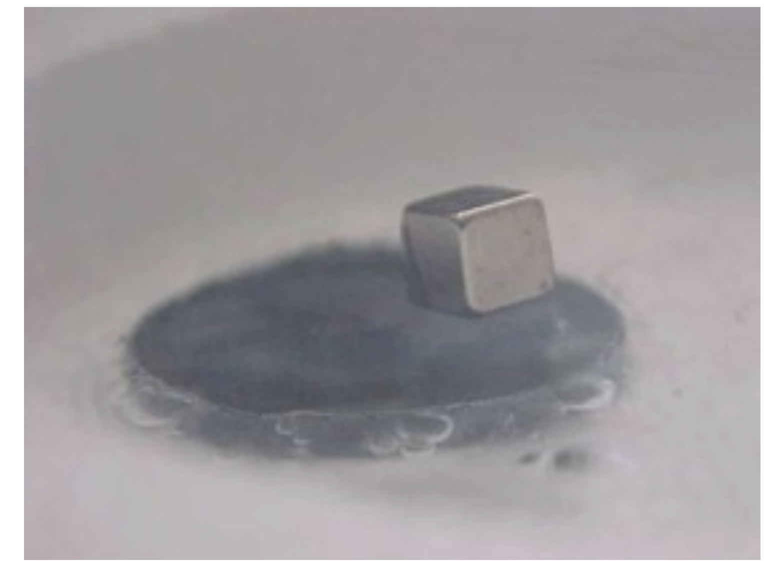
On-site Coulomb repulsion (~A)

complexity ~ 4^N

Antiferromagnetic correlations / nano-scale gap fluctuations



Gomes et al. (2007)

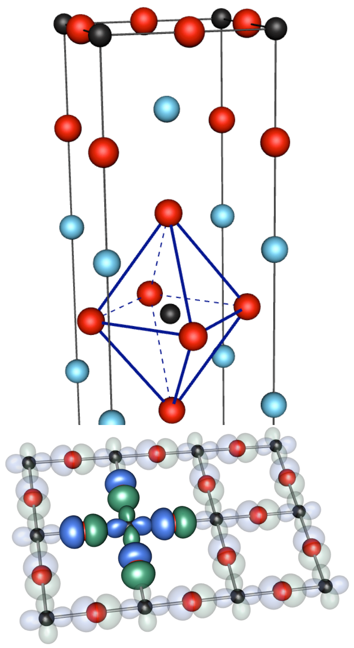


Superconductivity (macroscopic)

$N \sim 10^{23}$

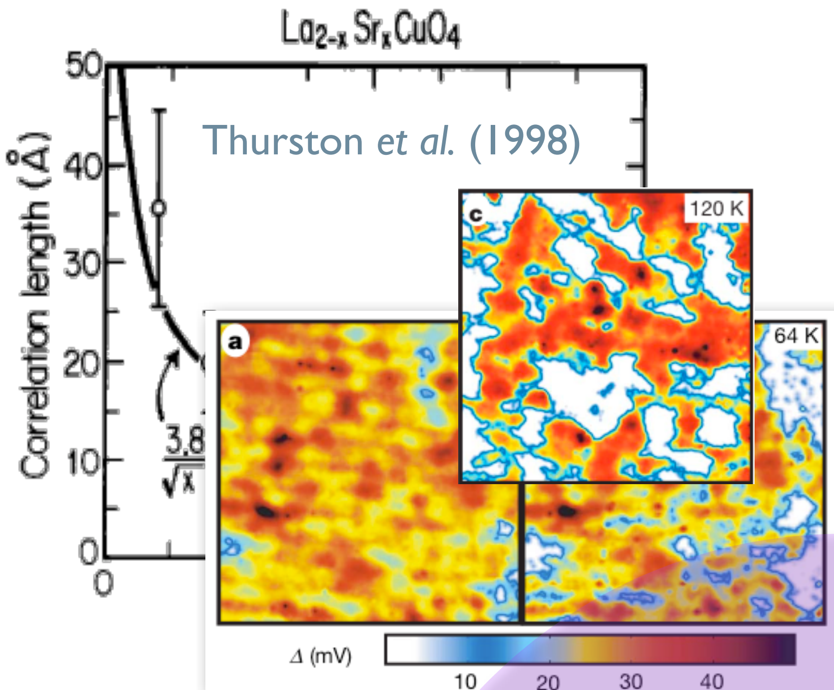
Quantum cluster theories

Maier *et al.*, Rev. Mod. Phys. ’05

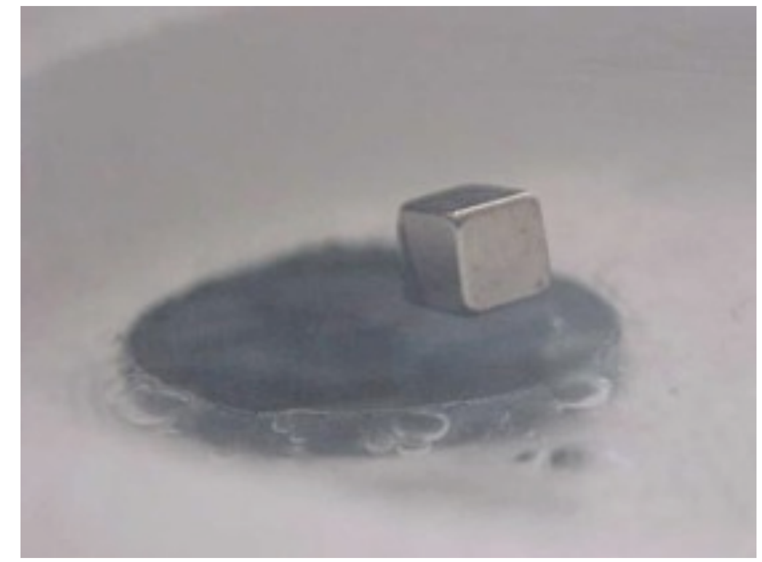


On-site Coulomb repulsion (~A)

Antiferromagnetic correlations / nano-scale gap fluctuations

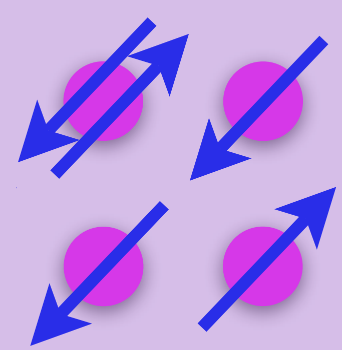


Gomes et al. (2007)



Superconductivity (macroscopic)

Explicitly treat correlations within a localized cluster

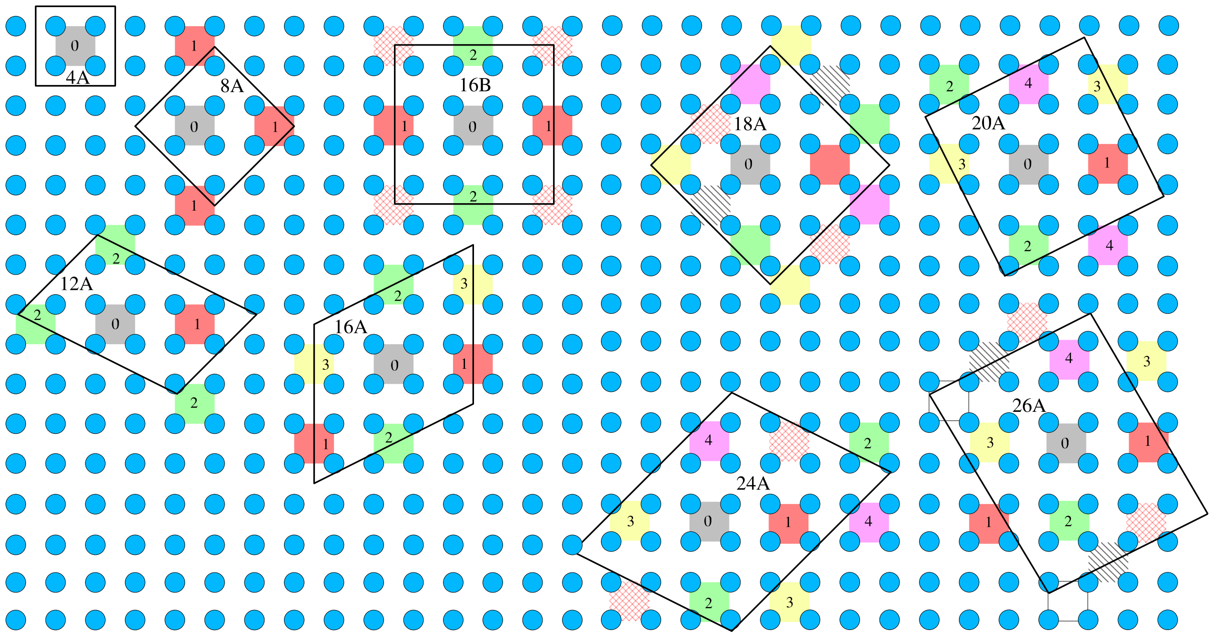


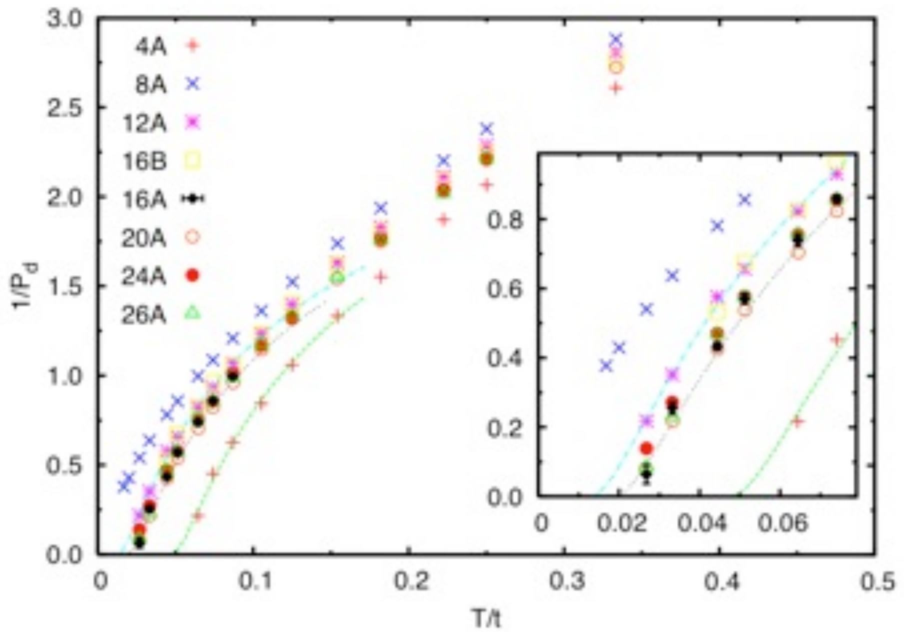
Treat macroscopic scales within mean-field

Coherently embed cluster into effective medium

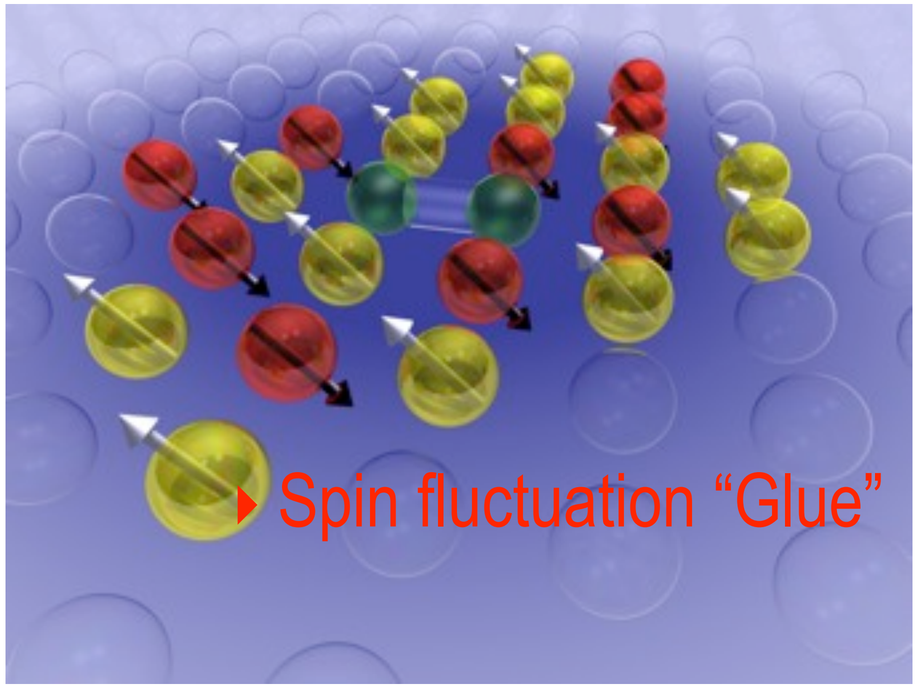
Systematic solution and analysis of the pairing mechanism in the 2D Hubbard Model

- First systematic solution demonstrates existence of a superconducting transition in 2D Hubbard model   Maier,et al., Phys. Rev. Lett. **95**, 237001 (2005)





- Study the mechanism responsible for pairing in the model
  - Analyze the particle-particle vertex
  - Pairing is mediated by spin fluctuations
    Maier, et al., Phys. Rev. Lett. **96** 47005 (2006)

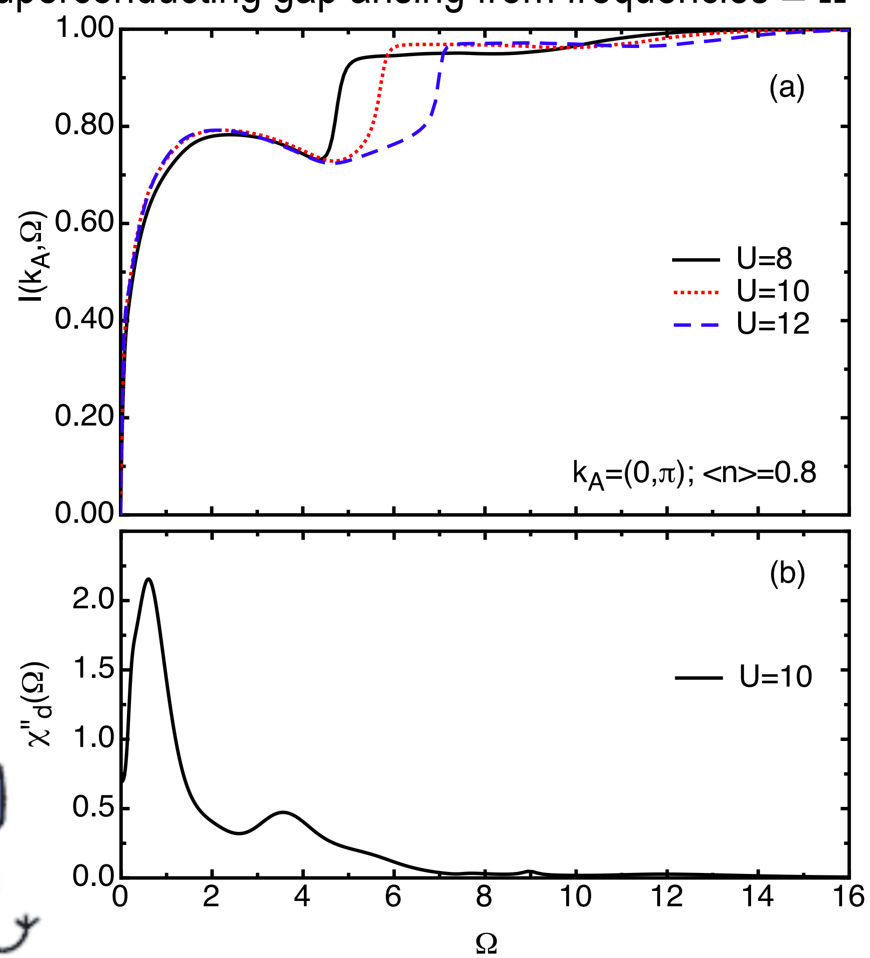


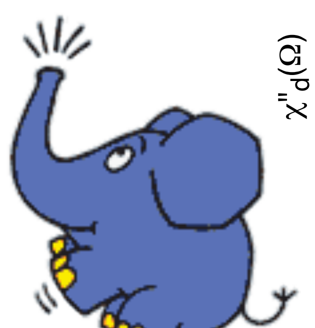
Moving toward a resolution of the debate over the pairing mechanism in the 2D Hubbard model

- "We have a mammoth (U) and an elephant (J) in our refrigerator - do we care much if there is also a mouse?"
  - P.W. Anderson, Science **316**, 1705 (2007)
  - see also www.sciencemag.org/cgi/eletters/316/5832/1705 "Scalapino is not a glue sniffer"

- Relative importance of resonant valence bond and spin-fluctuation mechanisms
  - Maier et al., Phys. Rev. Lett. **100** 237001 (2008)

Fraction of superconducting gap arising from frequencies ≤ Ω

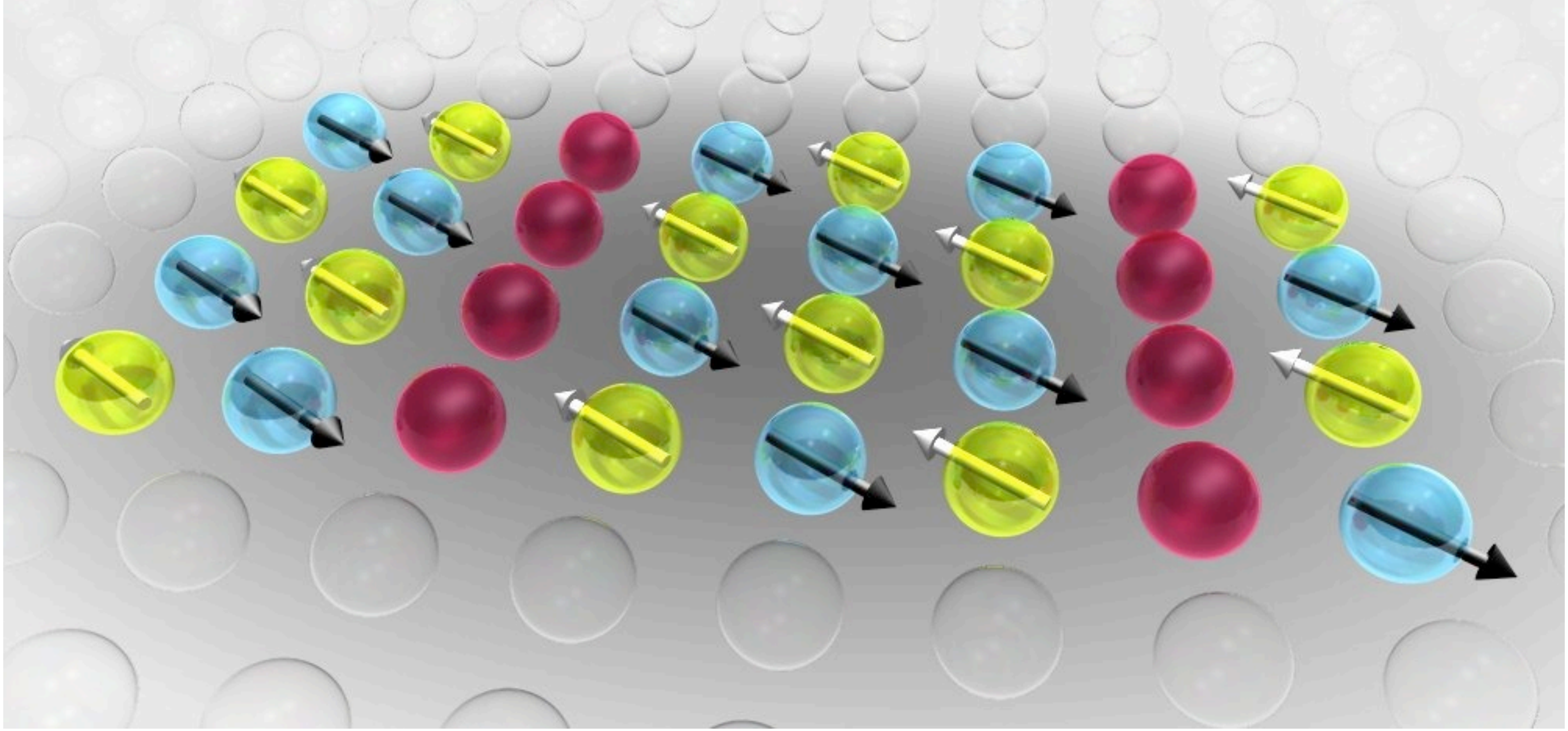




Both retarded spin-fluctuations and non-retarded exchange interaction J contribute to the pairing interaction

Dominant contribution comes from spin-fluctuations!

Significant increase of supercomputing transition temperature due to nanoscale stripe modulations



Maier, Alvarez, Summers and Schulthess Phys. Rev. Lett. in press (2010)

Hirsch-Fye Quantum Monte Carole (HF-QMC) for the quantum cluster solver

Hirsch & Fye, Phys. Rev. Lett. **56**, 2521 (1988)

Partition function & Metropolis Monte Carlo $Z = \int e^{-E[\mathbf{x}]/k_{\mathrm{B}}T} d\mathbf{x}$

Acceptance criterion for M-MC move: $\min\{1, e^{E[\mathbf{x}_k]-E[\mathbf{x}_{k+1}]}\}$

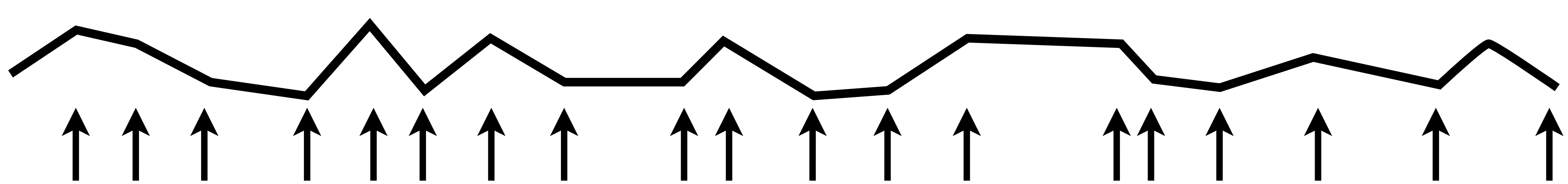
Partition function & HF-QMC: $Z \sim \sum_{s_i,l} \det[\mathbf{G}_c(s_i,l)^{-1}]$

N_c $N_l \approx 10^2$

matrix of dimensions $N_t \times N_t$

$N_t = N_c \times N_l \approx 2000$

Acceptance: $\min\{1, \det[\mathbf{G}_c(\{s_i,l\}_k)]/\det[\mathbf{G}_c(\{s_i,l\}_{k+1})]\}$

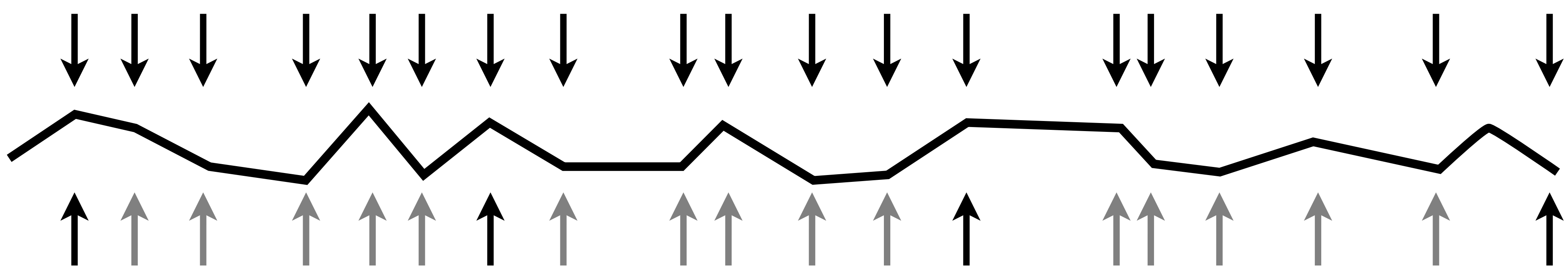


Update of accepted Green's function:

$$\mathbf{G}_c(\{s_i,l\}_{k+1}) = \mathbf{G}_c(\{s_i,l\}_k) + \mathbf{a}_k \times \mathbf{b}_k$$

HF-QMC with Delayed updates (or Ed updates)

$$\mathbf{G}_c(\{s_i,l\}_{k+1}) = \mathbf{G}_c(\{s_i,l\}_k) + \mathbf{a}_k \times \mathbf{b}_k^t$$

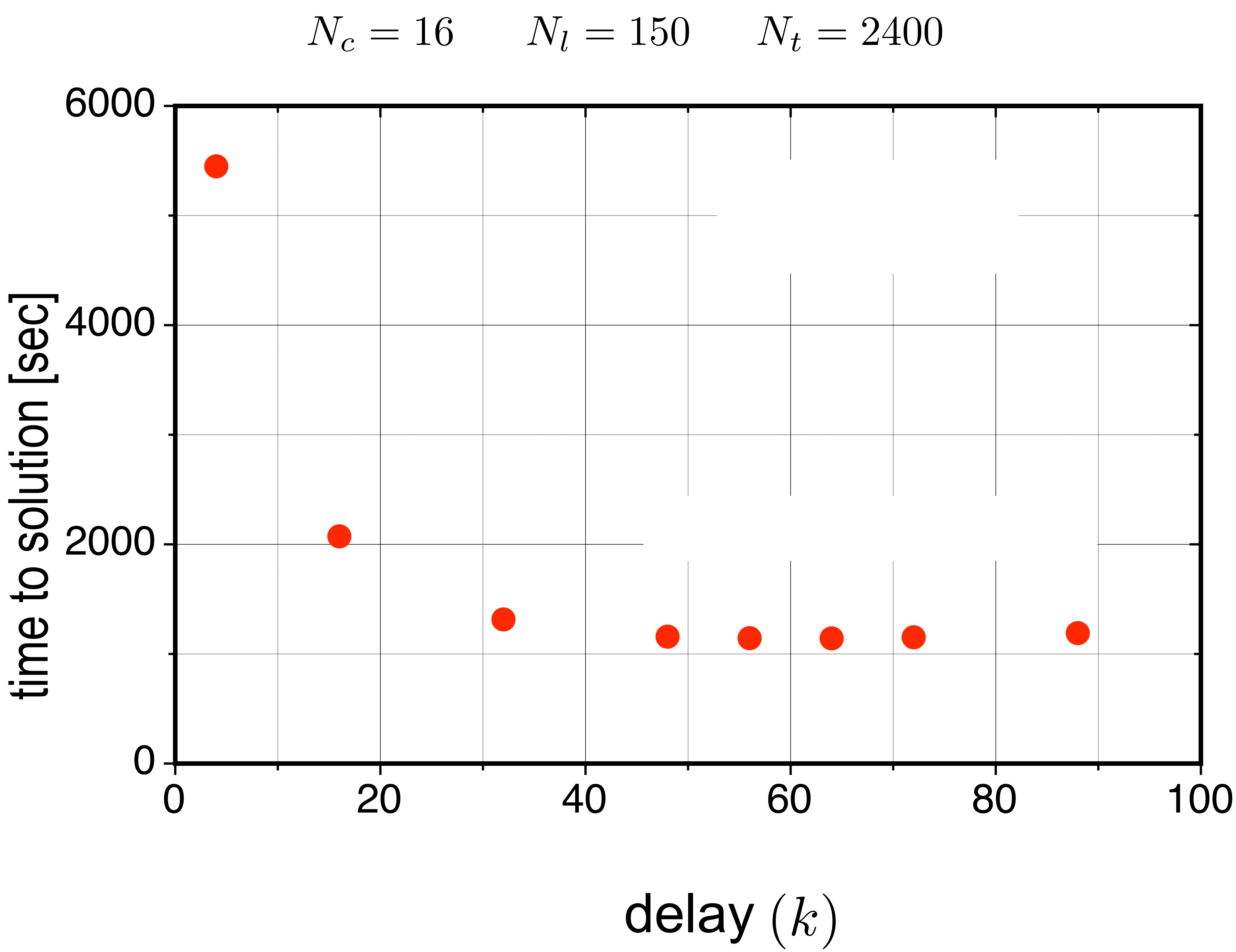


$$\mathbf{G}_c(\{s_i,l\}_{k+1}) = \mathbf{G}_c(\{s_i,l\}_0) + [\mathbf{a}_0|\mathbf{a}_1|...|\mathbf{a}_k] \times [\mathbf{b}_0|\mathbf{b}_1|...|\mathbf{b}_k]^t$$

Complexity for *k* updates remains $\mathcal{O}(kN_t^2)$

But we can replace *k* rank-1 updates with one matrix-matrix multiply plus some additional bookkeeping.

Performance improvement with delayed updates

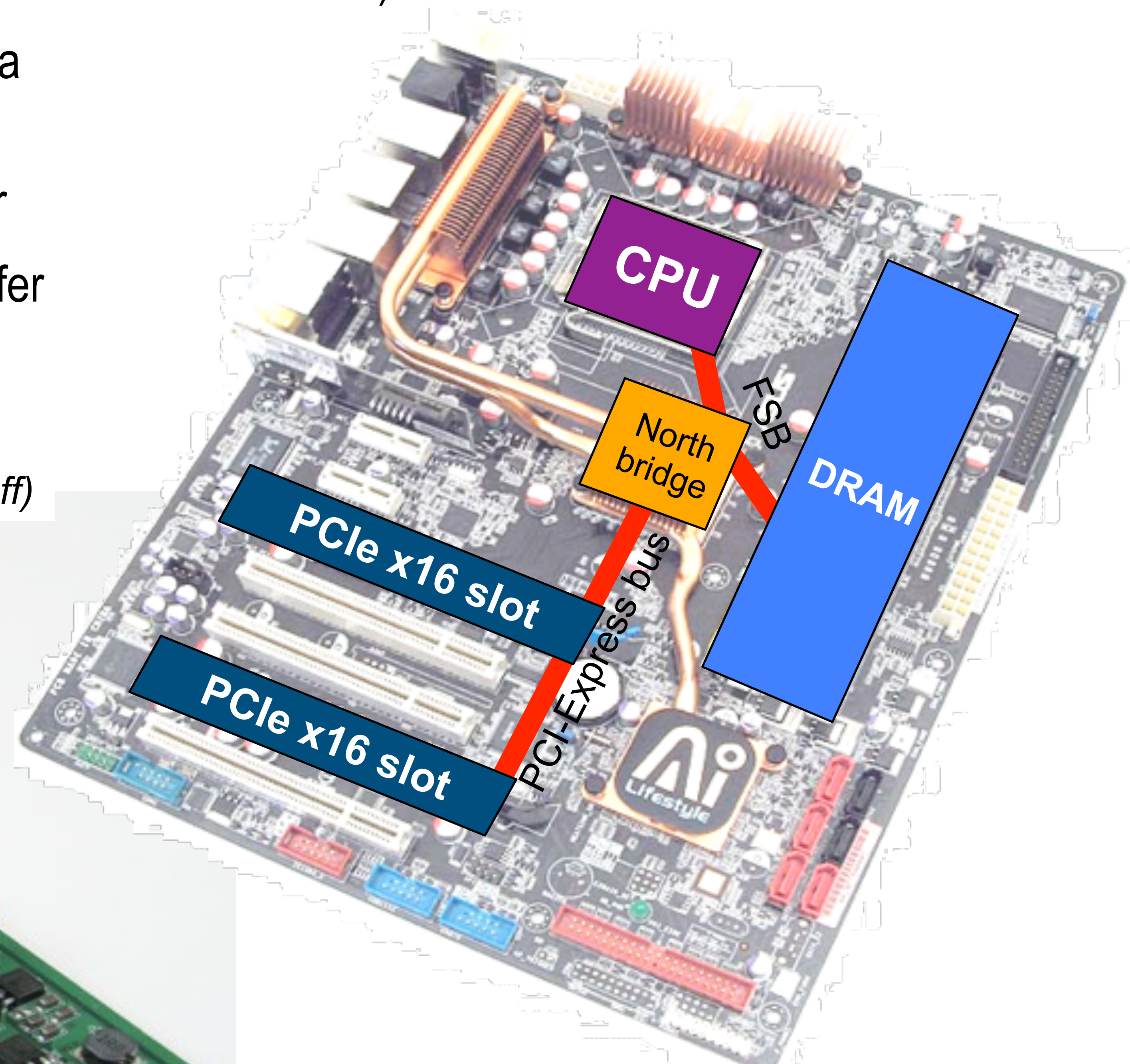


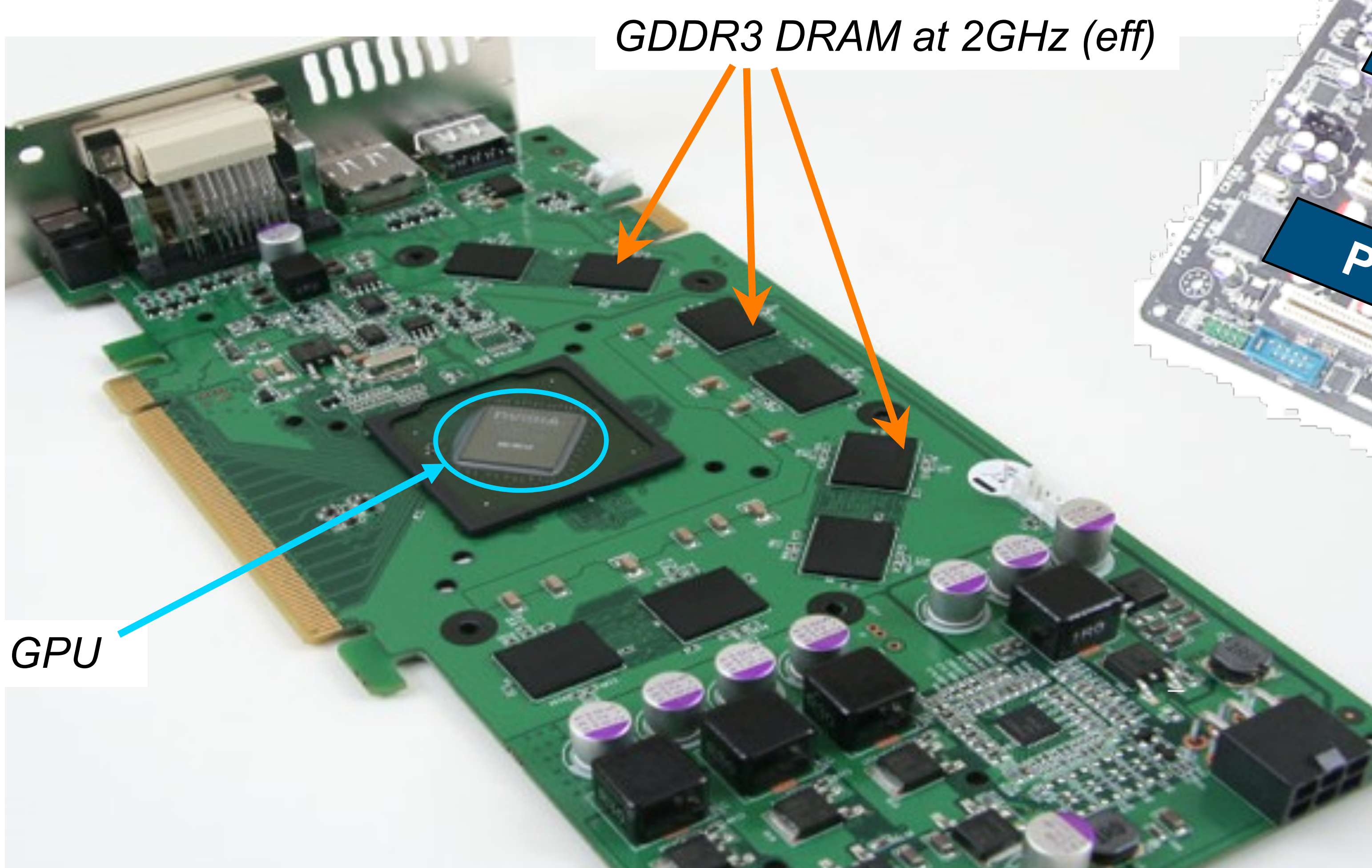
DCA++ speedup on GPU

Meredith et al., Par. Comp. **35**, 151 (2009)

Speedup of HF-QMC updates (2GHz Opteron vs. NVIDIA 8800GTS GPU):

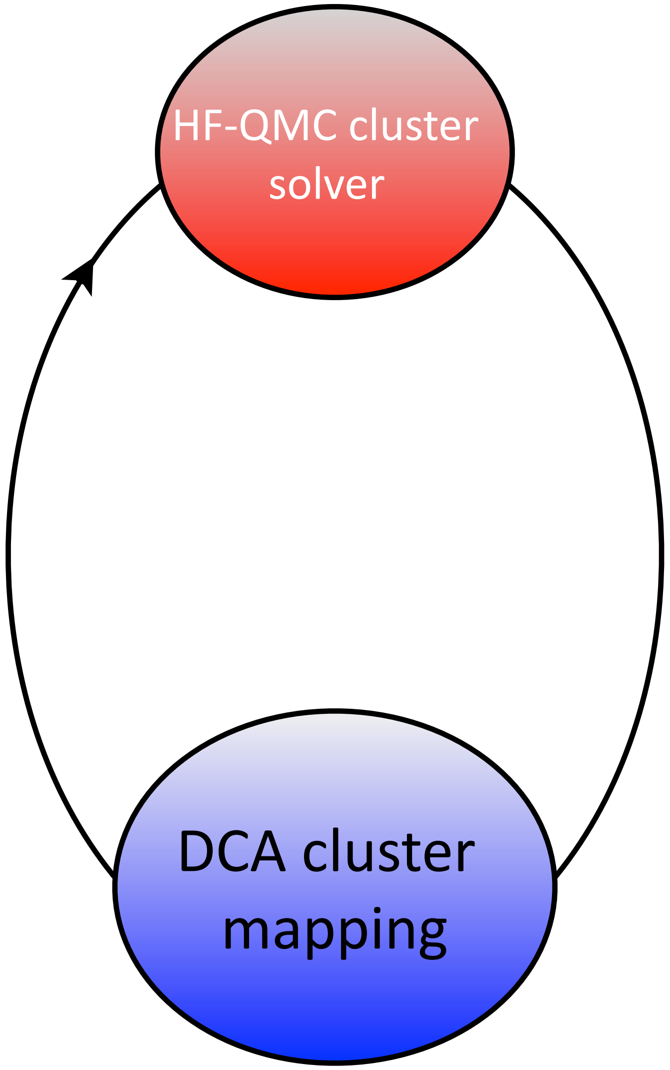
- 9x for offloading BLAS to GPU & transferring all data (completely transparent to application code)
- 13x for offloading BLAS to GPU & lazy data transfer
- 19x for full offload HF-updates & full lazy data transfer



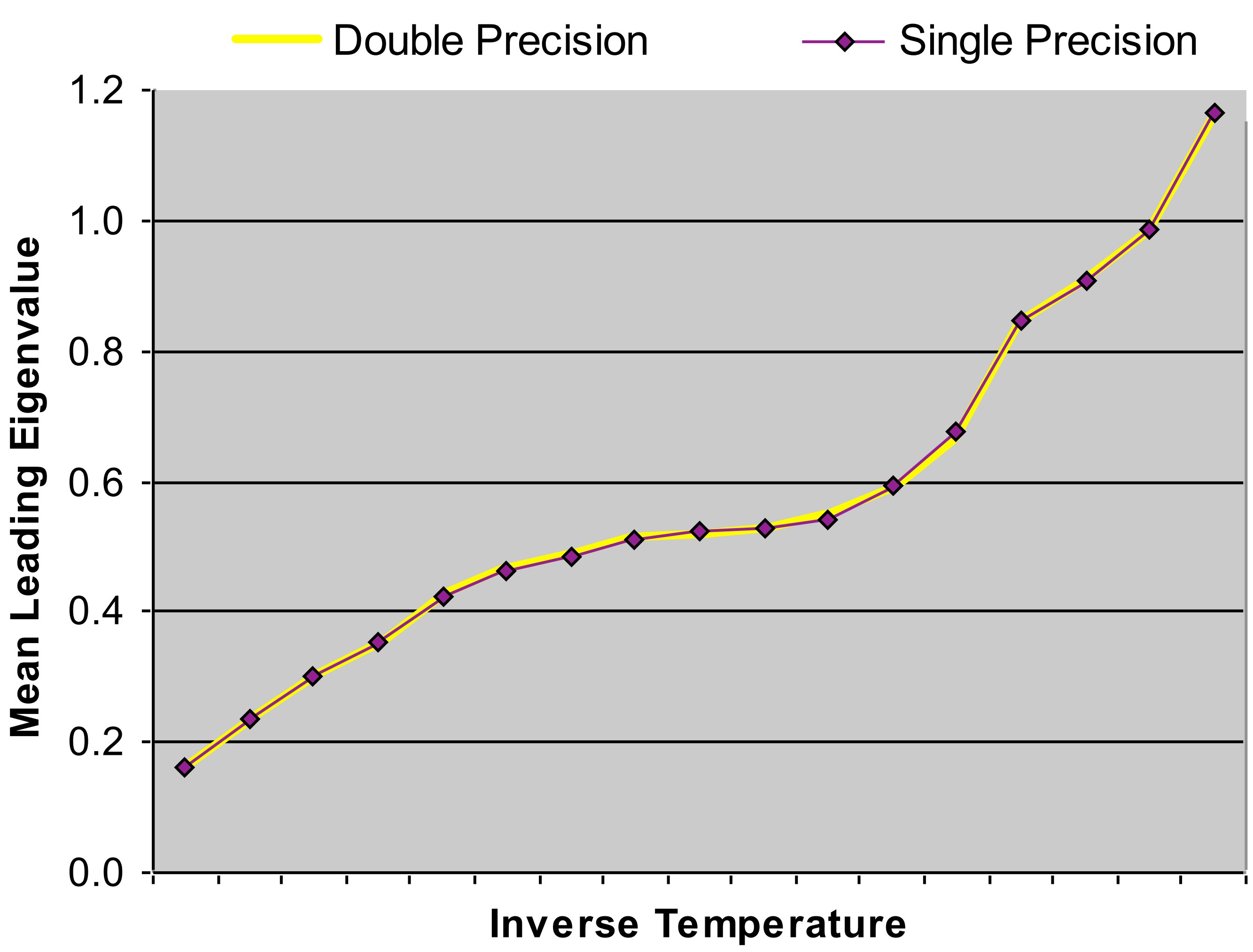


DCA++ with mixed precision

Run HF-QMC in single precision

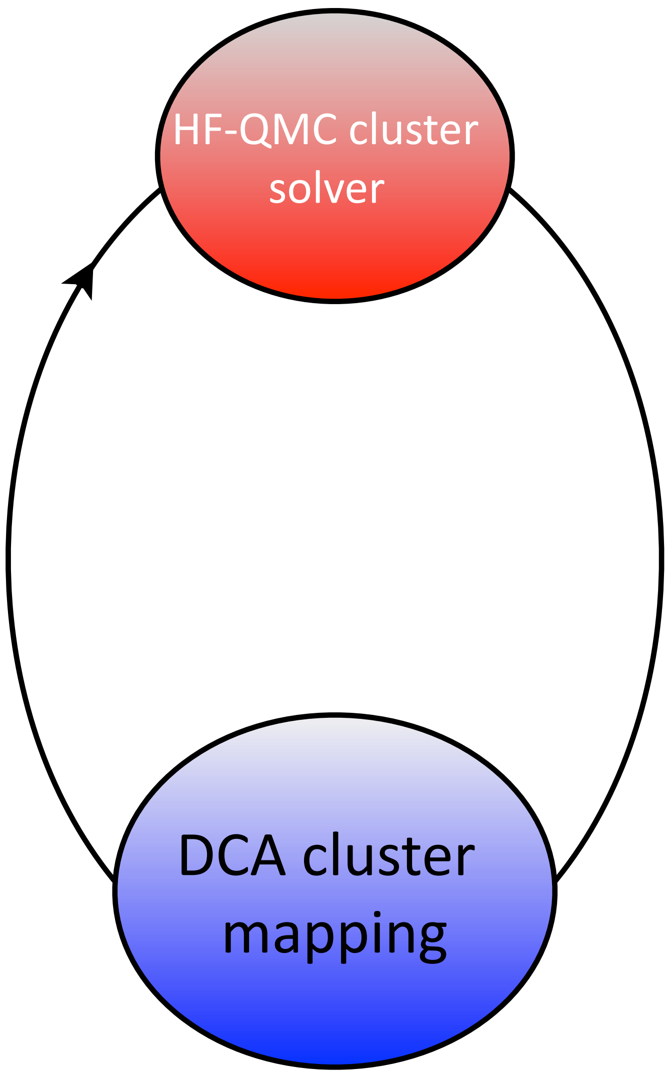


Keep the rest of the code, in particular cluster mapping in double precision



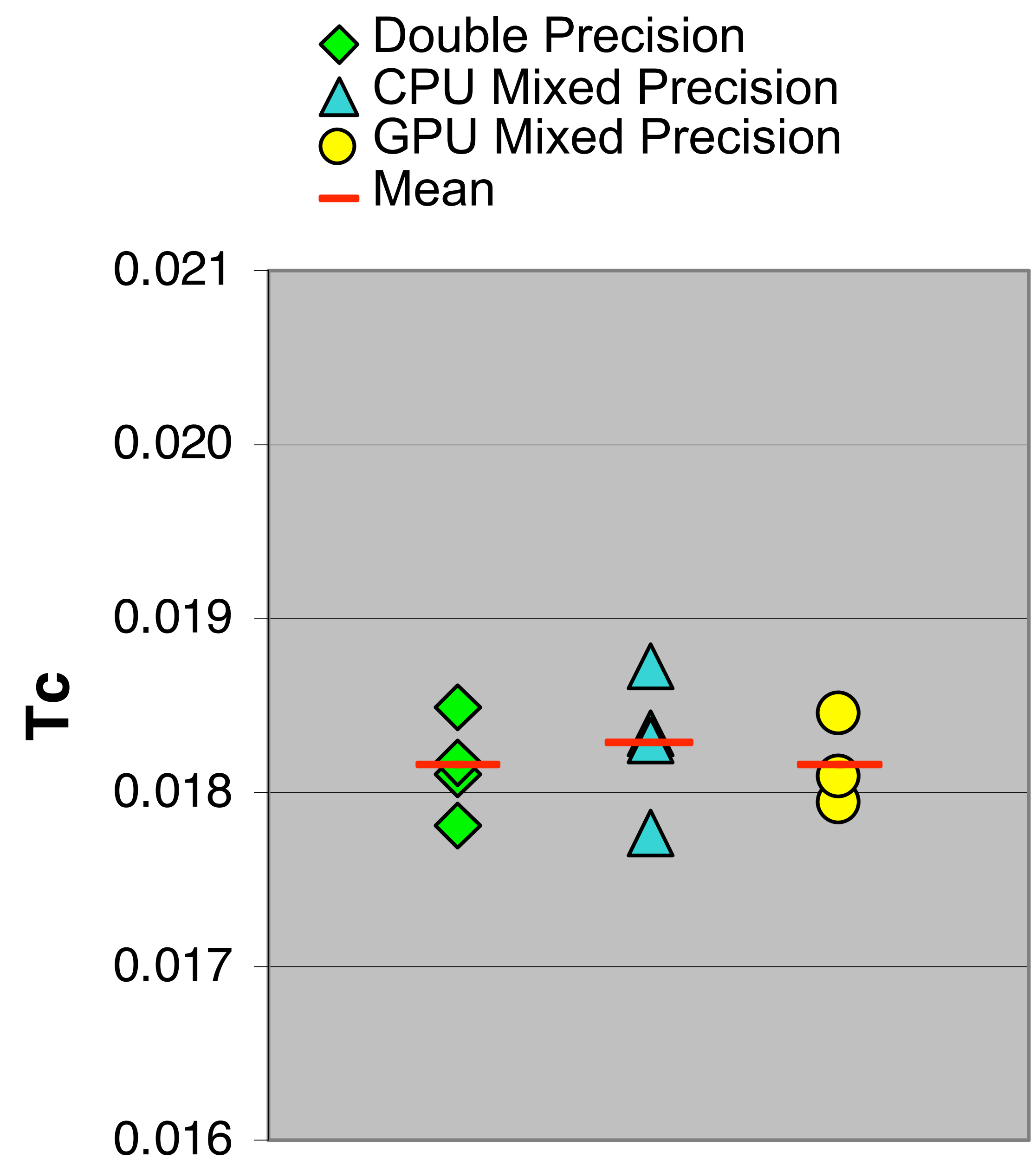
DCA++ with mixed precision

Run HF-QMC in single precision

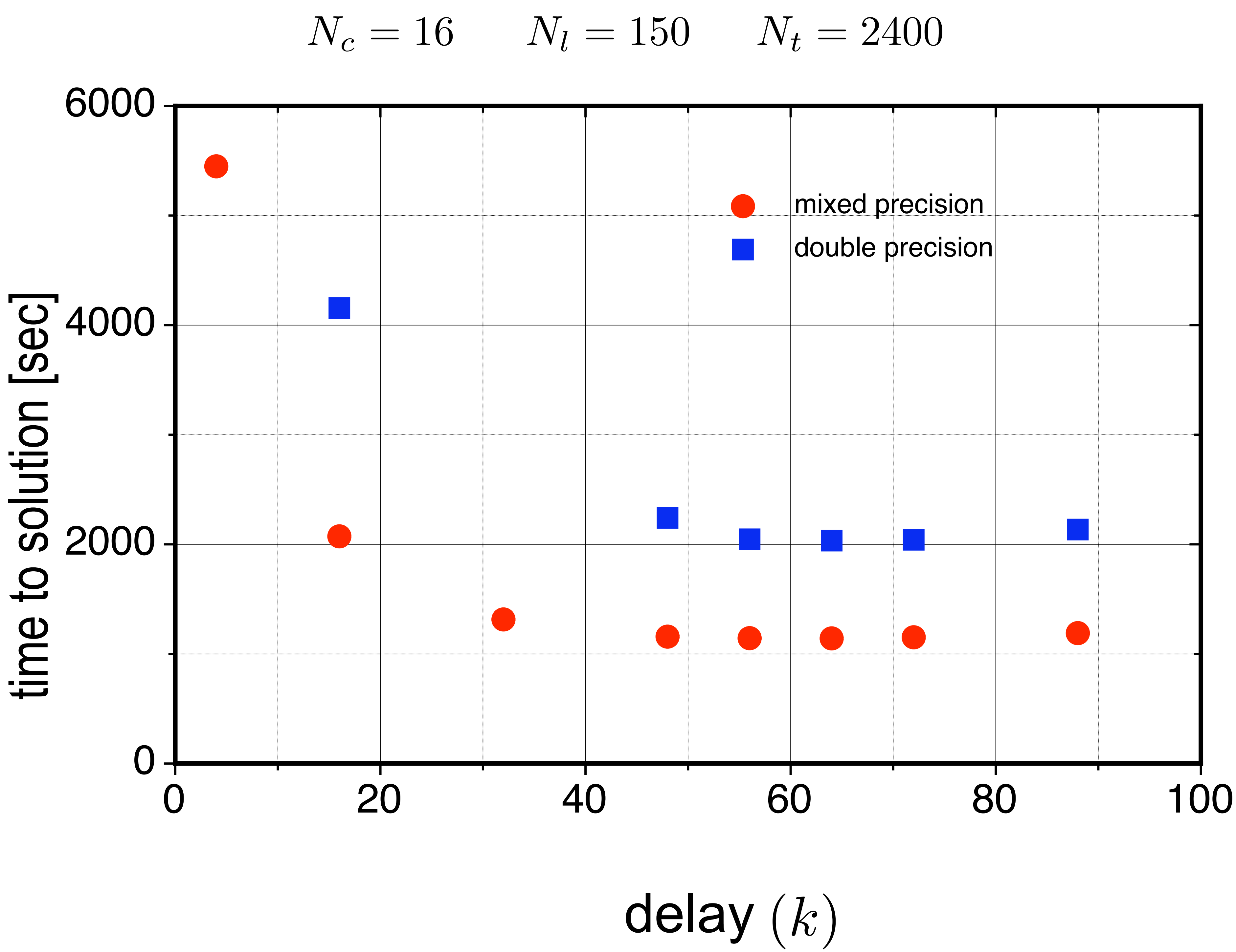


Keep the rest of the code, in particular cluster mapping in double precision

Multiple runs to compute T_c:



Performance improvement with delayed and mixed precision updates



High-T_c superconductivity: DCA/QMC simulations of the 2D Hubbard model

In 5 years, factor
10^3 X compute
10^{-4} X time to solution

First simulation proving model describes superconducting transition

Finally settled two-decade old debate over nature of pairing mechanism!

Realistic models of disorder and nanoscale inhomogeneities

High memory bandwidth helps performance of rank 1 update in DCA/QMC algortihm

Sustained performance of DCA/QMC

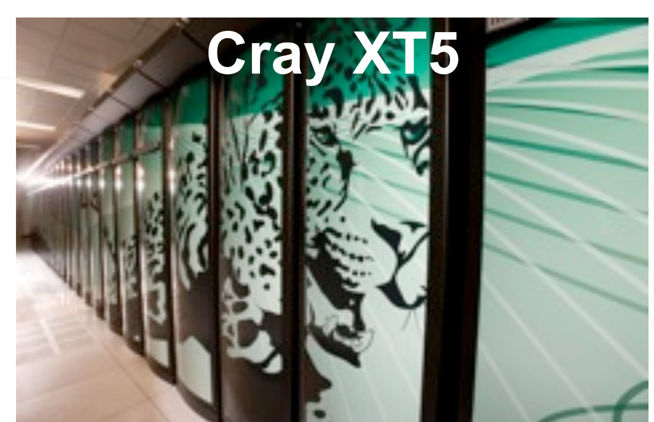
~1 TF — 2004
~6 TF — 2005
<<5 TF, ~26 TF — 2006
~60 TF — 2007
~140 TF, ~260 TF — 2008
1.34 PF, >2 PF — 2009

First sustained petaflop/s under production condition

Work with GPUs motivates change DCA/QMC algorithm to mixed precision

Modify QMC algorithm: replaced (delayed) rank 1 updates by matrix multiply

3 TF   18.5 TF
26 TF   54 TF   119 TF   263 TF
1.4 PF   2.4 PF



OLCF-3 Project:
10-20 PFlop/s Hybrid-Multi-Core systems based on NVIDIA Fermi
(2011/12)

Collaborators (superconductivity / DCA++):

Thomas Maier (ORNL)

Gonzalo Alvarez (ORNL)

Mike Summers (ORNL)

Paul Kent (ORNL)

Ed D'Azevedo (ORNL -- Comp. Math.)

Jeremy Meredith (ORNL -- future tech.)

Jeff Vetter (ORNL -- future tech.)

Trey White (ORNL -- NCCS)

Markus Eisenbach (ORNL -- NCCS)

Doug Scalapino (UCSB)

Mark Jarrell (U. of Cincinnati)

... many others

QUESTIONS?