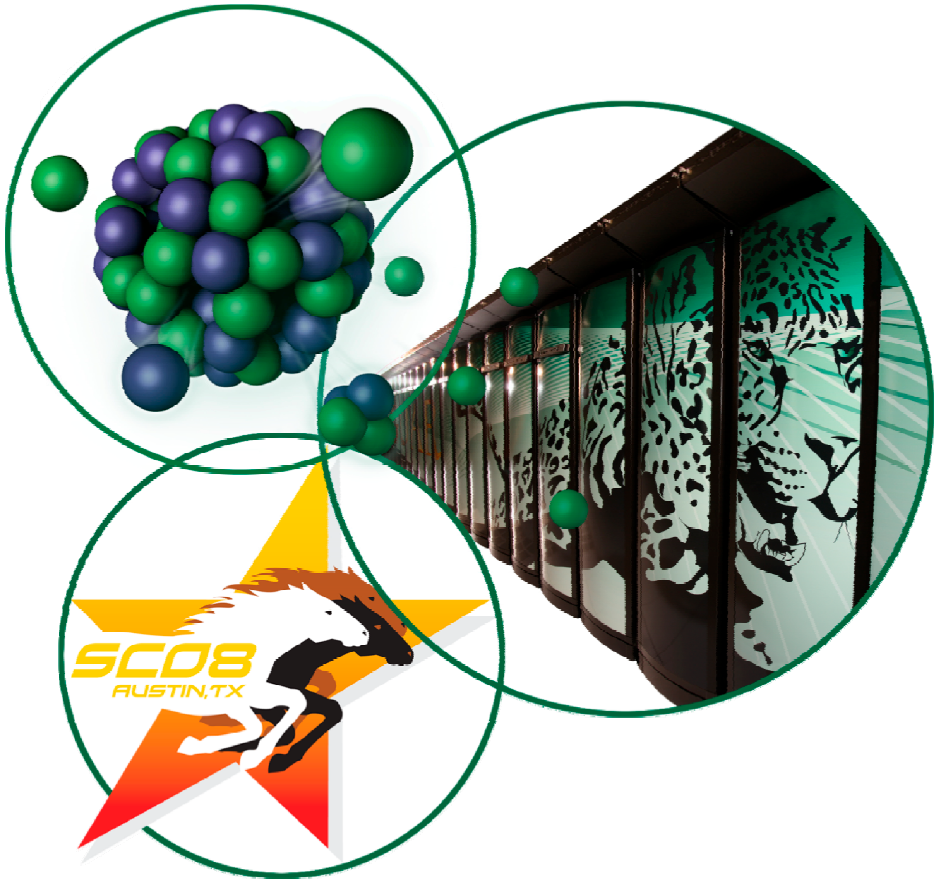
Fermion Glue in the Hubbard Model: New Insights into the Cuprate Pairing Mechanism with Advanced Computing



Presented by

Thomas C. Schulthess

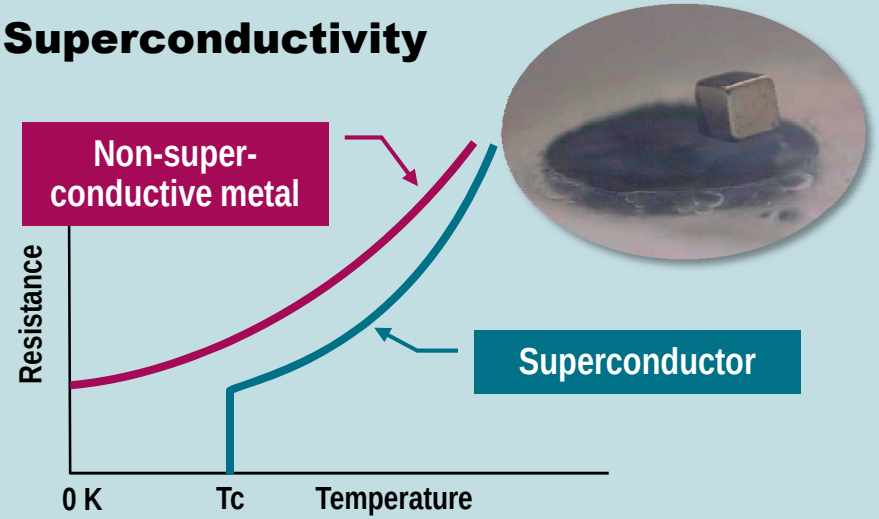
Computational Materials Sciences
Computer Science and Mathematics Division

Managed by UT-Battelle
for the Department of Energy

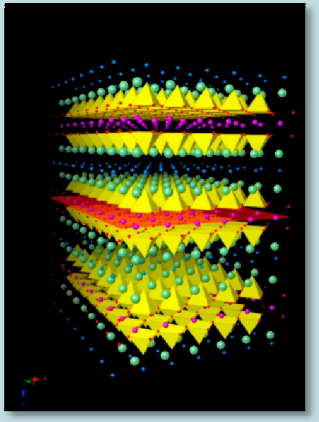
Oak Ridge National Laboratory

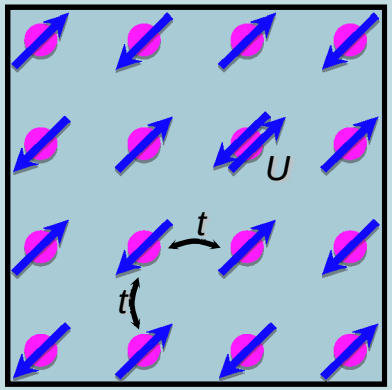
Outline

Superconductivity



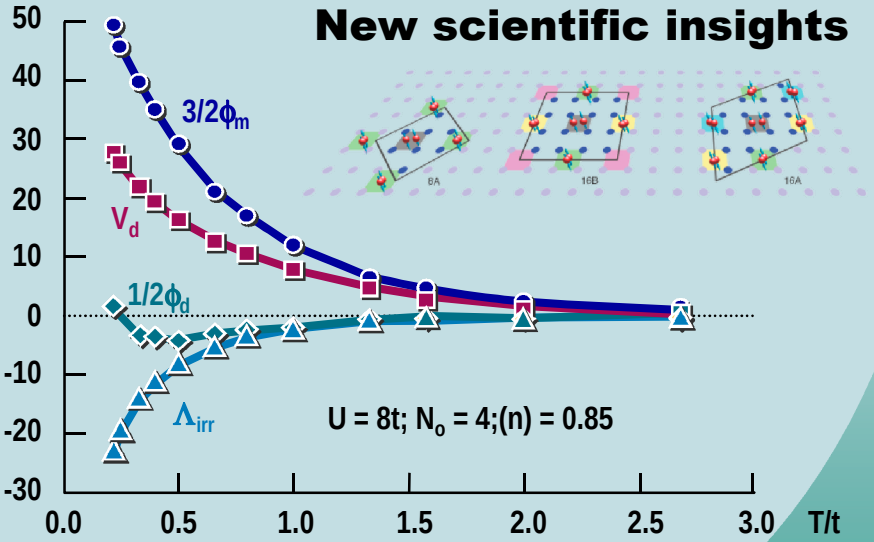
A model for high-temperature superconductors





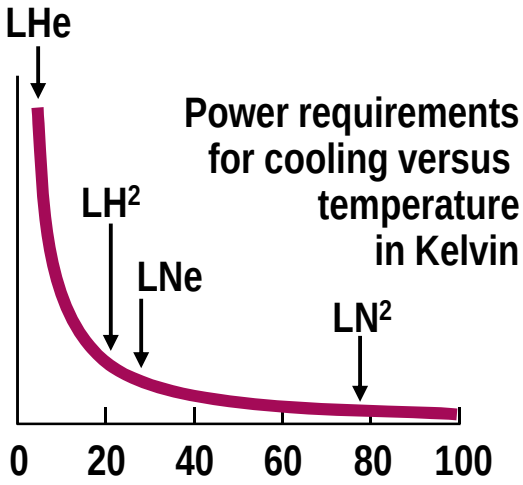
Algorithm and leadership computing

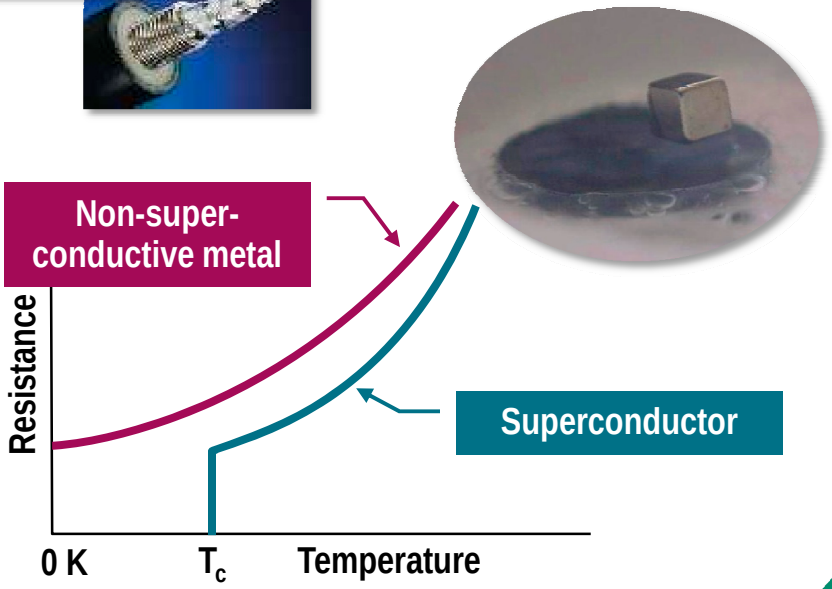
New scientific insights



What is superconductivity?

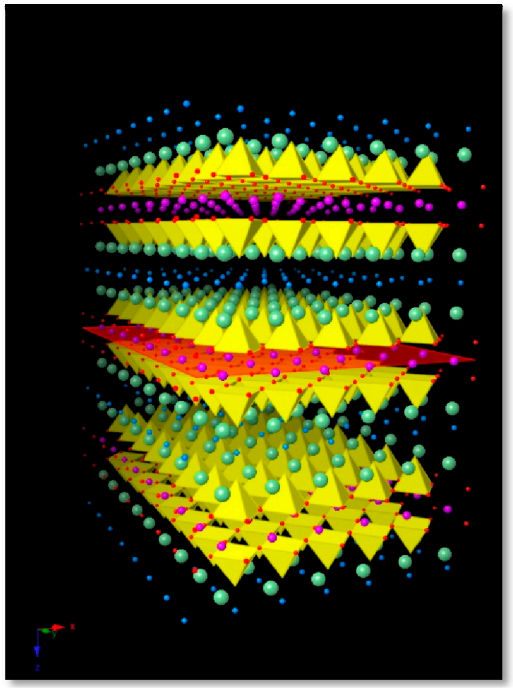
- A macroscopic quantum state with
  - Zero resistance
  - Perfect diamagnetism
- Applications
  - MAGLEV, MRI, power transmission, generators, motors
- Only disadvantage
  - Cooling necessary
  - Tc ≈ 150 K in high-temperature superconductivity
- Ultimate goal
  - Tc ≈ room temperature

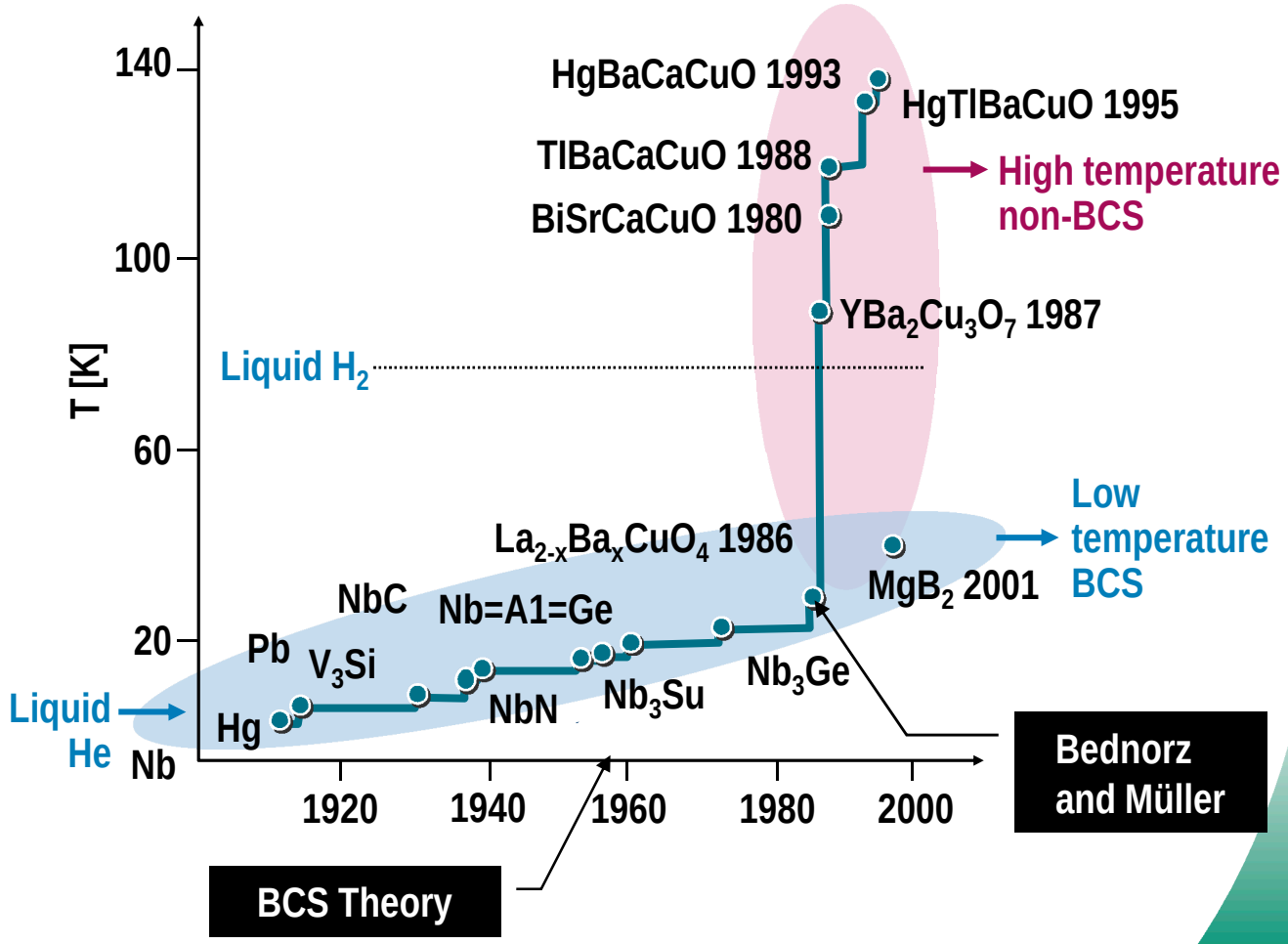




High-temperature superconductors

Discovered by Bednorz and Müller in 1986

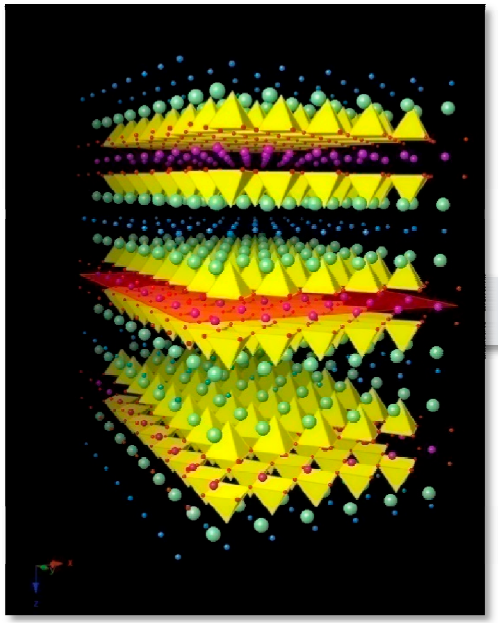




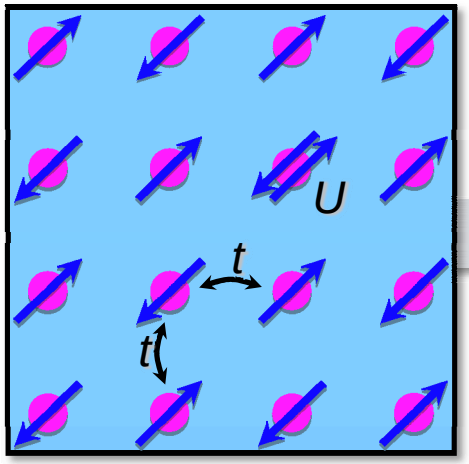
- **Highly anisotropic**
- **Superconducting CuO planes**

2-D Hubbard model of high-temperature superconductors

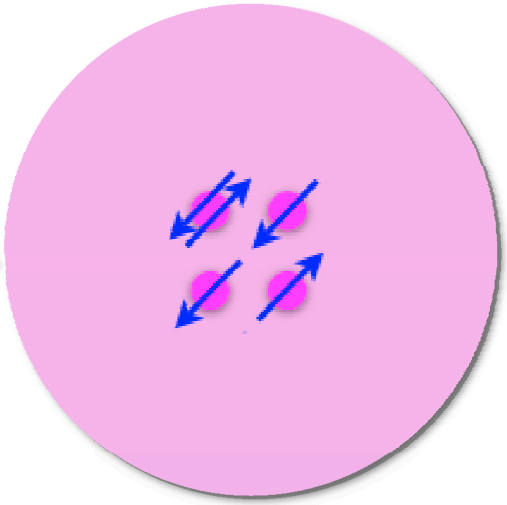
HTSC: 10^{23} interacting electrons



2-D Hubbard model for CuO planes



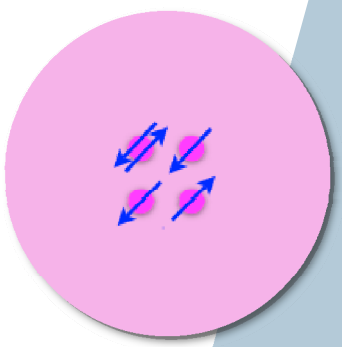
DCA/QMC: Map Hubbard model onto embedded cluster

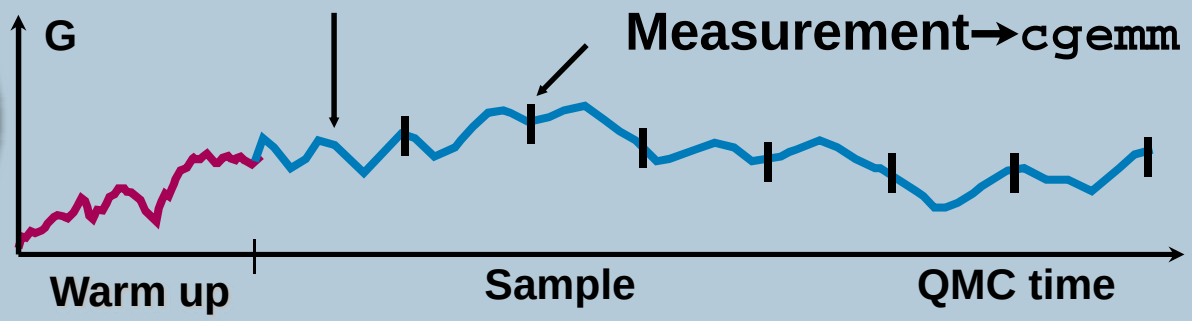


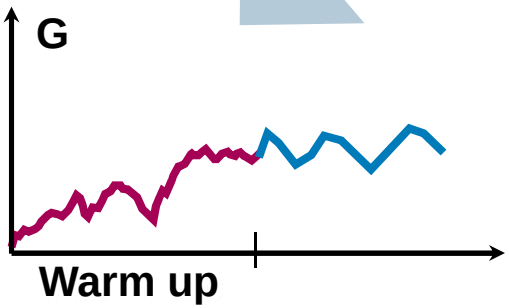
Algorithm and leadership computing:
Fixed startup cost favors fewer, faster processors → Cray X1E

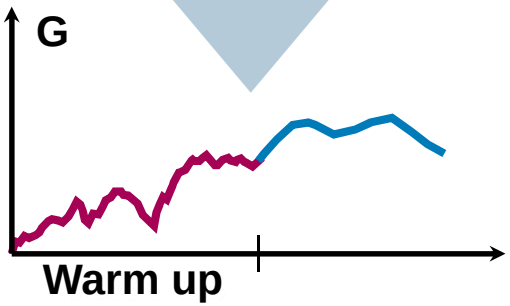
$\hat{G}' = \hat{G} + \vec{a} \times \vec{b}$ →`dger` (N = 4480)

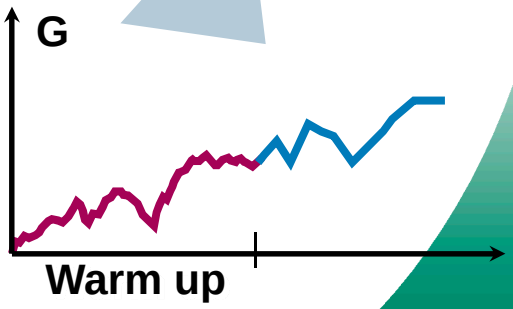
or delay updating→`dgemm` (4480 x 32)



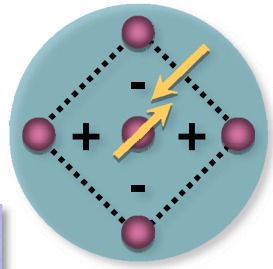


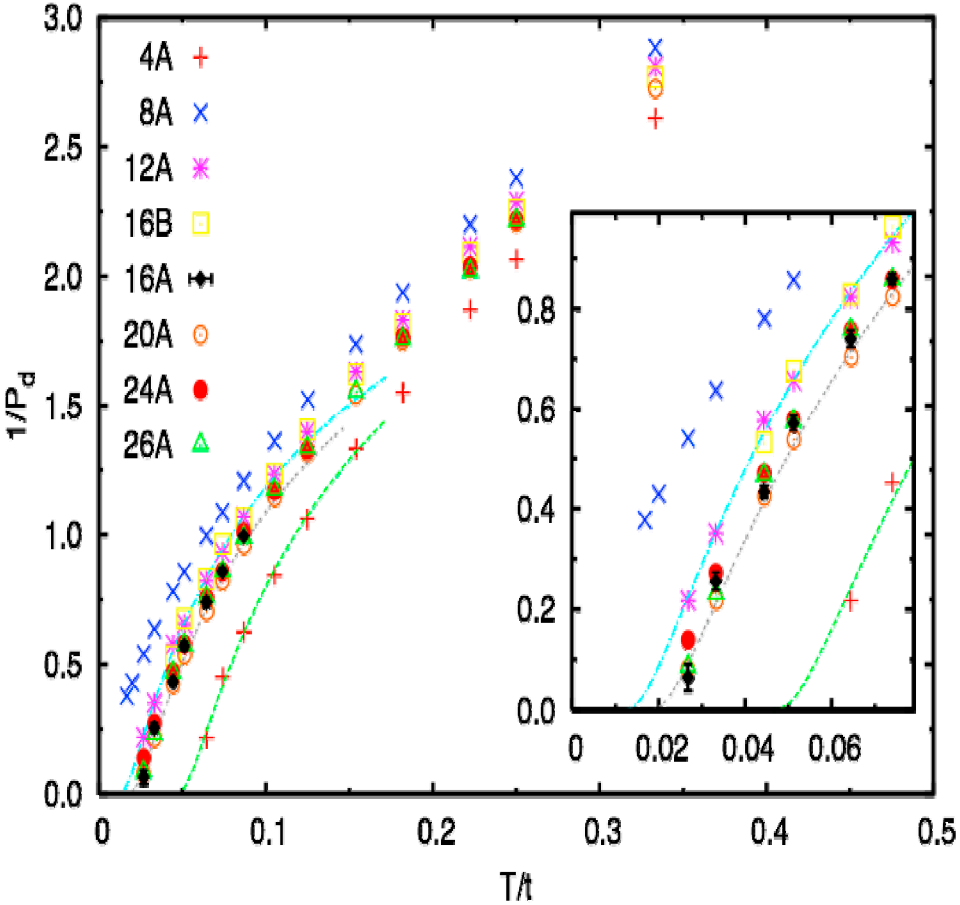


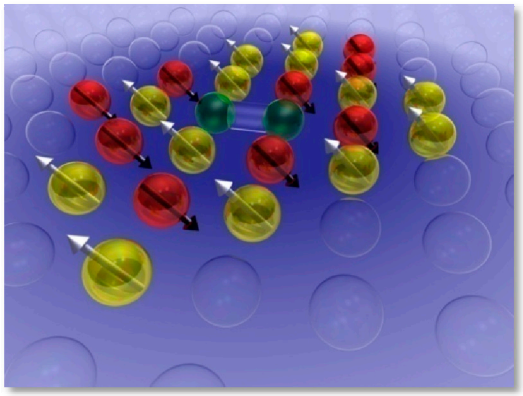




Superconductivity as a consequence of strong electronic correlations



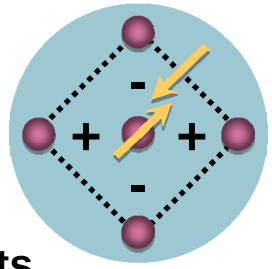


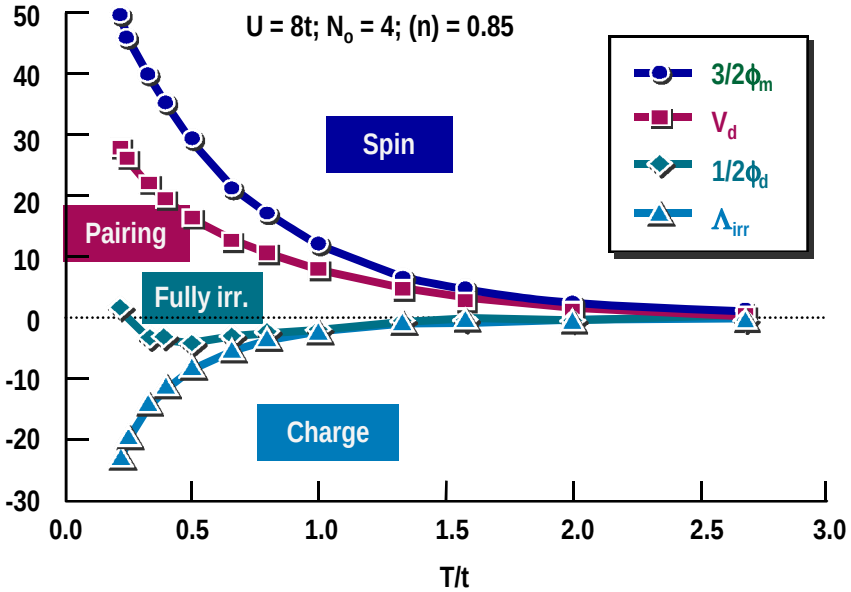


N_c	Z_d	T_c
4A	0	0.056
8A	1	-0.006
12A	2	0.016
16B	2	0.015
16A	3	0.025
20A	4	0.022
24A	4	0.020
26A	4	0.023

T. A. Maier, M. Jarrell, T. C. Schulthess, P. R. C. Kent, J. B. White, Systematic study of D-wave superconductivity in the 2D repulsive Hubbard model, *Phys. Rev. Lett.* **95**, 237001 (2005).

Magnetic origin of pairing interaction





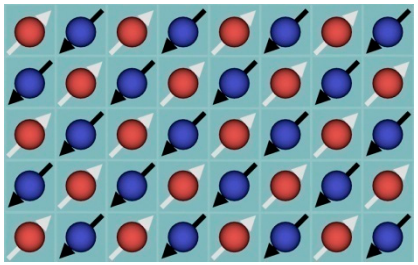
- **Attractive pairing interaction between nearest neighbor singlets**
- **Pairing mediated by electron spin**

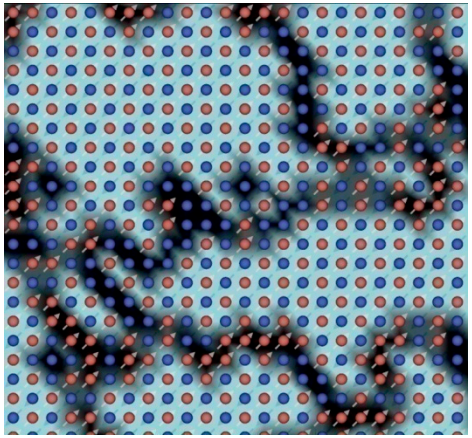
T. A. Maier, M. S. Jarrell, and D. J. Scalapino, Structure of the pairing interaction in the two-dimensional Hubbard Model, *Phys. Rev. Lett*. **96**, 047005 (2006).

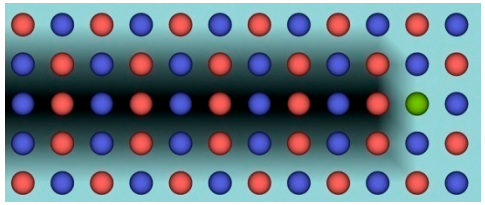
T. A. Maier, M. Jarrell, and D. J. Scalapino, Pairing interaction in the two-dimensional Hubbard model studied with a dynamic cluster quantum Monte Carlo approximation, *Phys. Rev. B* **74**, 094513 (2006).

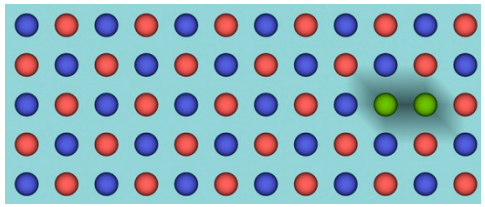
T. A. Maier, M. Jarrell, and D. J. Scalapino, Spin susceptibility representation of the pairing interaction for the two-dimensional Hubbard model, *Phys. Rev. B* **75**, 134519 (2007).

T. A. Maier, A. Macridin, M. Jarrell and D. J. Scalapino, Systematic analysis of a spin susceptibility representation of the pairing interaction in the 2D Hubbard Model, *Phys. Rev. B* **76**, 144516 (2007).

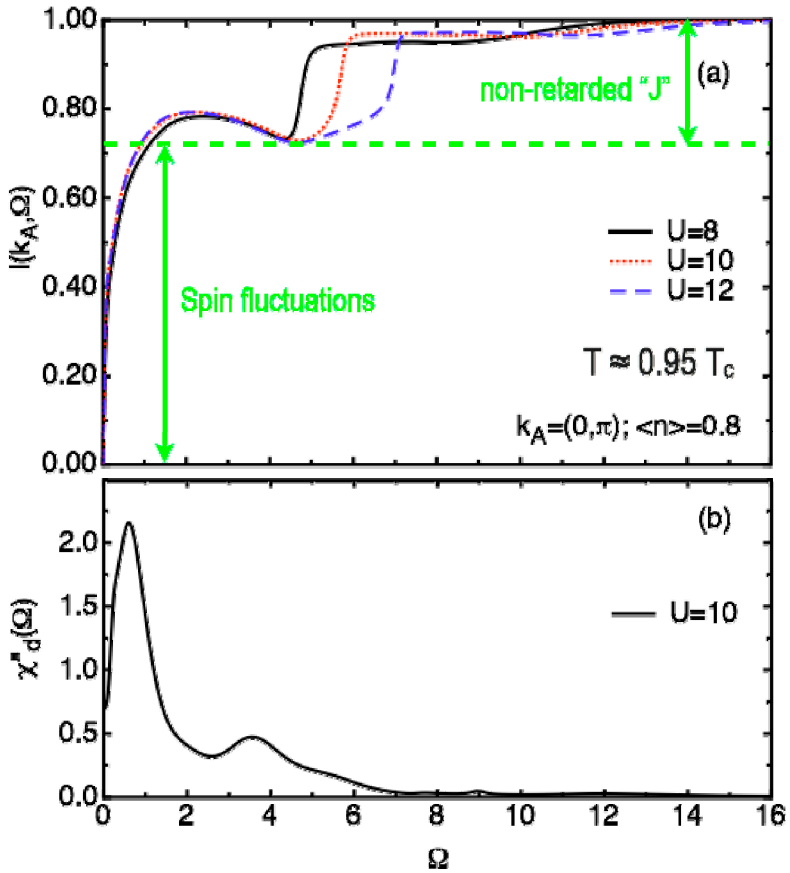








Dynamics of the pairing interaction—"Pairing glue" or not?



- **Pairing interaction contains retarded and non-retarded contributions**
- **Retarded contribution associated with dynamic spin fluctuations**
- **Non-retarded (instantaneous) contribution due to antiferromagnetic exchange interaction and related to excited states due to local Coulomb repulsion**
- **Phenomenological form for the pairing interaction:**

$$\frac{3}{2}\bar{U}^2\chi(k-k',w-w') - \bar{J}(\cos k_x - \cos k_y)(\cos k'_x - \cos k'_y)$$

T. A. Maier, D. Poilblanc and D. J. Scalapino, Dynamics of the pairing interaction in the Hubbard and t-J models of high-temperature superconductors, *Phys. Rev. Lett.* **100**, 237001 (2008).

Summary/conclusions/outlook

- Superconductivity: A macroscopic quantum effect
- 2-D Hubbard model for strongly correlated high-temperature superconducting cuprates
- Dynamic cluster quantum Monte Carlo simulations on Cray X1E and Cray XT3/4
- Superconductivity as a result of strong correlations
- Pairing mediated by electron spin
- Non-retarded and retarded contributions to pairing interaction
- Verification by neutron scattering experiments?
- Role of inhomogeneities?

Contacts

Thomas Maier

Computational Materials Sciences
Computer Science and Mathematics Division
(865) 576-3597
maierta@ornl.gov

Paul Kent

Computational Materials Sciences
Computer Science and Mathematics Division
(865) 574-4845
kentpr@ornl.gov

Thomas Schulthess

Computational Materials Sciences
Computer Science and Mathematics Division
(865) 574-4344
schulthesstc@ornl.gov

The team

University of California

D. Scalapino

University of Cincinnati

M. Jarrell

Oak Ridge National Laboratory

Paul Kent
Thomas Maier
Thomas Schulthess