New Insights into High-Temperature Superconductivity from a Computational Solution of the 2D Hubbard Model

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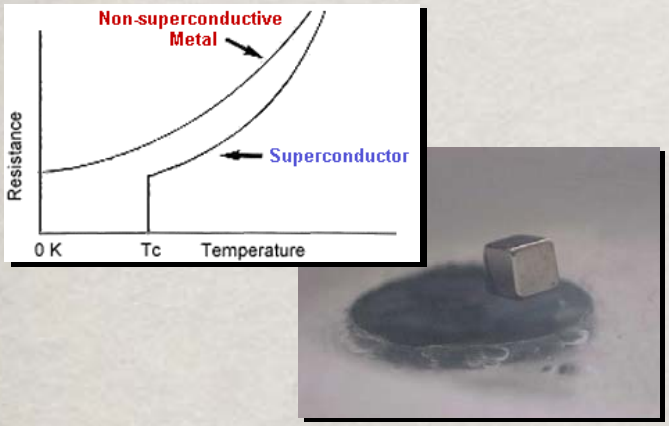
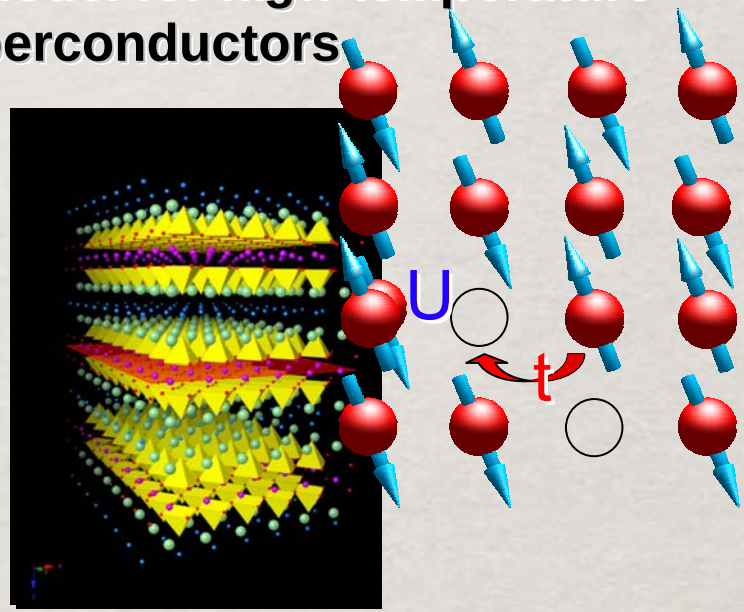
Outline

Superconductivity

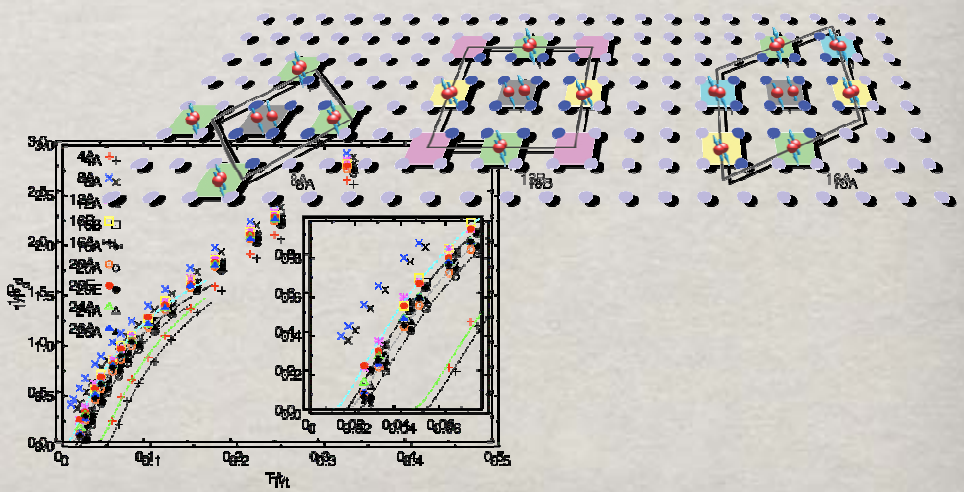


A model for high-temperature superconductors



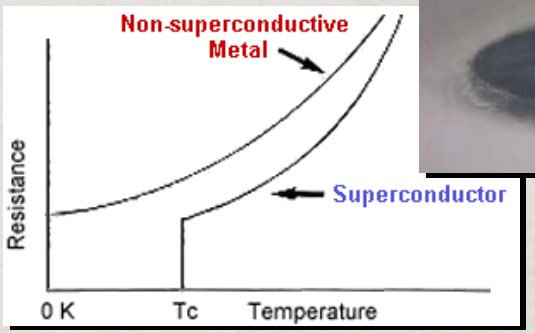
Algorithm and leadership computing

New scientific insights

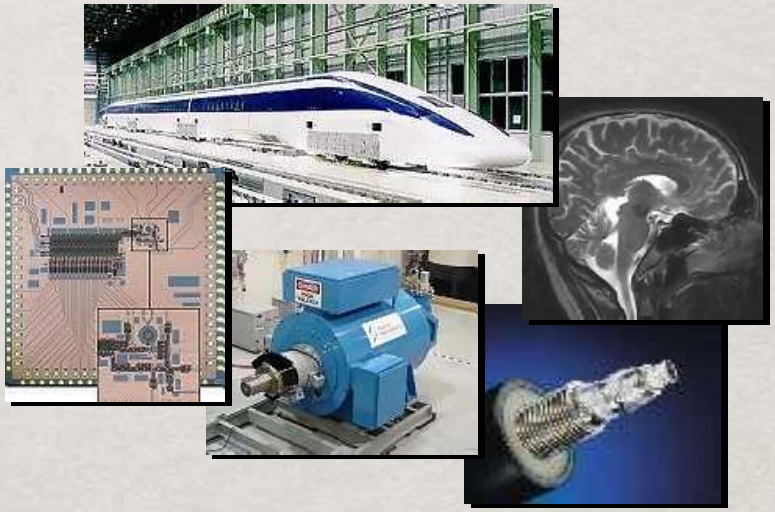


Superconductivity in a nutshell

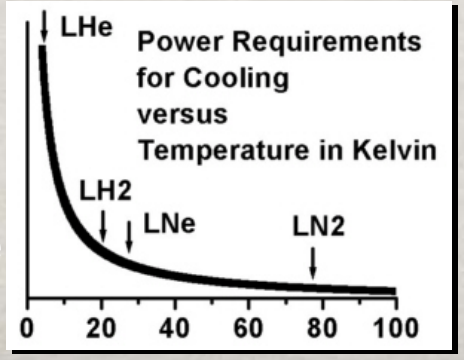
- **Superconductivity = macroscopic quantum state**
  - zero resistance
  - perfect diamagnetism



- **Applications**
  - MAGLEV
  - MRI
  - Power transmission
  - Generators
  - Motors

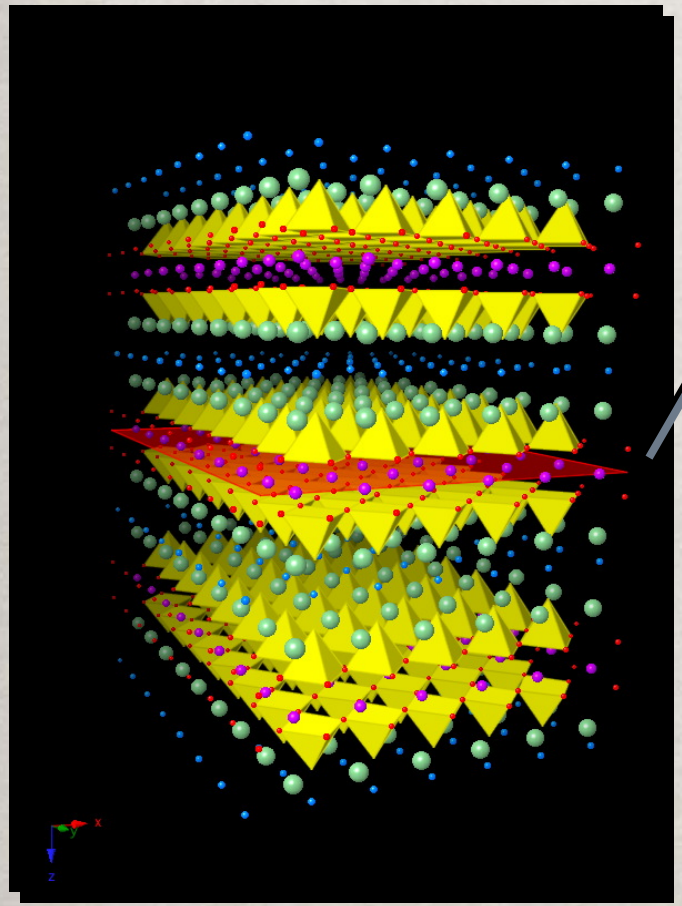


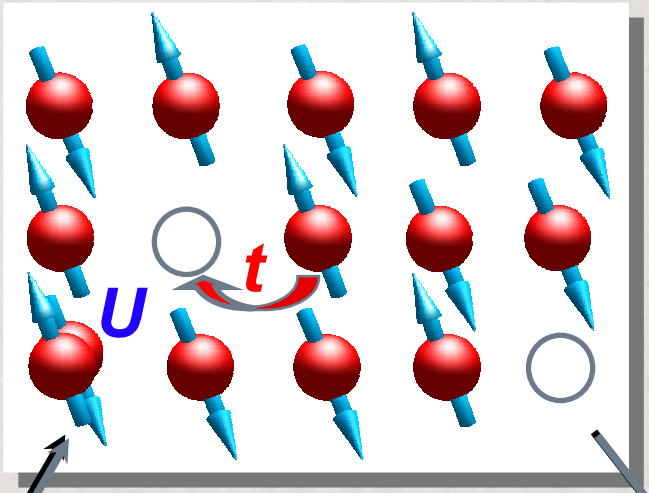
- **Only disadvantage**
  - Cooling necessary
  - $T_c \approx 150K$ in HTSC
- **Ultimate Goal**
  - $T_c \approx$ room temperature



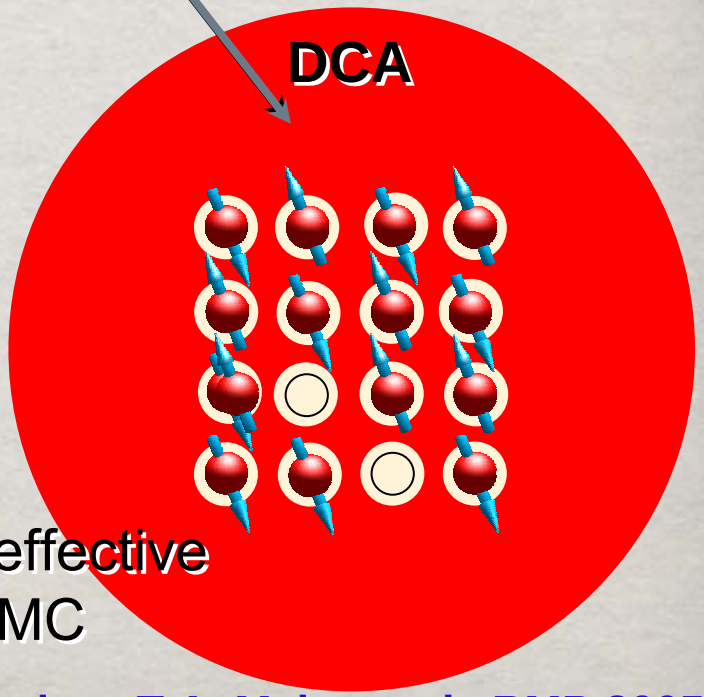
A model for high-temperature superconductors

HTSC compounds:
10^{23} correlated electrons





2D Hubbard model
for superconducting
CuO_2-planes



DCA/QMC: Solve DCA effective cluster problem using QMC

Review: T.A. Maier et al., RMP 2005

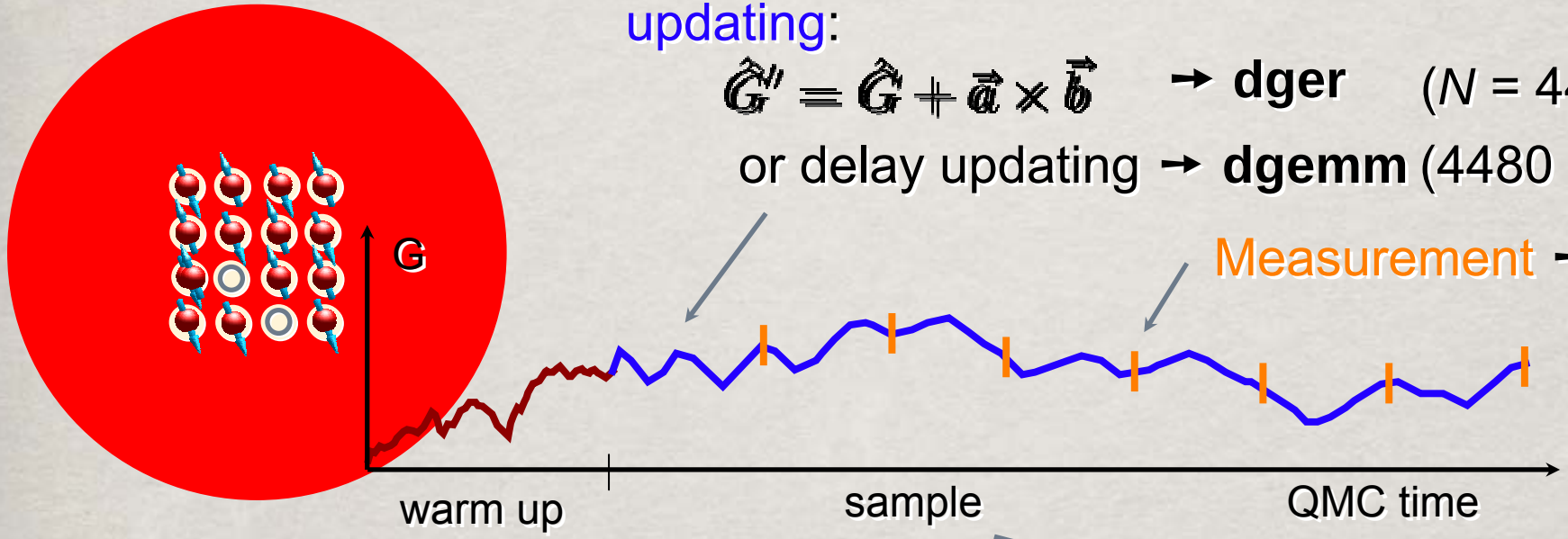
Algorithm and leadership computing: Fewer, more powerful processors are better

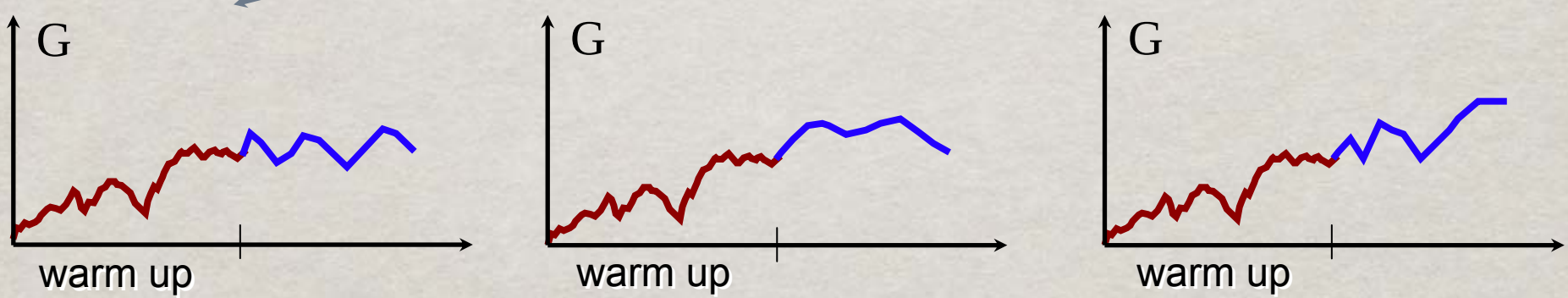
updating:

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

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

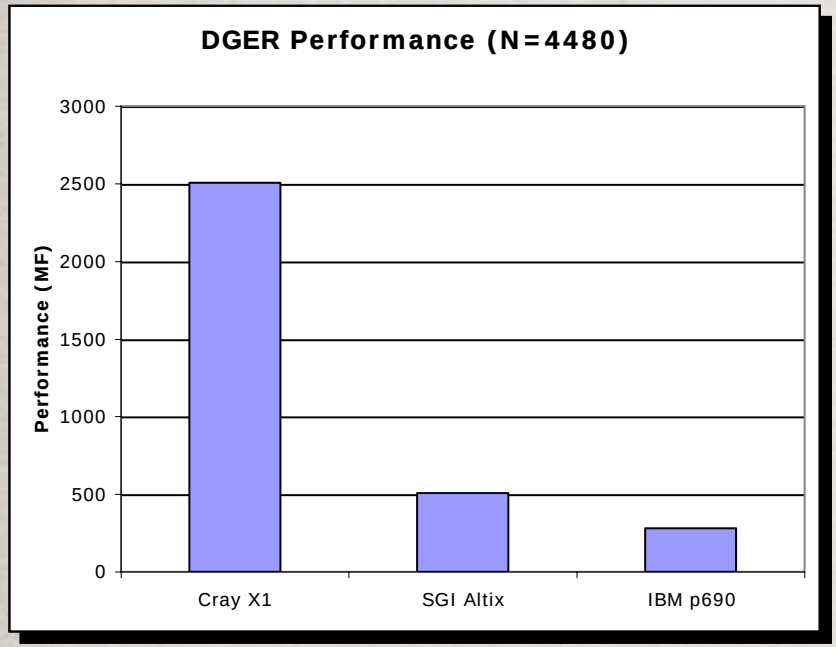
Measurement → **cgemm**

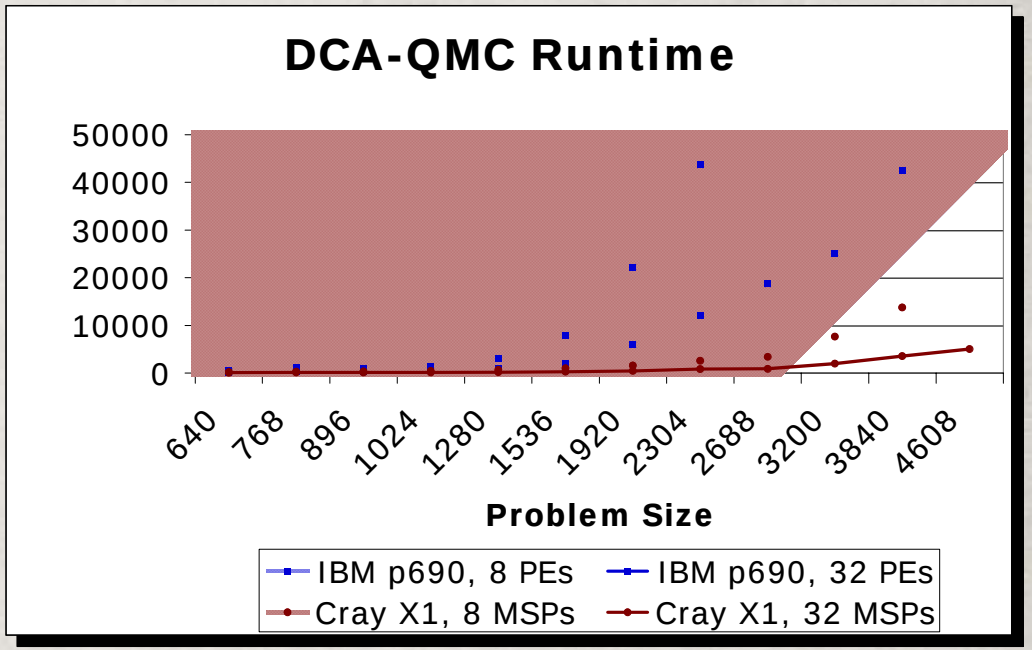




→ Fixed startup cost favors fewer, faster processors

QMC/DCA: Performance

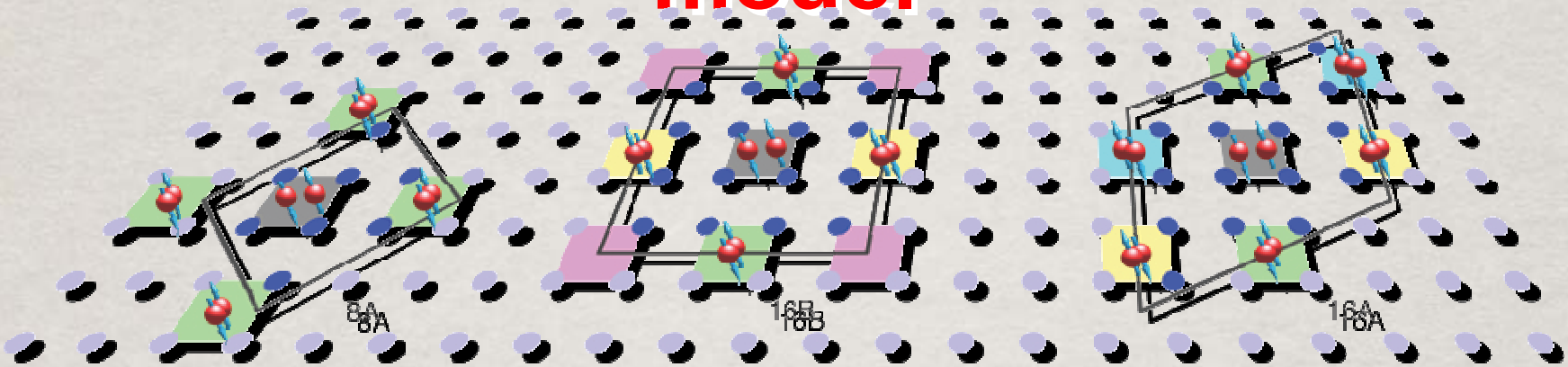


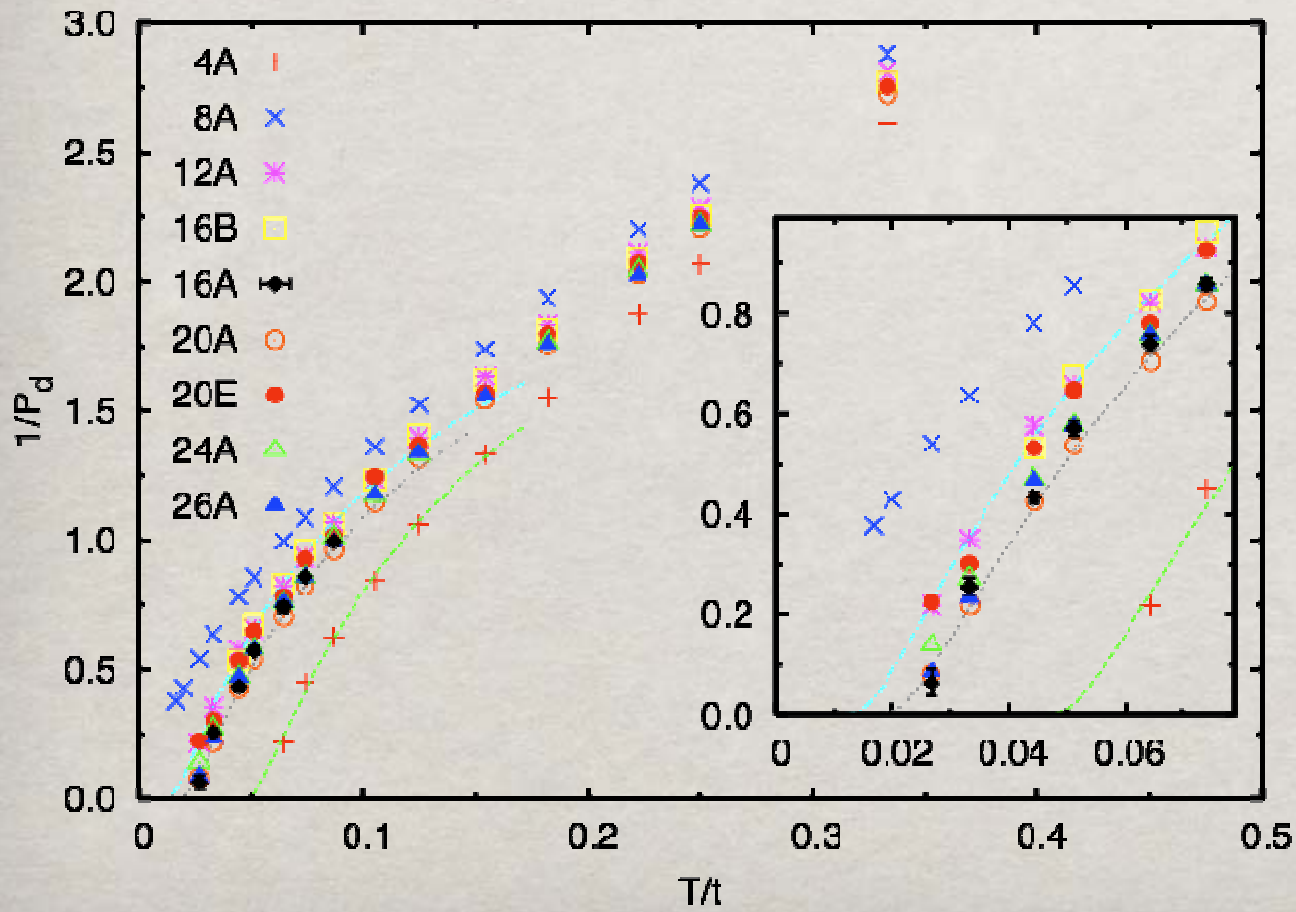


- **Cray X1(E) advantage:**
  - dger requires high-memory bandwidth
  - cgemm and dgemm benefit from high peak-rate
  - Code runs at 30-60% efficiency and scales to > 500 MSPs

- → Cray X1(E) provides capability for new science

Superconductivity in 2D Hubbard model





Cluster	Z_d	T_c/t
4	0 (MF)	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

→ $T_c \approx 0.023t$

T.A. Maier et al., to appear in PRL

Pairing mechanism: T.A. Maier et al., preprint cond-mat/0508361)