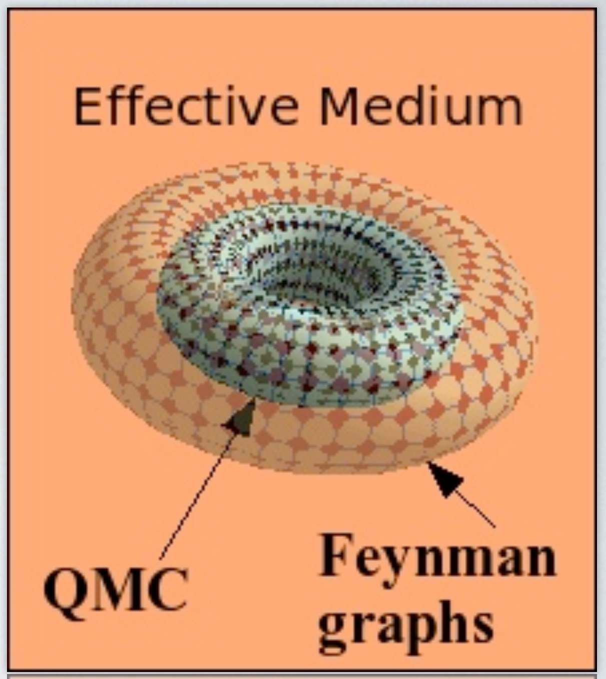
ADVANCING OUR UNDERSTANDING OF HIGH-TEMPERATURE SUPERCONDUCTORS THROUGH EXTREME SCALE COMPUTING

Thomas A. Maier
Oak Ridge National Laboratory

SCIDAC PROJECT ACCOMPLISHMENTS

Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials

Mark Jarrell (PI), Z. Bai, Ed D'Azevedo, T.A. Maier, S.Y. Savrasov, R.T. Scalettar, K. Tomko



- **Order of magnitude increase in number of electrons that can be simulated using Quantum Monte Carlo (QMC) codes.**

- **New QMC solver for dynamic mean field theory that scales linearly in inverse temperature rather than cubic.**

- **Highly parallel solver for multi-scale parquet quantum modeling of correlated materials**

- **INCITE 2010 award: 17M hours on ORNL Cray XT**

See posters by Ed D'Azevedo & Z. Bai!

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SCIDAC PROJECT PUBLICATIONS

Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials

Mark Jarrell (PI), Z. Bai, Ed D'Azevedo, T.A. Maier, S.Y. Savrasov, R.T. Scalettar, K. Tomko

"High Precision Quantum Monte Carlo Study of the 2D Fermion Hubbard Model at Half-Filling," C.N. Varney, C.R. Lee, Z.J. Bai, S. Chiesa, M. Jarrell, and R.T. Scalettar, Phys. Rev. B80, 075116 (2009).

"Dynamical Mean Field Theory Cluster Solver with Linear Scaling in Inverse Temperature", E. Khatami, C.R. Lee, Z.J. Bai, R.T. Scalettar, and M. Jarrell, Phys. Rev. E81, 056703 (2009).

"Magnetism and pairing of two-dimensional trapped fermions", S. Chiesa, R.T. Scalettar, C.N. Varney and M. Rigol, submitted to Physical Review Letters.

"Parquet approximation for the 4x4 Hubbard cluster," S. X. Yang, H. Fotso, J. Liu, T. A. Maier, K. Tomko, E. F. D'Azevedo, R. T. Scalettar, T. Pruschke, and M. Jarrell, Phys. Rev. E80, 046706 (2009).

"The screening of 4f moments and delocalization in the compressed light rare earths", A.K. McMahan, R.T. Scalettar, and M. Jarrell, Phys. Rev. B80, 235105 (2009).

"Quantum Criticality Due to Incipient Phase Separation in the 2D Hubbard Model", E. Khatami, K. Mikelsons, D. Galanakis, A. Macridin, J. Moreno, R.T. Scalettar, and M. Jarrell, Phys. Rev. B81, 201101 (2010).

"High Quality Preconditioning Technique for Multi-Length-Scale Symmetric Positive Definite Linear Systems", I. Yamazaki, Z. Bai, W. Chen, and R. Scalettar, Numerical Mathematics: Theory, Methods and Applications 2, 469 (2009).

"Self consistent GW determination of the interaction strength: application to the iron arsenide superconductors ", A. Kutepov, K. Haule, S.Y. Savrasov, G. Kotliar, arXiv: 1005.0885 (2010).

"Dimensional trend in CePt2In7, Ce-115 compounds, and CeIn3" , M. Matsumoto, M.J. Han, J. Otsuki, S.Y. Savrasov , arXiv:1004.5457 (2010)

"Calculated Magnetic and Electronic Properties of Pyrochlore Iridates", Xiangang Wan, Jinming Dong, Sergej Y. Savrasov arXiv:1003.3414 (2010).

"First Principle Simulations of Heavy Fermion Cerium Compounds Based on the Kondo Lattice", M. Matsumoto, M.J. Han, J. Otsuki, S. Y. Savrasov, Phys. Rev Lett. 103, 096403 (2009);

"Doping Driven (pi, 0) Nesting and Magnetic Properties in Iron Chalcogenide Superconductors", M.J. Han, S. Y. Savrasov, Phys. Rev. Lett. 103, 067001 (2009);

"Anisotropy, Itineracy, and Magnetic Frustration in High-TC Iron Pnictides", M. J. Han, Q. Y., W. E. Pickett, and S. Y. Savrasov, Phys. Rev. Lett. 102, 107003 (2009)

"Calculated Magnetic Exchange Interactions in High-Temperature Superconductors", X. Wan, T. A. Maier, S. Y. Savrasov, Phys. Rev. B 79, 155114 (2009);

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ACKNOWLEDGEMENTS

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Thomas Schulthess	ETH Zürich & CSCS
Mike Summers	ORNL

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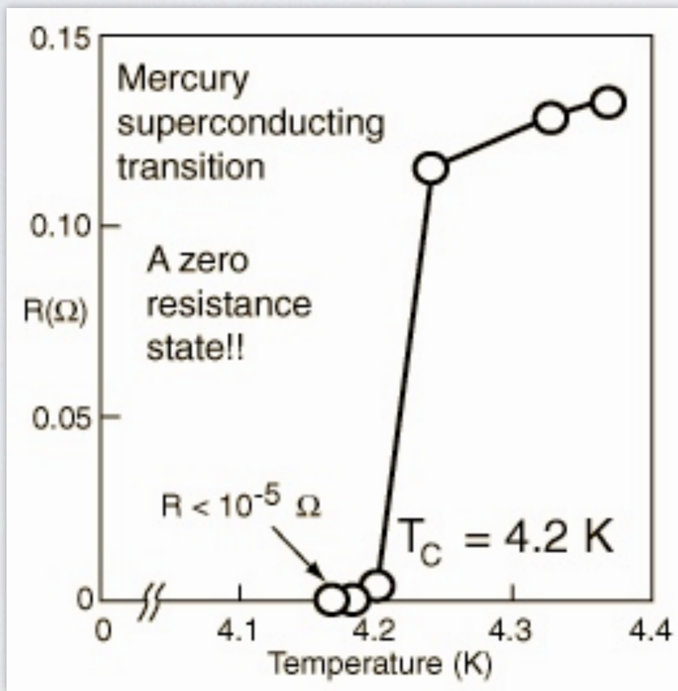
Computational resources:
NCCS @ ORNL

SUPERCONDUCTIVITY - ZERO RESISTANCE STATE

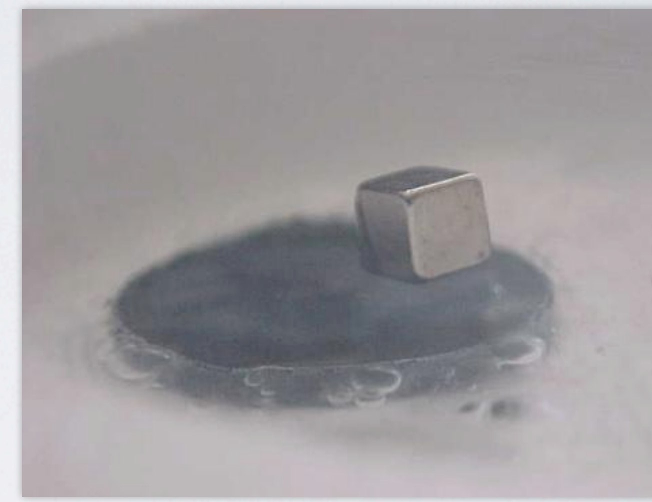
Discovery:

- Zero resistance state
  H. Kamerlingh Onnes (1911)



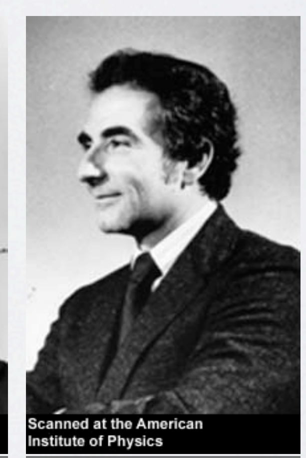
Meissner-Ochsenfeld effect:

- Superconductors repel magnetic fields
  Meissner & Ochsenfeld (1933)



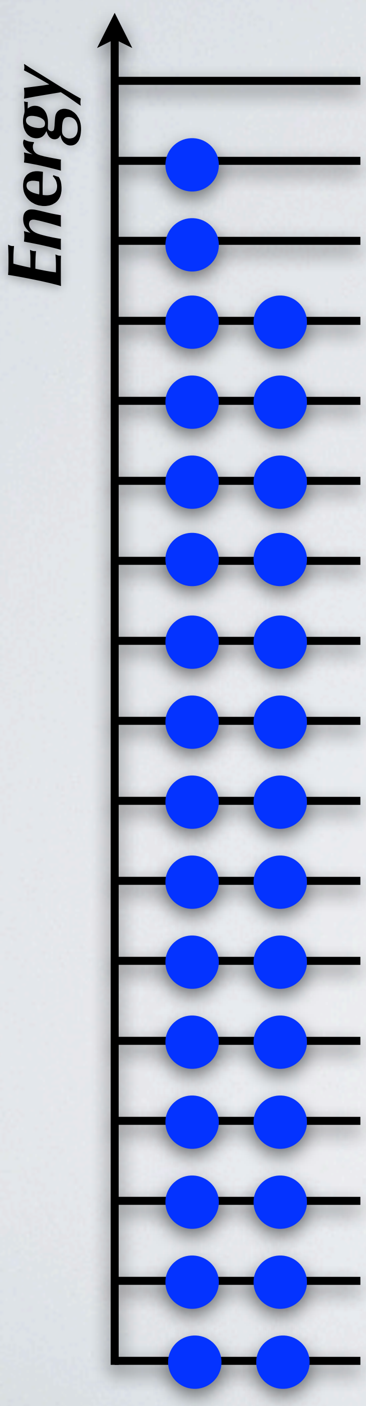
Explanation:

- Bardeen-Cooper-Schrieffer theory (1957)
- BCS theory generally accepted in early 1970s



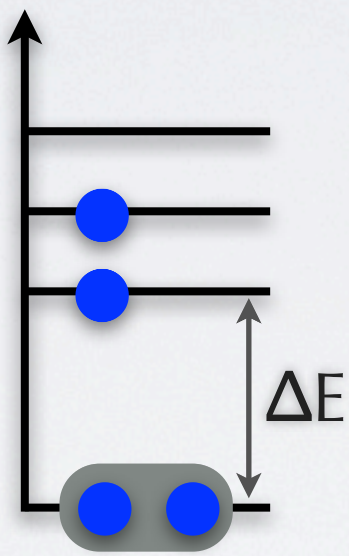
BCS THEORY - FERMIONS, BOSONS AND COOPER PAIRS

Fermions (Electrons)

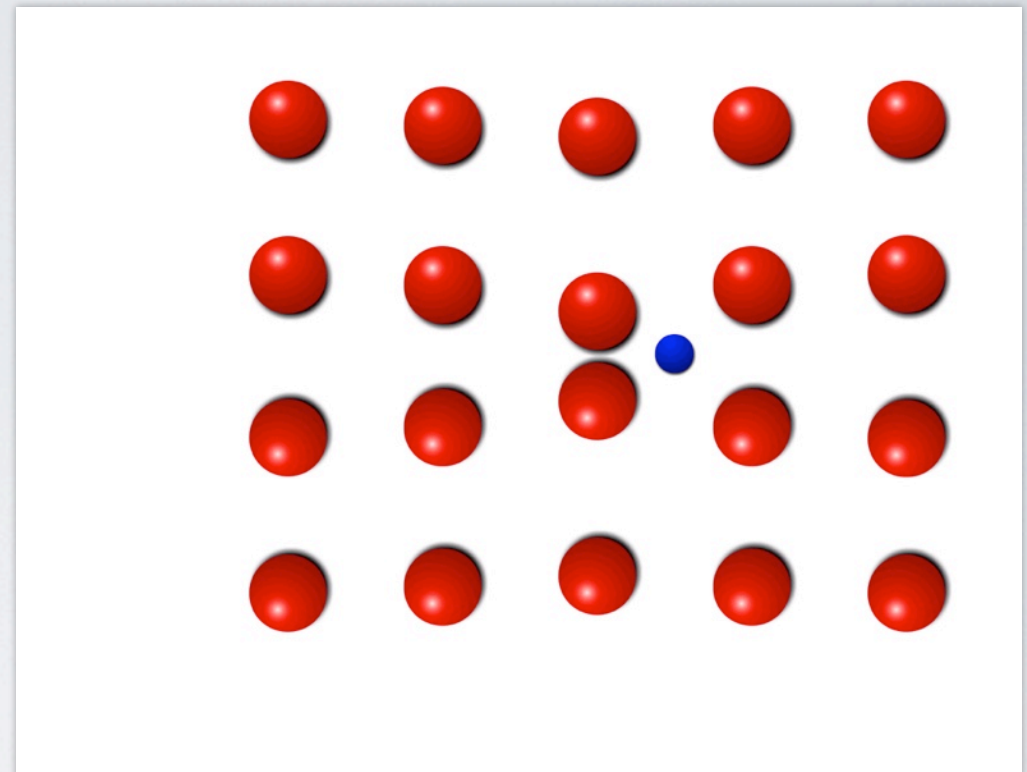


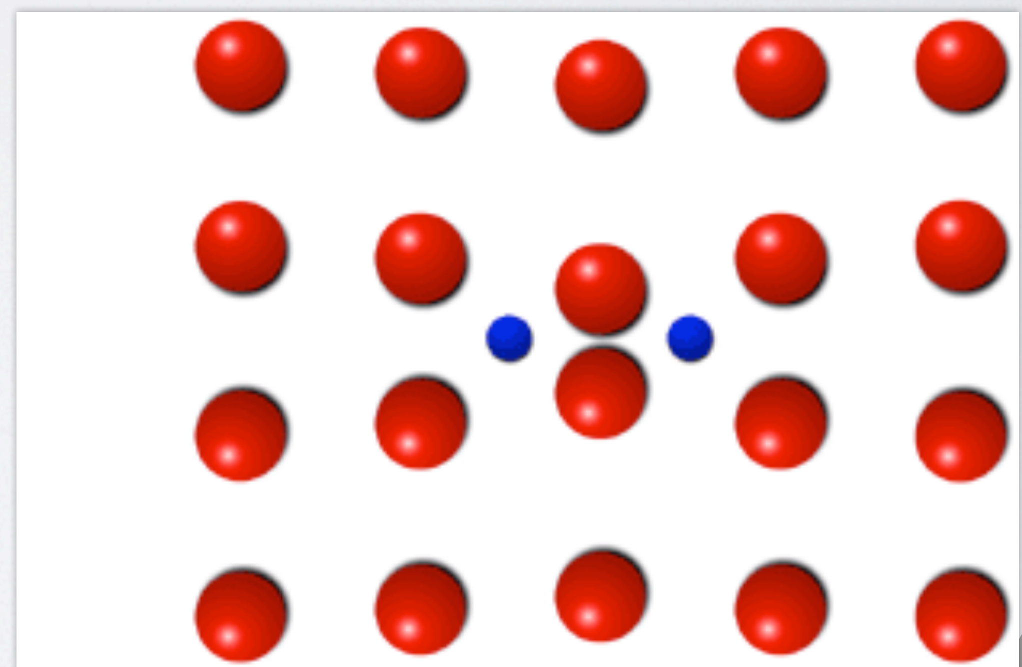
Bosons

Phonos (lattice vibrations) glue fermions into Cooper pairs (boson-like)



Energy gap prevents scattering that leads to resistivity





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CUPRATE HIGH-TEMPERATURE SUPERCONDUCTORS

– Discovery:

- Bednorz & Müller (1986)

– Properties:

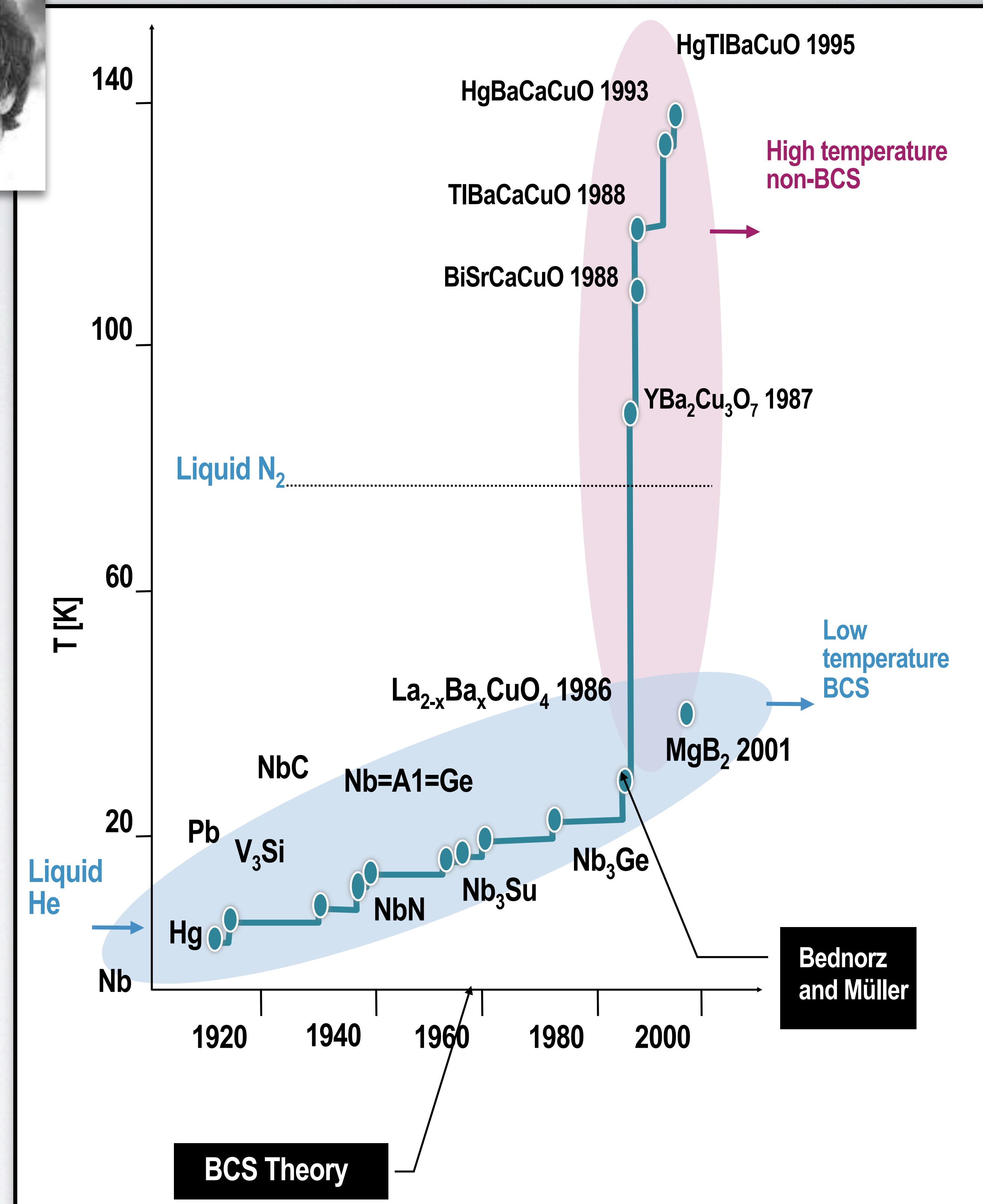
- Insulators or bad metals (conv. superconductors are good metals)
- Many complex phenomena

– Critical temperatures:

- T_c ~ 40K - 150K (well above liquid nitrogen boiling point)

– 25 years of intense research:

- No consensus on a general theory
- No predictive power for T_c in known materials
- No guidance for design of new materials



OUTLINE

- Brief introduction into superconductivity
- Background: 2D Hubbard model & dynamic cluster quantum Monte Carlo approximation (DCA-QMC)
- Gaining insight into superconductivity through computing

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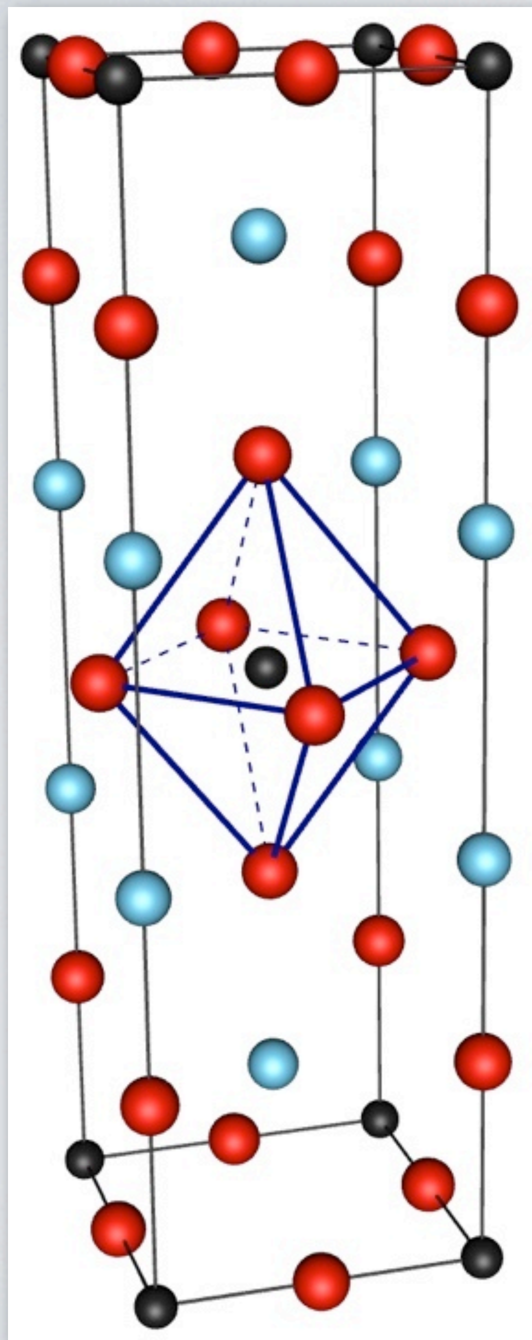
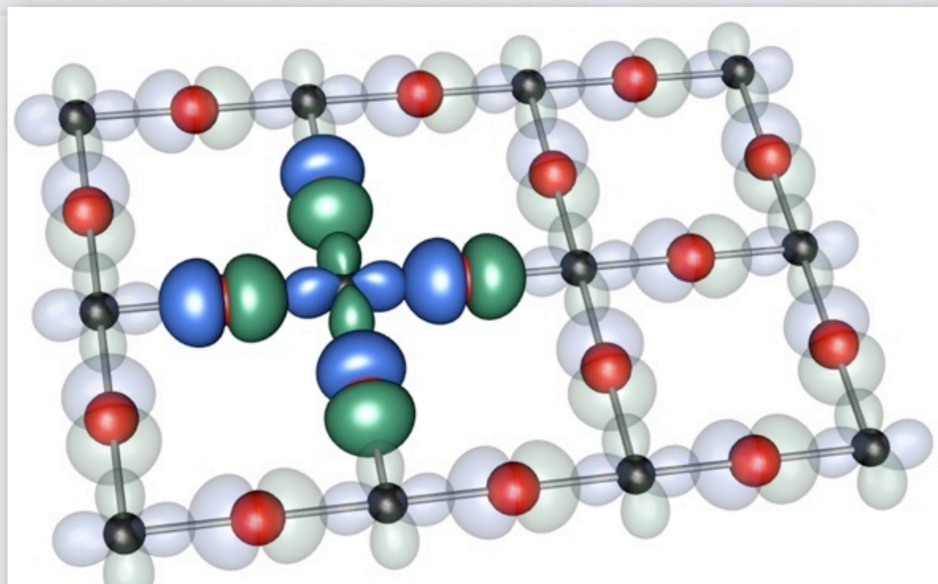
FROM CUPRATE MATERIALS TO THE HUBBARD MODEL

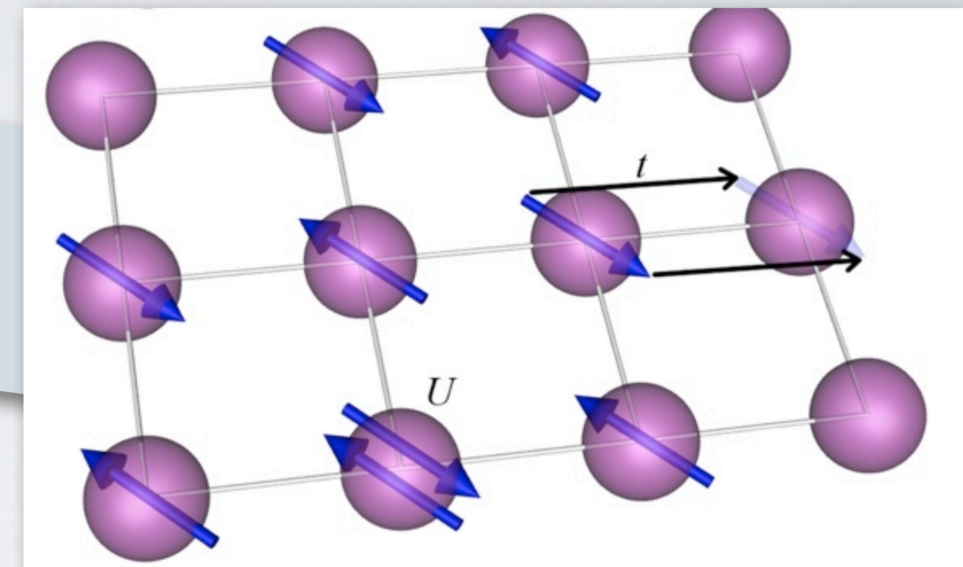
Cuprate structure



CuO-planes



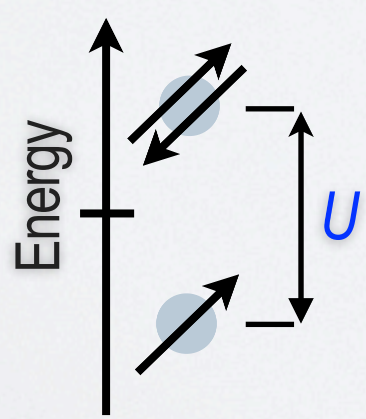
2D Hubbard Model



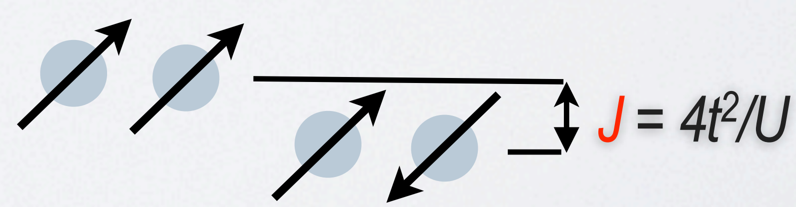
$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Basic properties:

- Moment formation

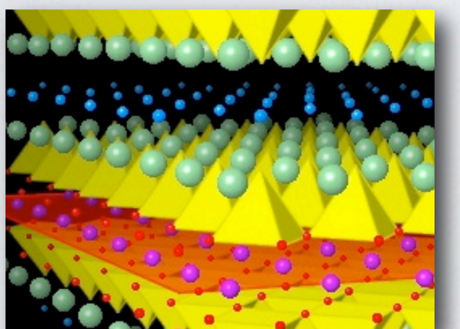


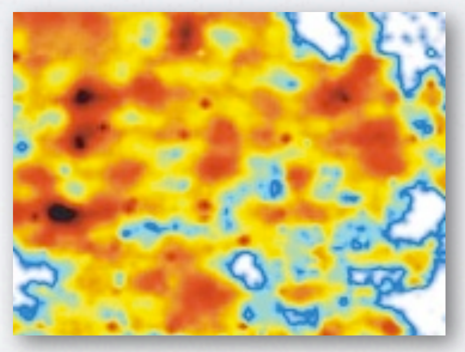
- Antiferromagnetic exchange



A QUANTUM MULTISCALE PROBLEM

Atomic scale		*Nano-scale*		*Macro-scale*
• Strong local correlations • Moment formation	~ nm	• Antiferromagnetic correlations • Cooper pairs • Inhomogeneities	~ μm	• Macroscopic quantum effects





Theory:

Atomistic description →

← Thermodynamics
Continuum description

Complexity ~ 4^N

$N \sim 10^{23}$

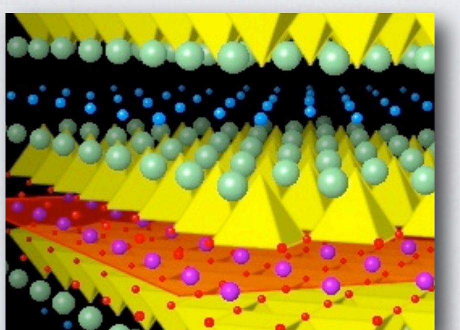
CLUSTER DYNAMIC MEAN FIELD METHODS

Atomic scale ~ nm ***Nano-scale*** ~ μm ***Macro-scale***

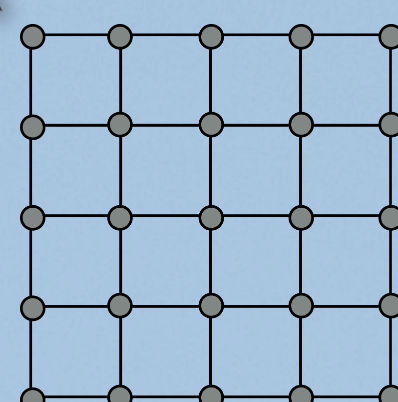
- Strong local correlations
- Moment formation

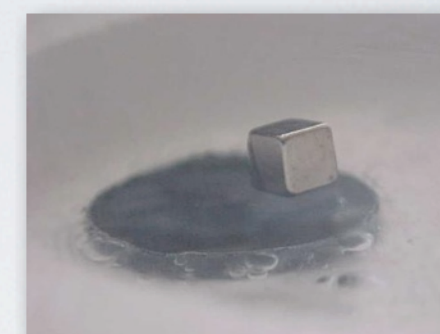
- Antiferromagnetic correlations
- Cooper pairs
- Inhomogeneities

- Macroscopic quantum effects



Explicitly treat correlations within a localized cluster





Treat macroscopic scales within mean-field

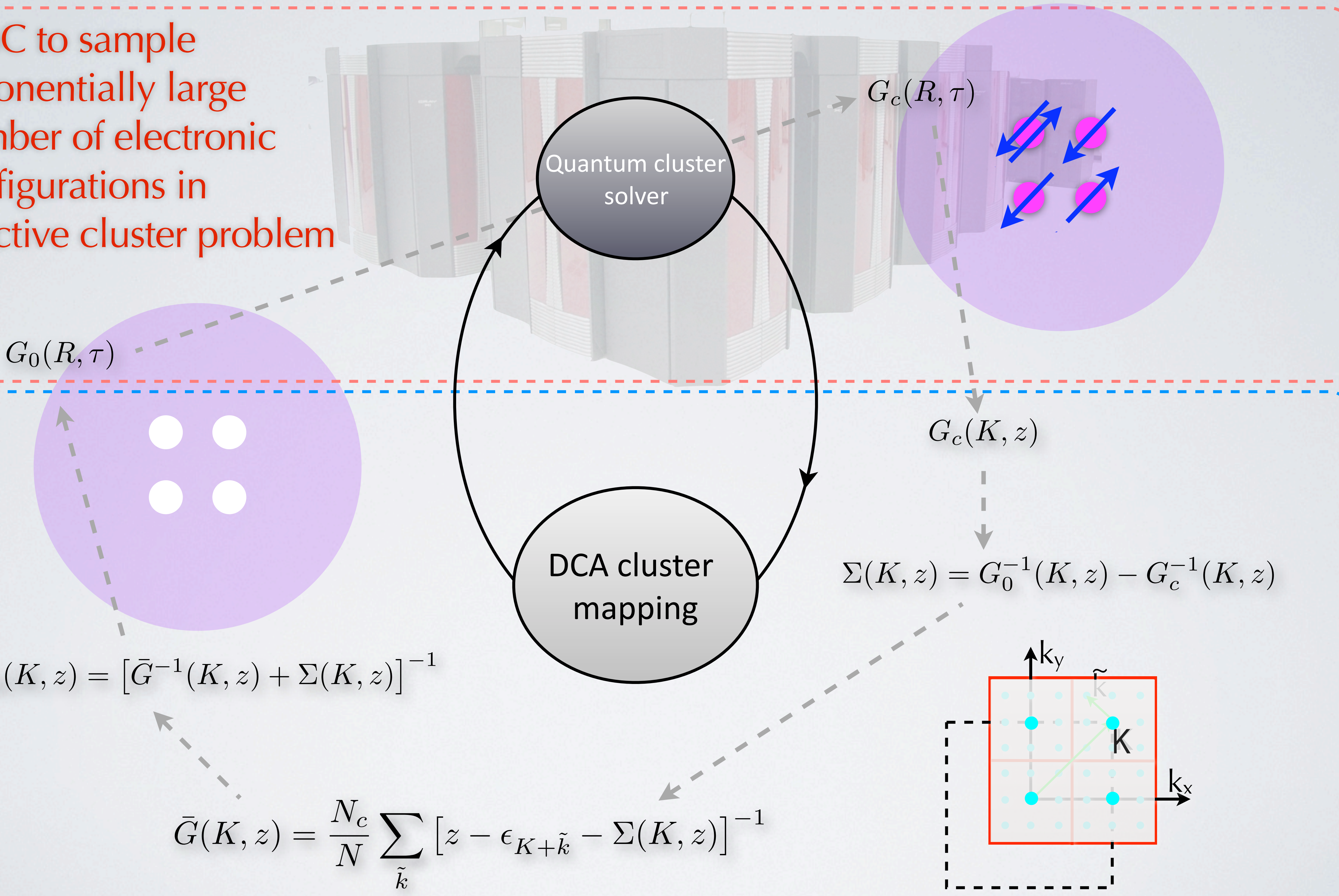
Coherently embed cluster into effective medium

DMFT:
Metzner & Vollhardt, PRL ’89;
Müller-Hartmann, Z. Phys. ’89; Georges *et al.*, RMP ’96

Quantum cluster theories review:
Maier, Jarrell, Pruschke & Hettler, Rev. Mod. Phys. ‘05

DCA: SELFCONSISTENCY

QMC to sample exponentially large number of electronic configurations in effective cluster problem



$$\Sigma(K,z) = G_0^{-1}(K,z) - G_c^{-1}(K,z)$$

$$\bar{G}(K,z) = \frac{N_c}{N} \sum_{\tilde{k}} \left[z - \epsilon_{K+\tilde{k}} - \Sigma(K,z) \right]^{-1}$$

$$G_0(K,z) = \left[\bar{G}^{-1}(K,z) + \Sigma(K,z) \right]^{-1}$$

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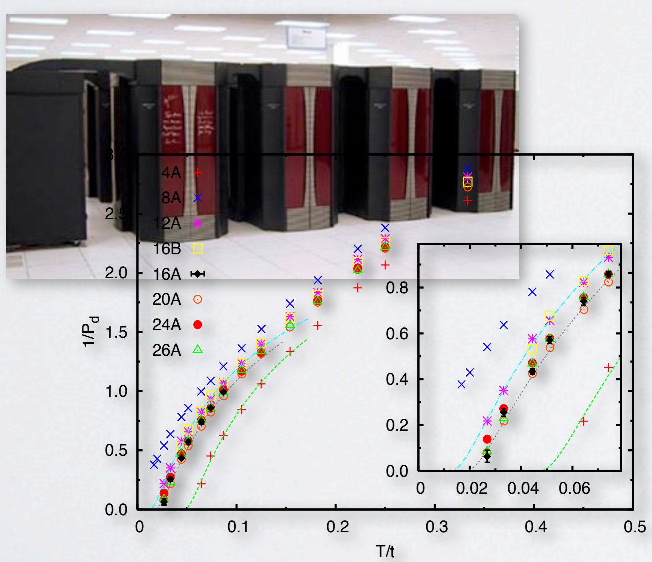
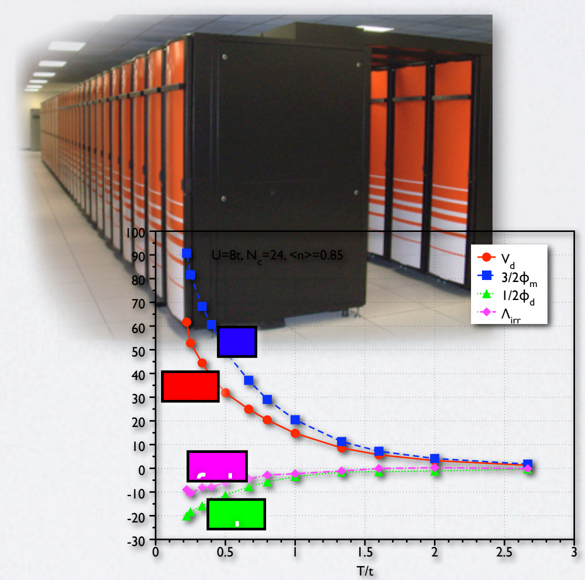
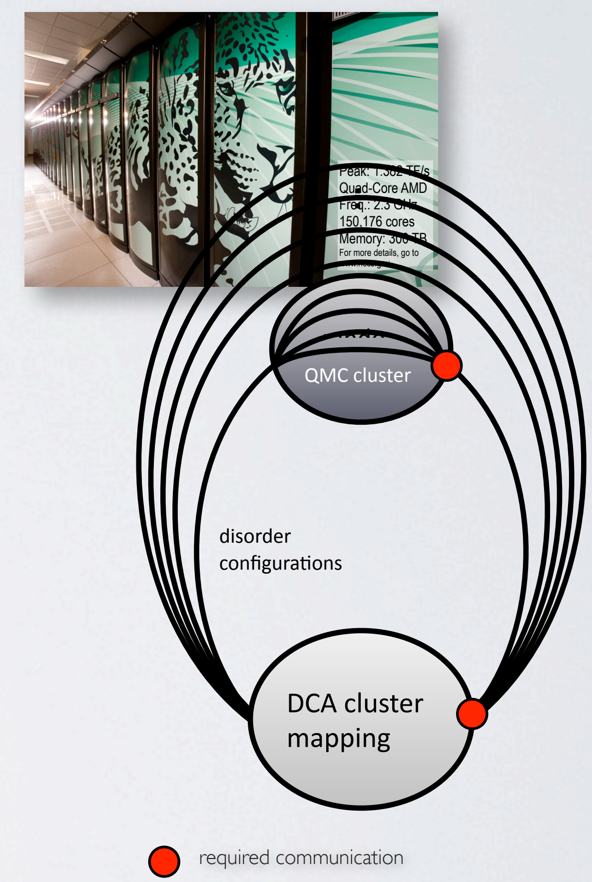
Superconductivity in Hubbard model
on Cray X1(E)



Pairing mechanism in Hubbard model
on Cray XT3/4

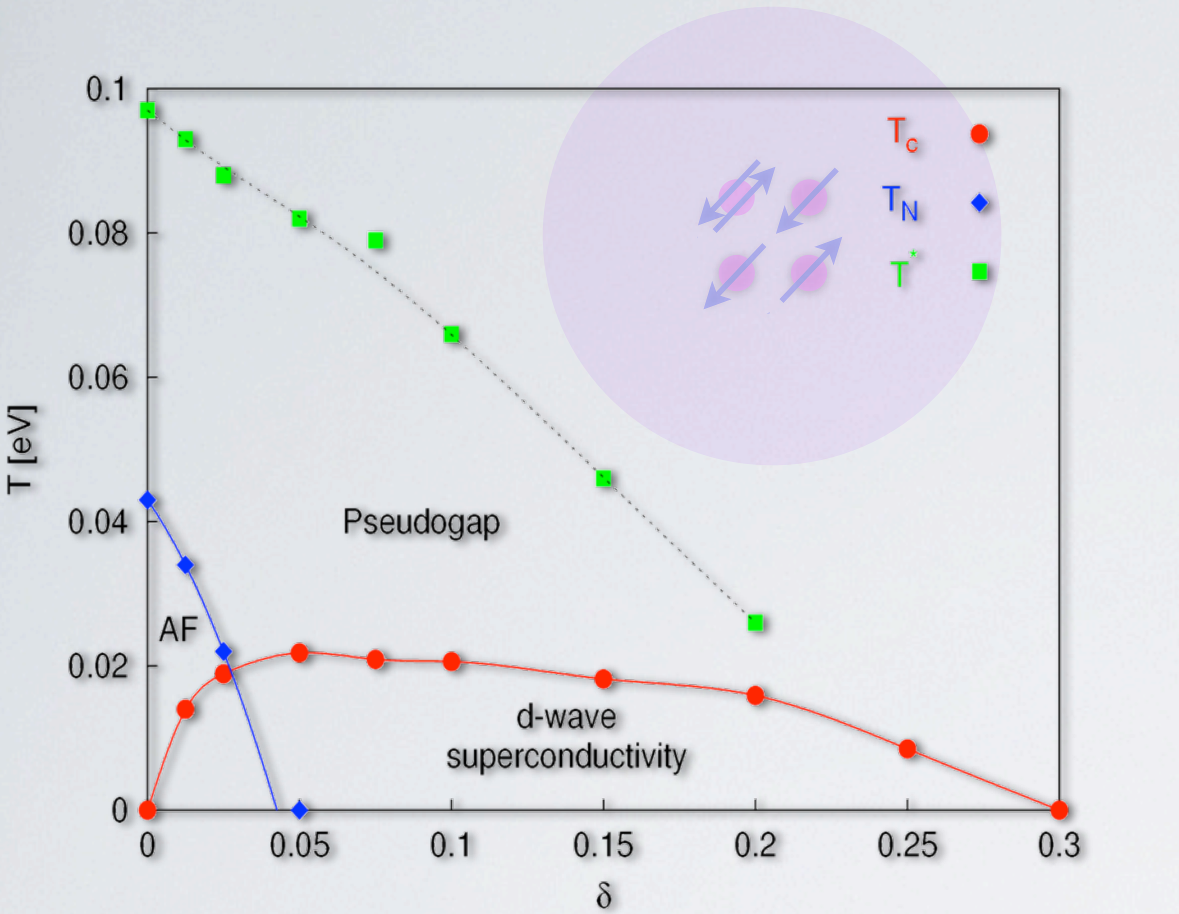


Role of inhomogeneities
on Cray XT5



2005 — 2006-2008 — 2009 -

SUPERCONDUCTIVITY IN 2D HUBBARD MODEL



– *4-site cluster: Antiferromagnetism, pseudogap & superconductivity*

Jarrell, Maier *et al.*, EPL '01

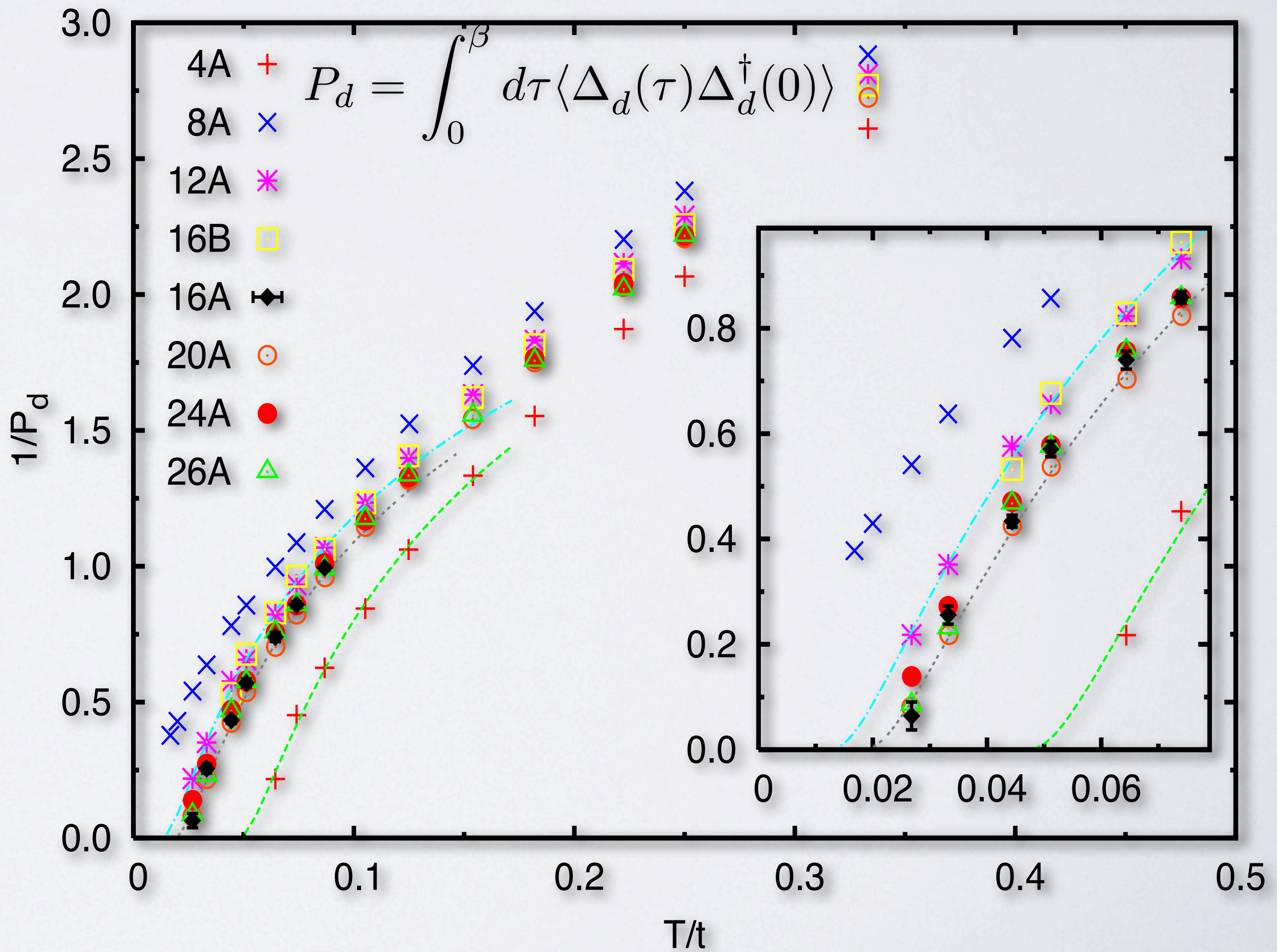
(Simulations on IBM Power4 "Cheetah")

– *2005 on Cray X1(E):*

- Superconducting transition in largest accessible clusters

→ *T_c ~ 0.025t for U=4t, <n>=0.9*

Maier, Jarrell, Schulthess, Kent & White, PRL '05



OUTLINE

Superconductivity in Hubbard model
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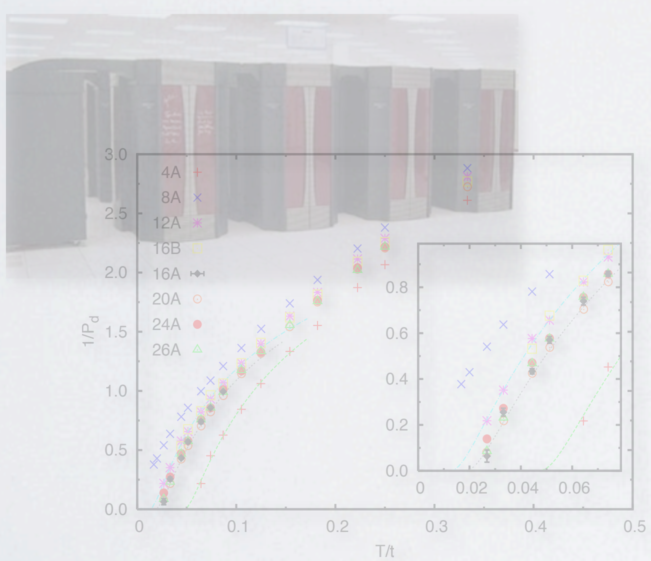

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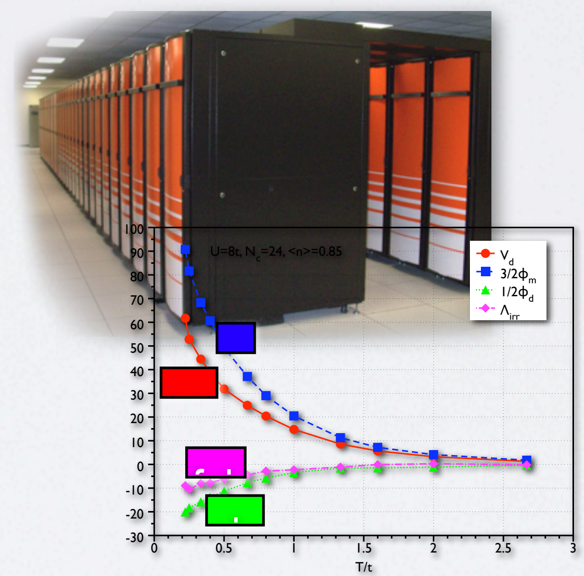

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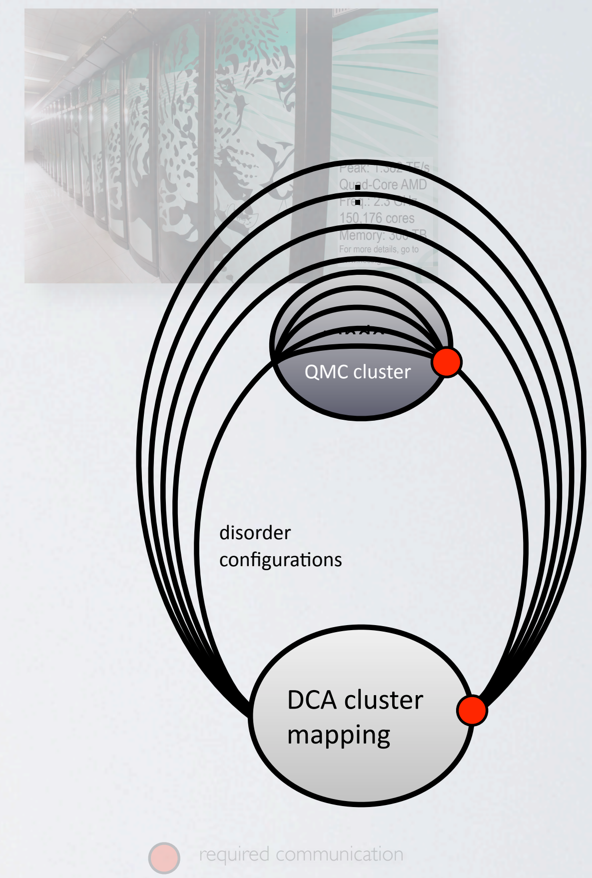
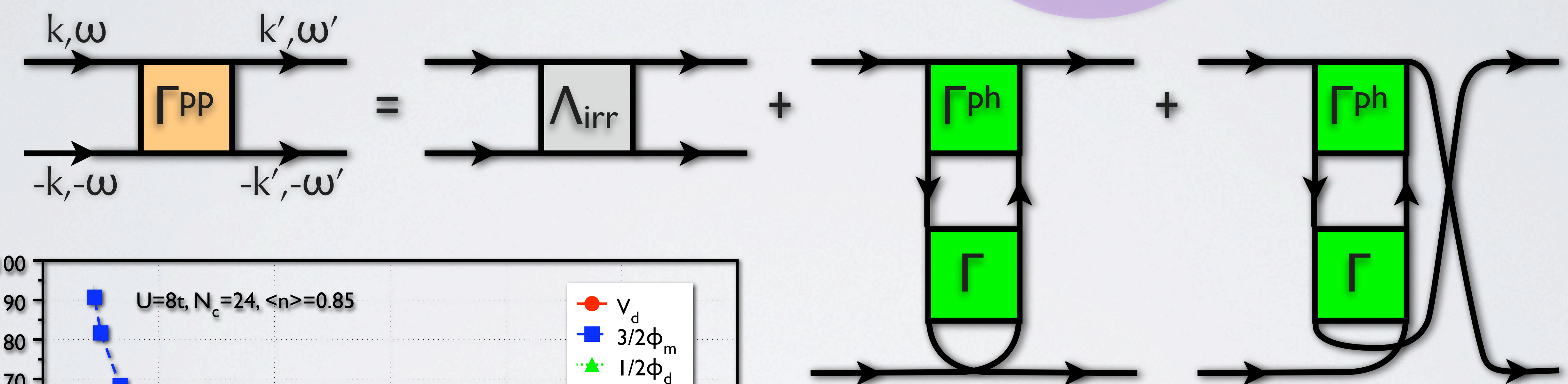


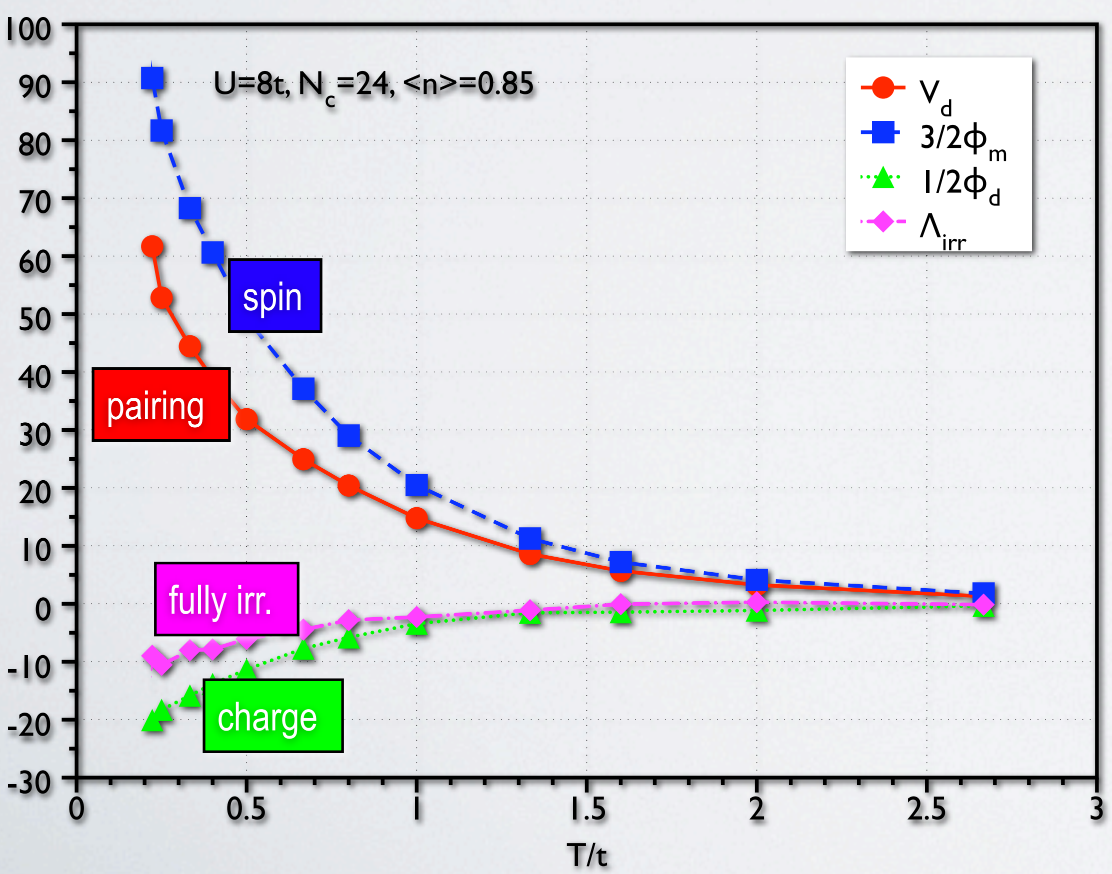
2005 2006-2008 2009 -

PAIRING MECHANISM

– *2006 - 2008 on Cray XT3/4:*

- Study of mechanism responsible for superconductivity in the Hubbard model
- Analyze the particle-particle irreducible vertex function





– *Electron spin is responsible for pairing*

Maier et al., Phys. Rev. Lett. 96, 047005 (2006)
Maier et al., Phys. Rev. B 74, 094513 (2006)

SPIN-MEDIATED PAIRING

Doping a Mott insulator:
Physics dominated by Coulomb energy, kinetic energy is frustrated

Brinkman & Rice, PRB (1970)

SPIN-MEDIATED PAIRING

Doping a Mott insulator:
Physics dominated by Coulomb energy, kinetic energy is frustrated

(Brinkman & Rice, PRB '70)

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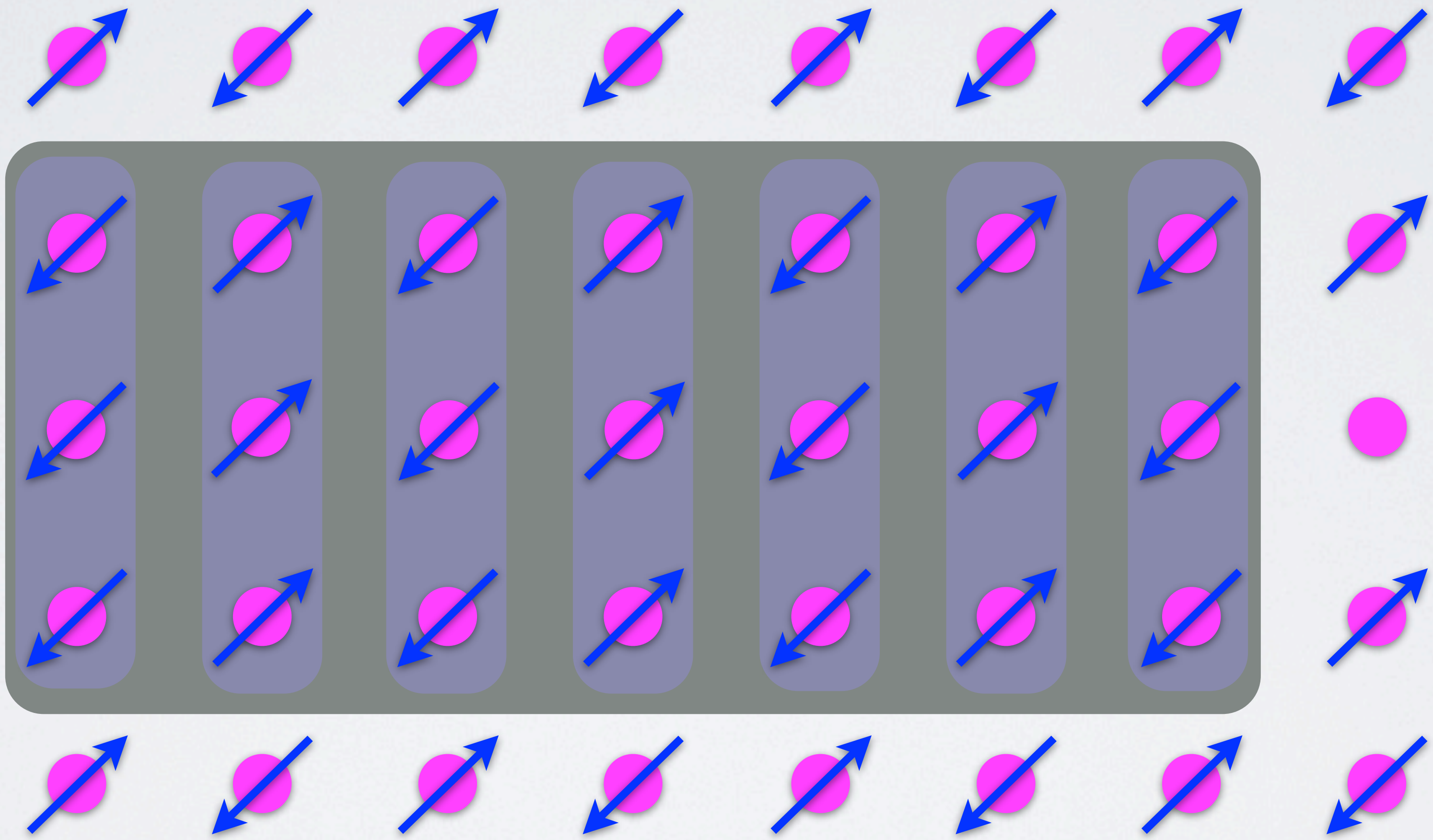

Hole localization due to increase in exchange energy!

RELIEVE KINETIC FRUSTRATION THROUGH PAIRING

Paired hole restores antiferromagnetic background

(Hirsch, PRL ’87; Bonca et al., PRB ‘89; Dagotto et al., PRB ‘90)

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DETAILS OF PAIRING MECHANISM

– *Further characterization of pairing interaction*

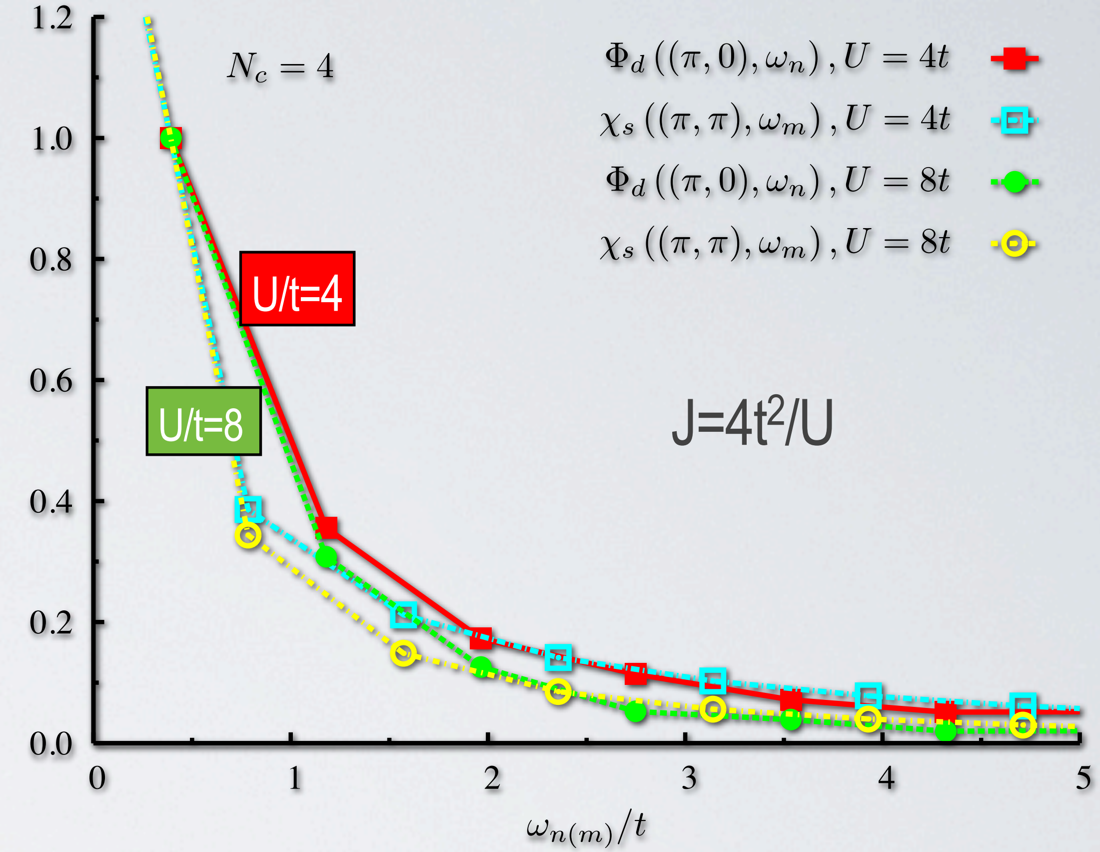
- Dynamics associated with spin-fluctuation spectrum

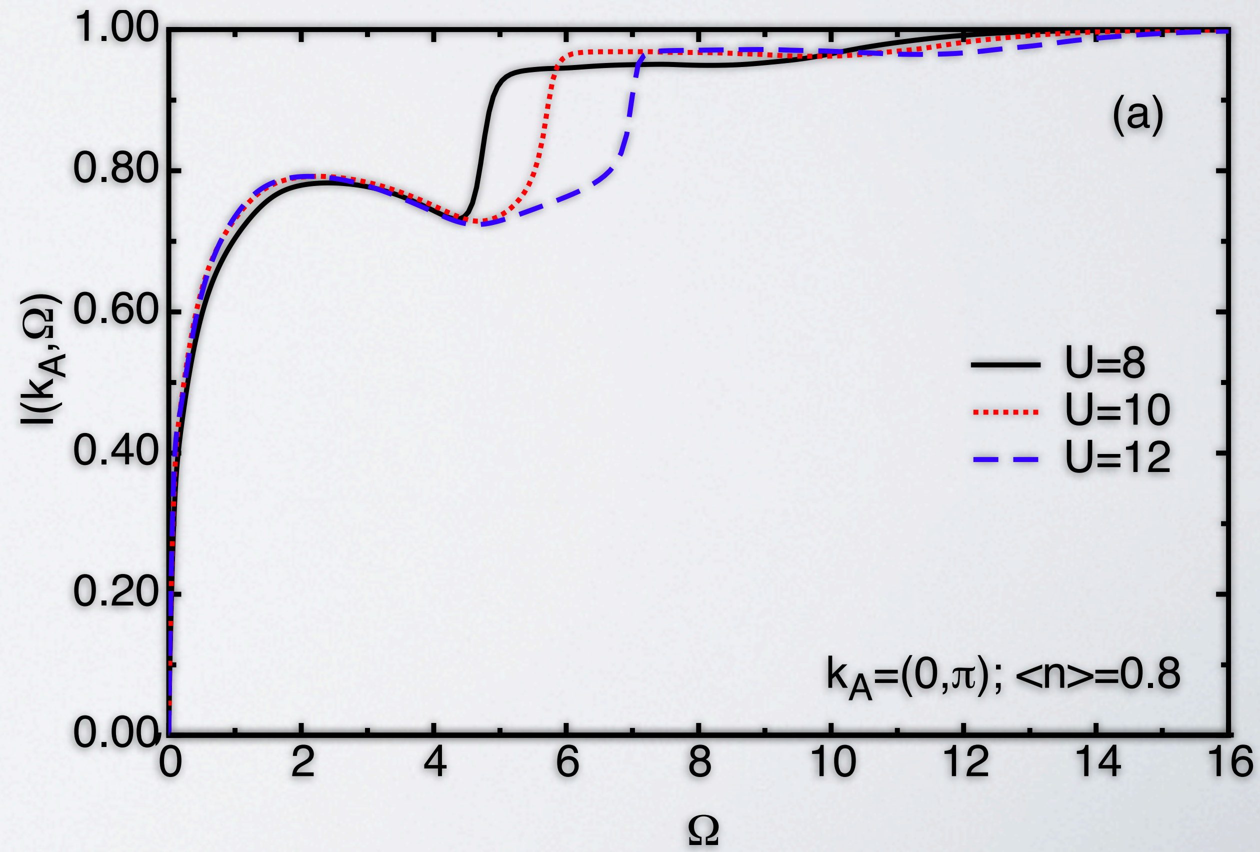
$$\Gamma^{pp}(\omega,\omega') \sim \chi_s(\omega-\omega')$$

- Spin-fluctuation representation reproduces T_c within 30%

$$\Gamma^{pp}(k,k') \approx \frac{3}{2}\bar{U}^2\chi_s(k-k')$$

- Relative importance of spin-fluctuation and instantaneous resonating valence bond mechanism

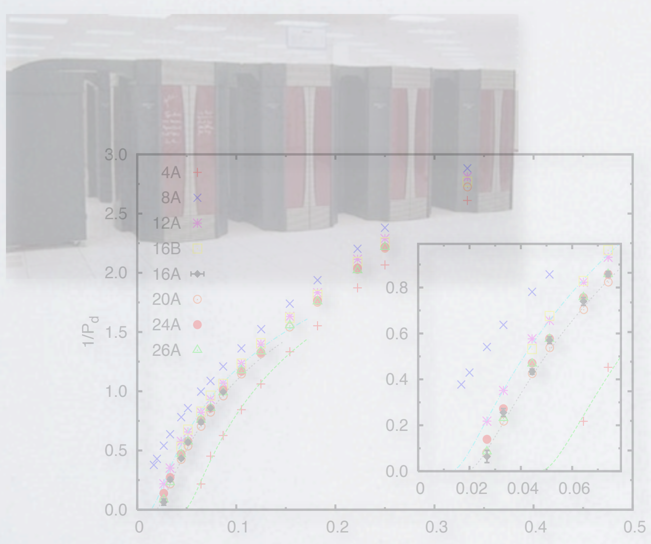




Maier *et al.*, Phys. Rev. B **74**, 094513 (2006),
Maier *et al.*, PRB 75, 134519 (2007), PRB 76, 144516 (2007)
Maier, Poilblanc & Scalapino, PRL ’08

OUTLINE

Superconductivity in Hubbard model
on Cray X1(E)



Pairing mechanism in Hubbard model
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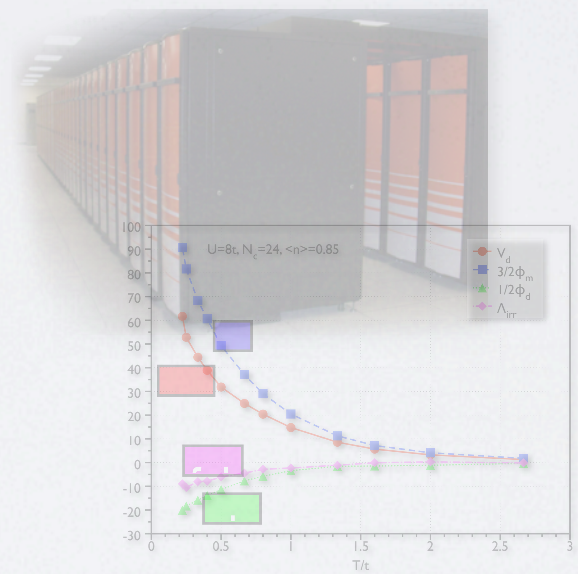

Role of inhomogeneities
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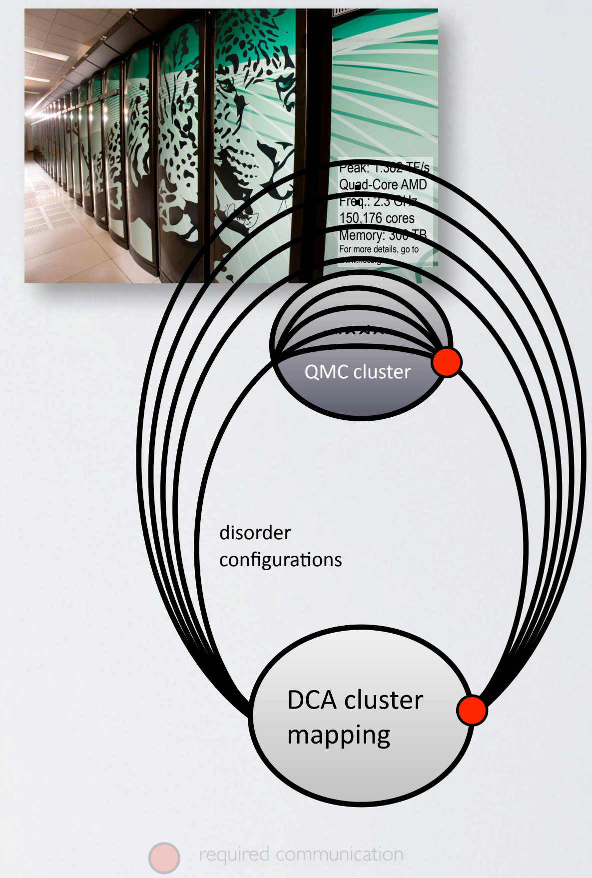


2005

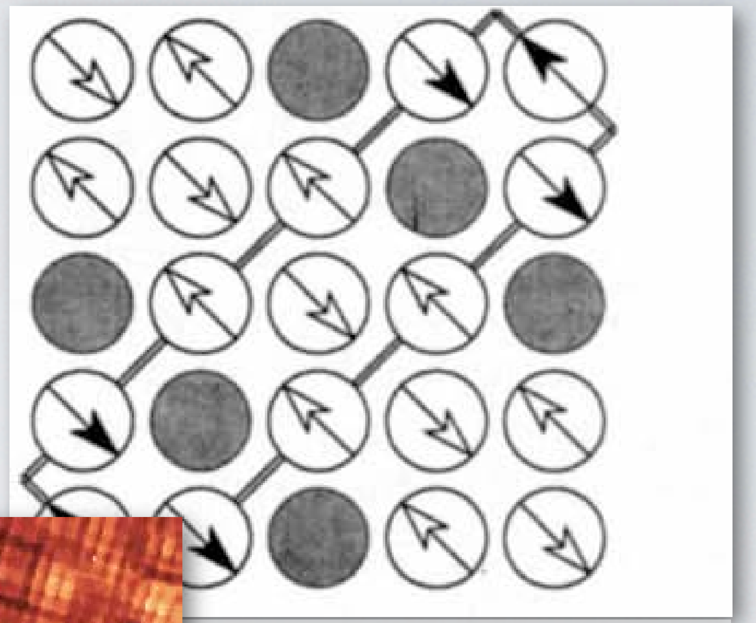
2006-2008

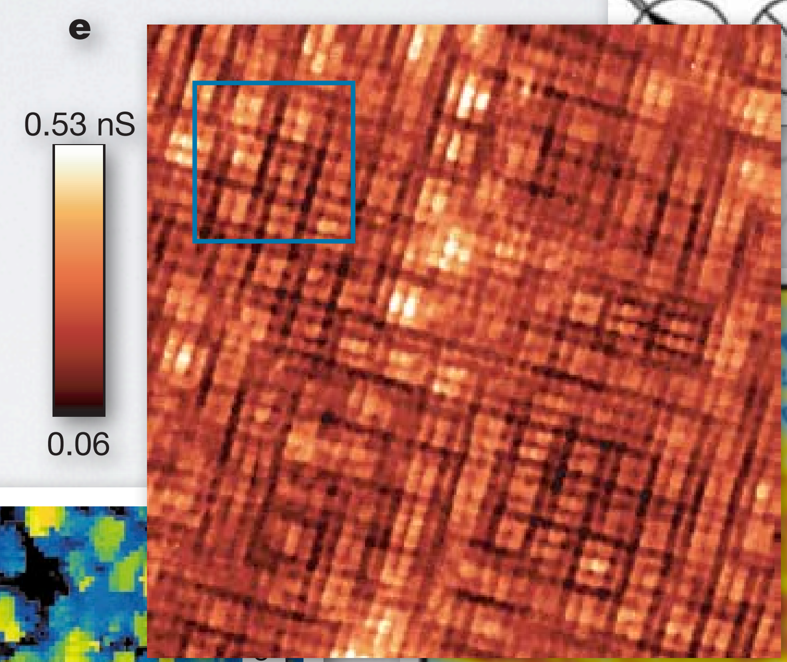
2009 -

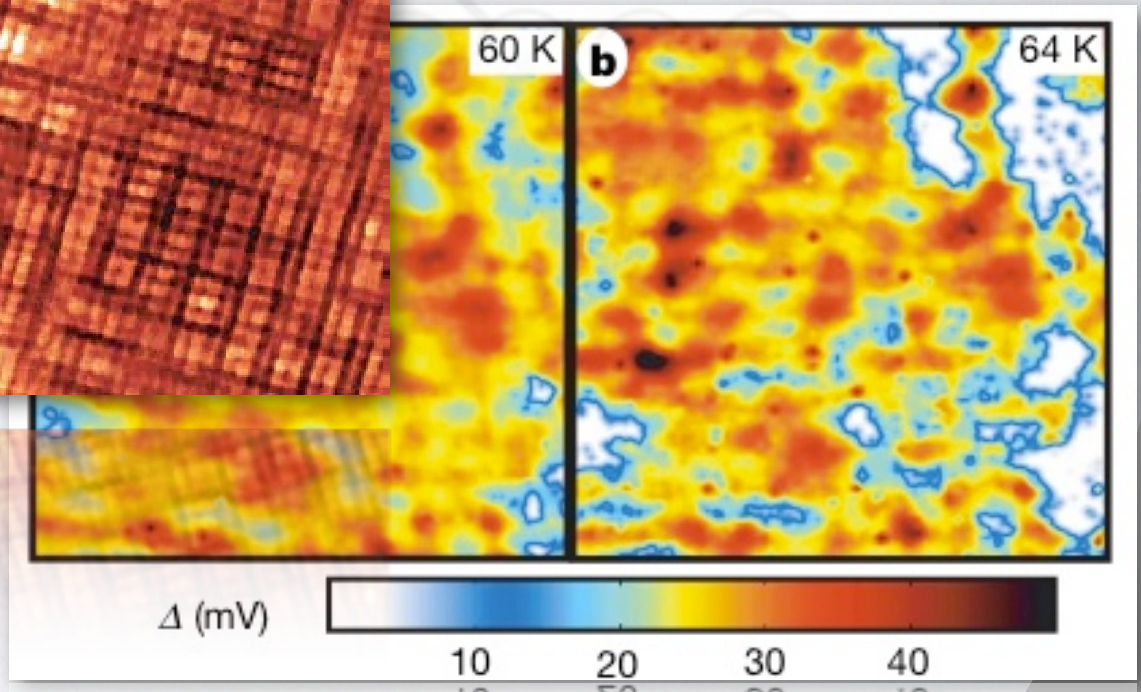
ROLE OF INHOMOGENEITY?

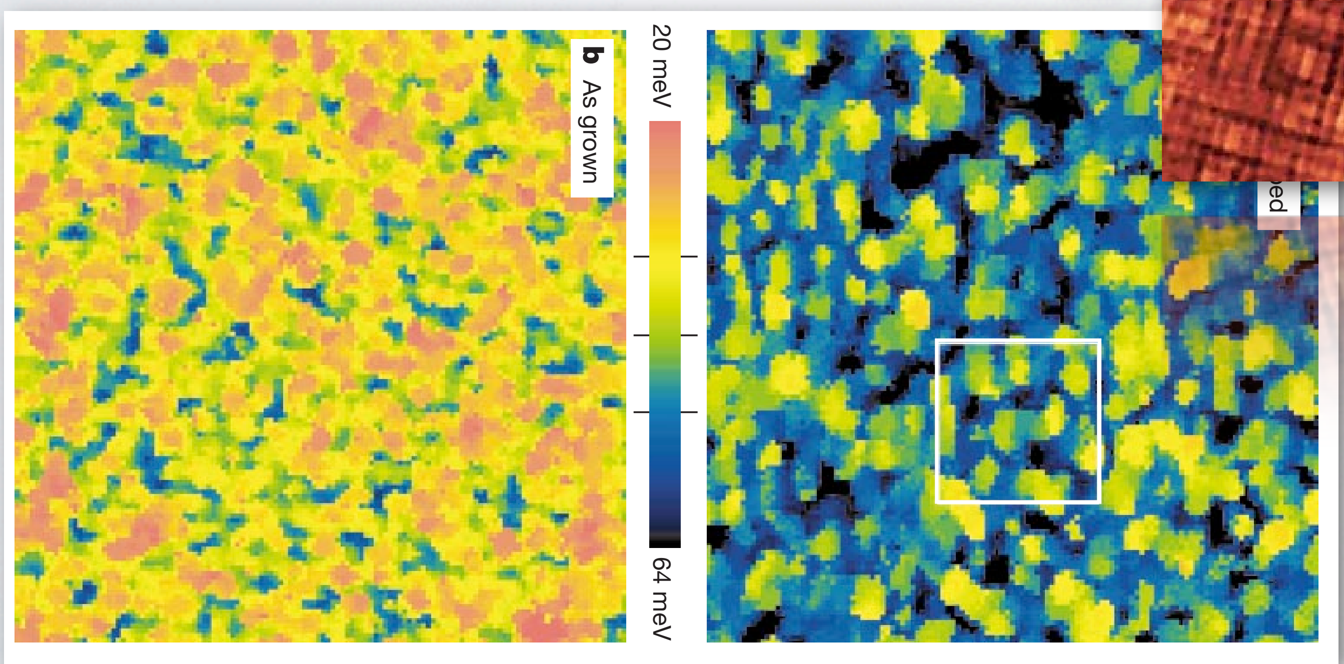
– *Nanoscale electronic inhomogeneity*

- Stripes
  (Tranquada *et al.* '95, Mook *et al.*, '00)
- Checkerboard charge modulations
  (Hanaguri, Davis *et al.*, '04)
- Random SC gap modulations
  (Lang, Davis *et al.*, '02,
  Gomes, Yazdani *et al.*, '07)





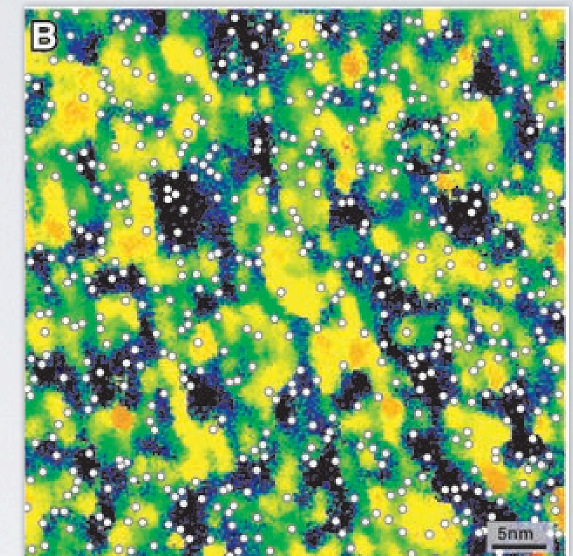




INTRODUCING RANDOM DISORDER INTO DCA

– Hubbard model with diagonal disorder:

$$H^{(\nu)} = -t \sum_{<ij>,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U_i^{(\nu)} n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} V_i^{(\nu)} n_{i\sigma}$$



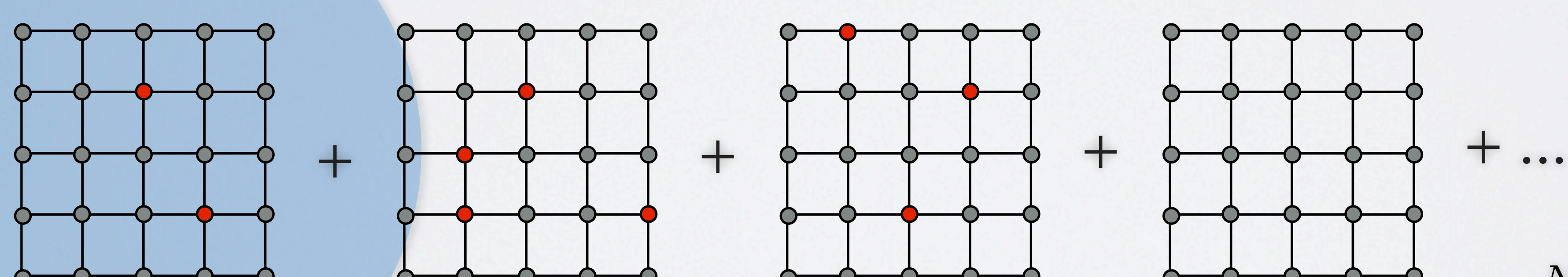
McElroy et al., Science **309** 1048 (2005)

$$V_i \in \{V, 0\}$$

$$P(\{V_i\}) = \prod_{i=1}^{N_c} P_i(V_i) \qquad P_i(V_i) = \begin{Bmatrix} x & V_i = V \\ (1-x) & V_i = 0 \end{Bmatrix}$$

– Disorder-average cluster Green's function

$$N_c = 16 \rightarrow N_d = 2^{16}$$



$$G_c(X_i - X_j, z) = \frac{1}{N_c} \sum_{\nu=1}^{N_d} G_c^\nu(X_i, X_j, z)$$

➠ *Peta- or exascale problem!*

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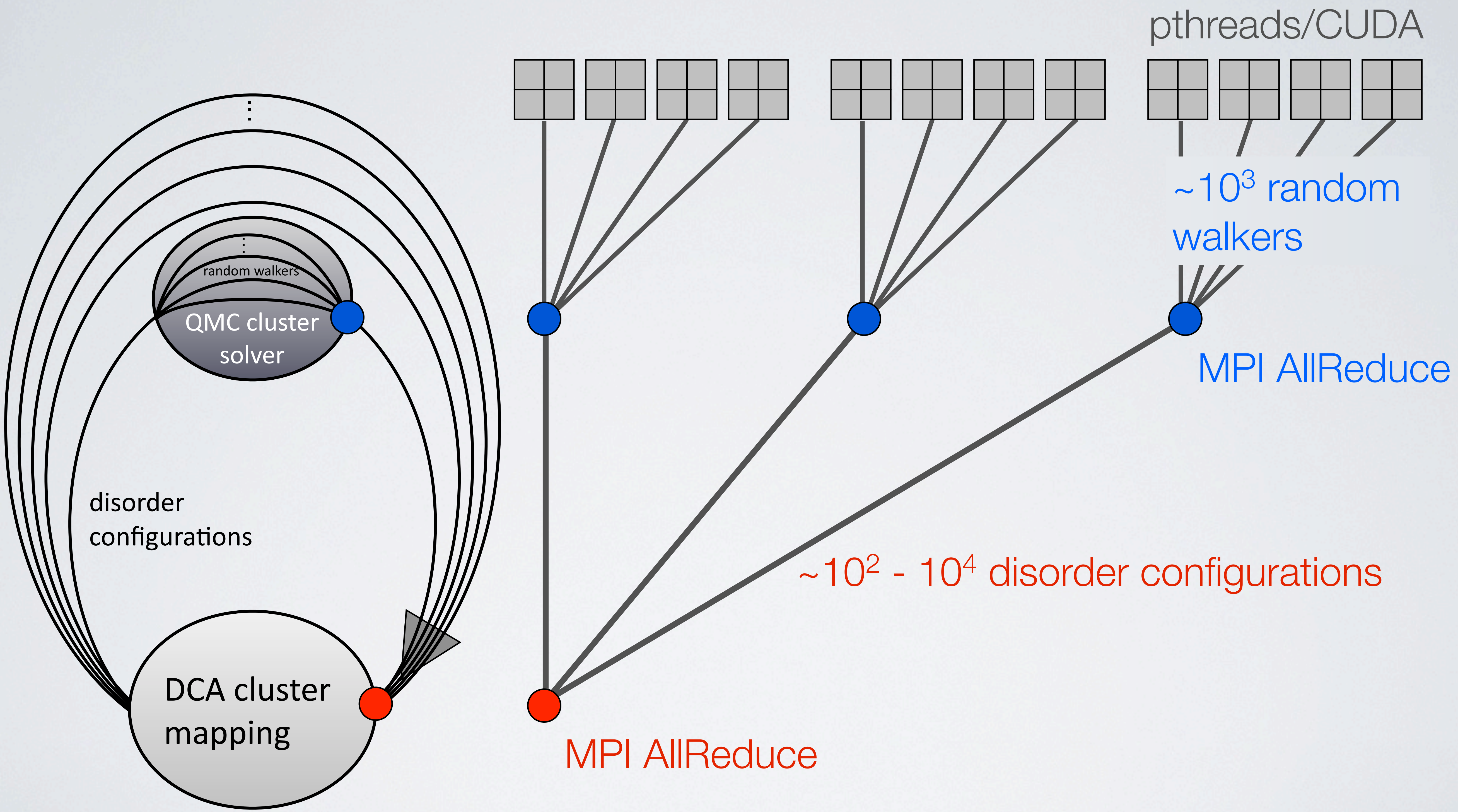
DCA++ CODE: EFFICIENCY



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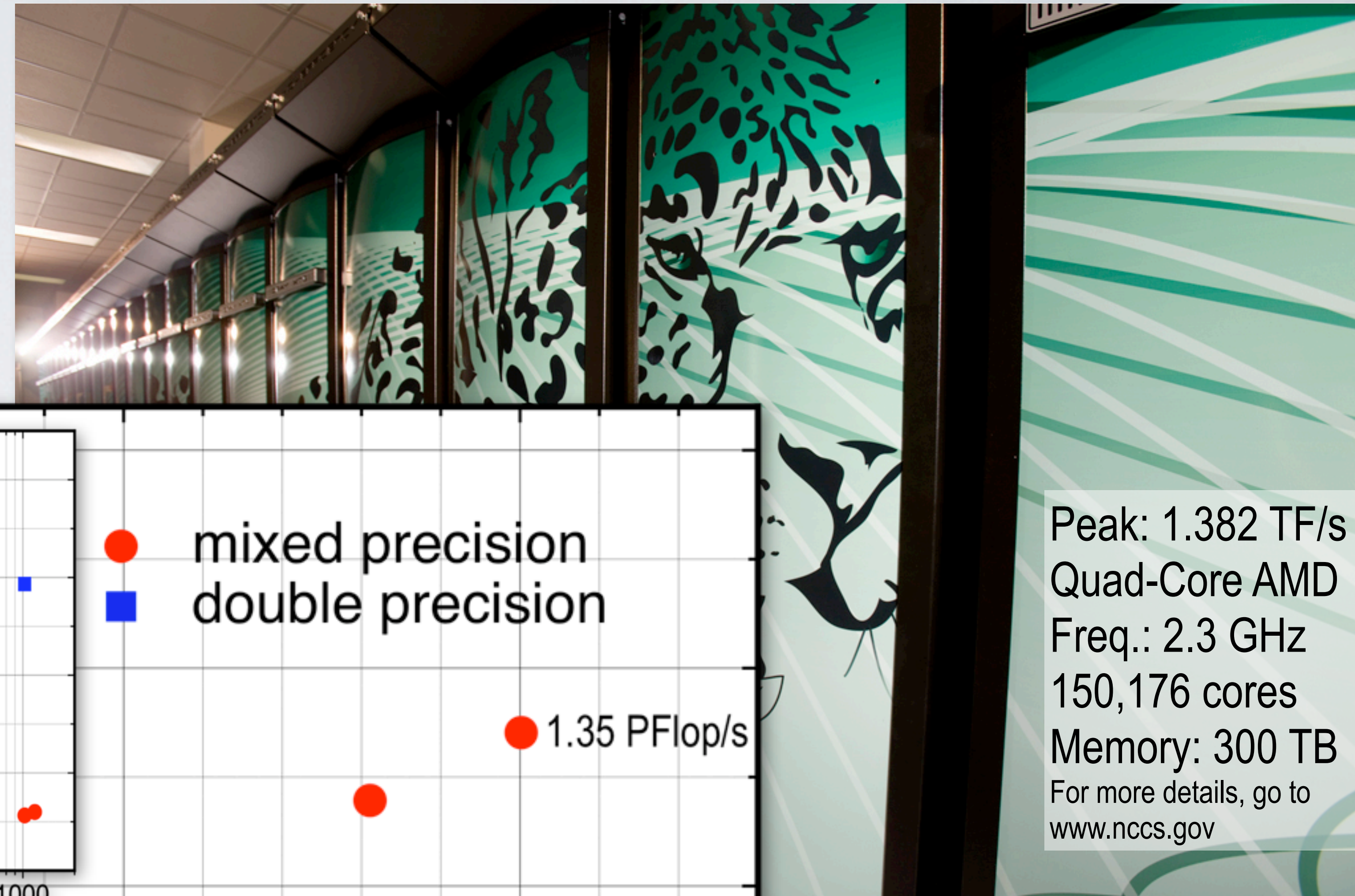
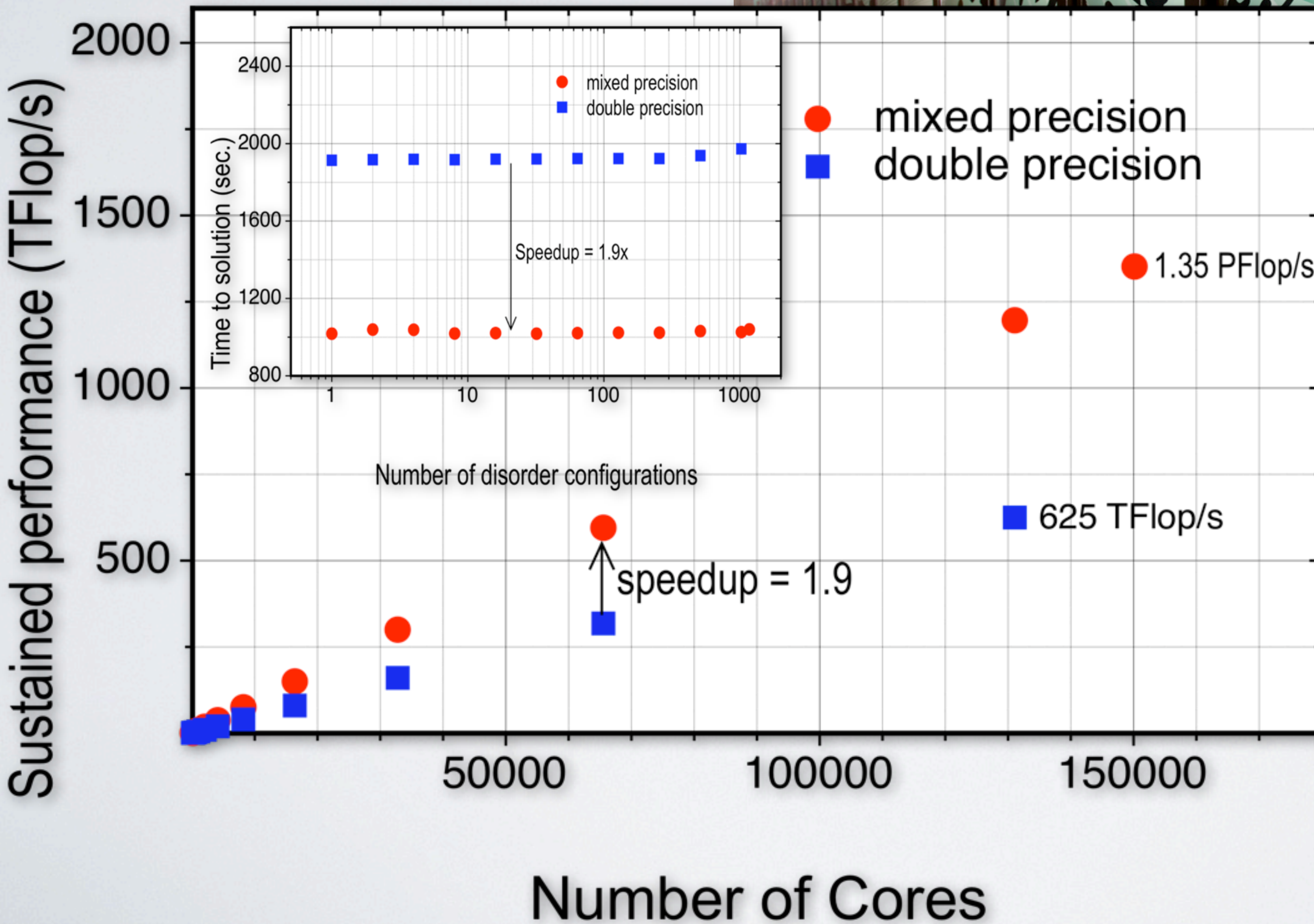
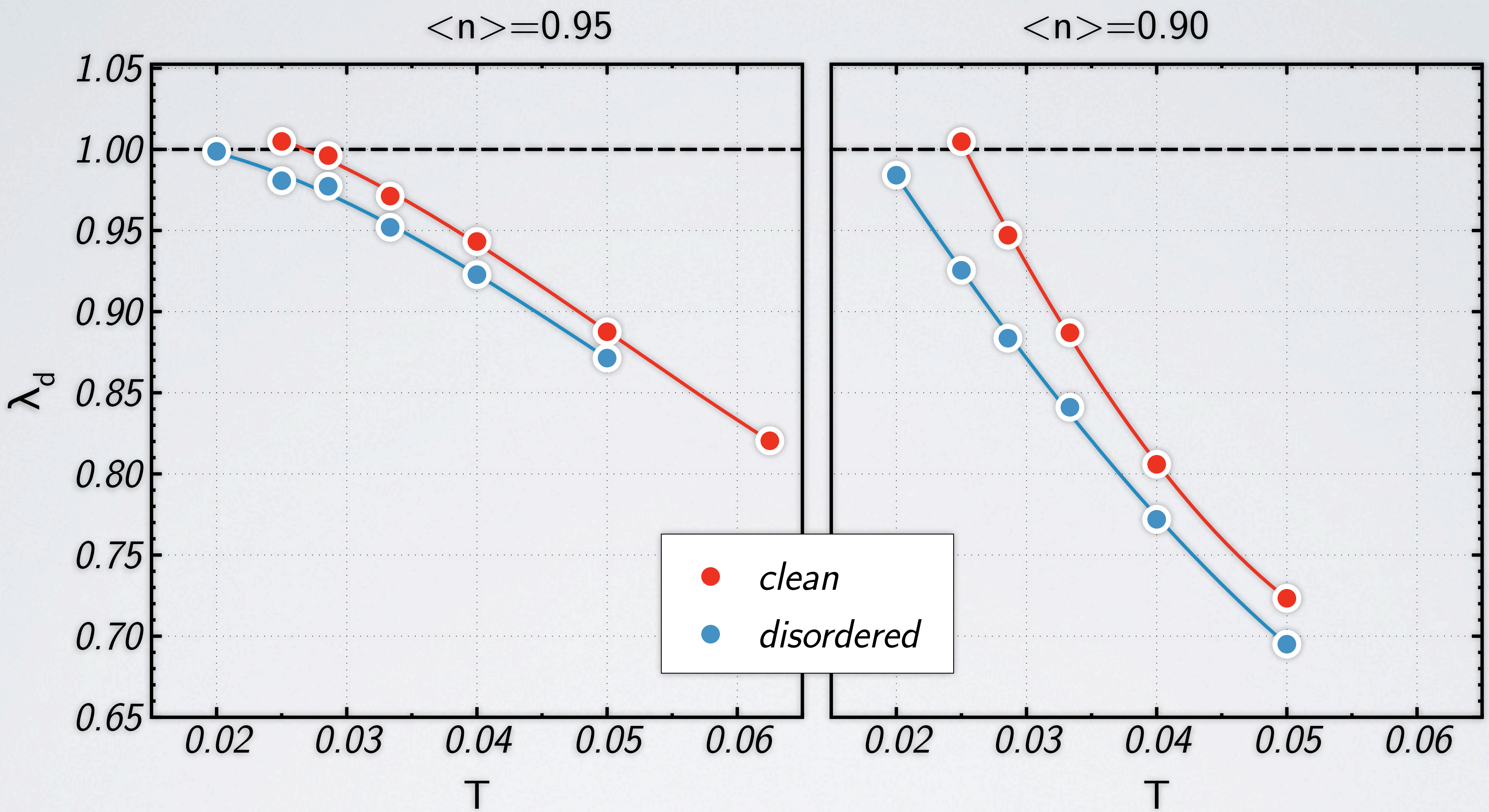




RANDOM DISORDER SUPPRESSES SC

Leading d-wave eigenvalue; U=4t, N_c=16A



λ_d leading eigenvalue of $\Gamma^{pp} P_d^0$ $$P_d = \frac{P_d^0}{1 - \Gamma^{pp} P_d^0}$$

– Random disorder reduces T_c, but only by about 20%

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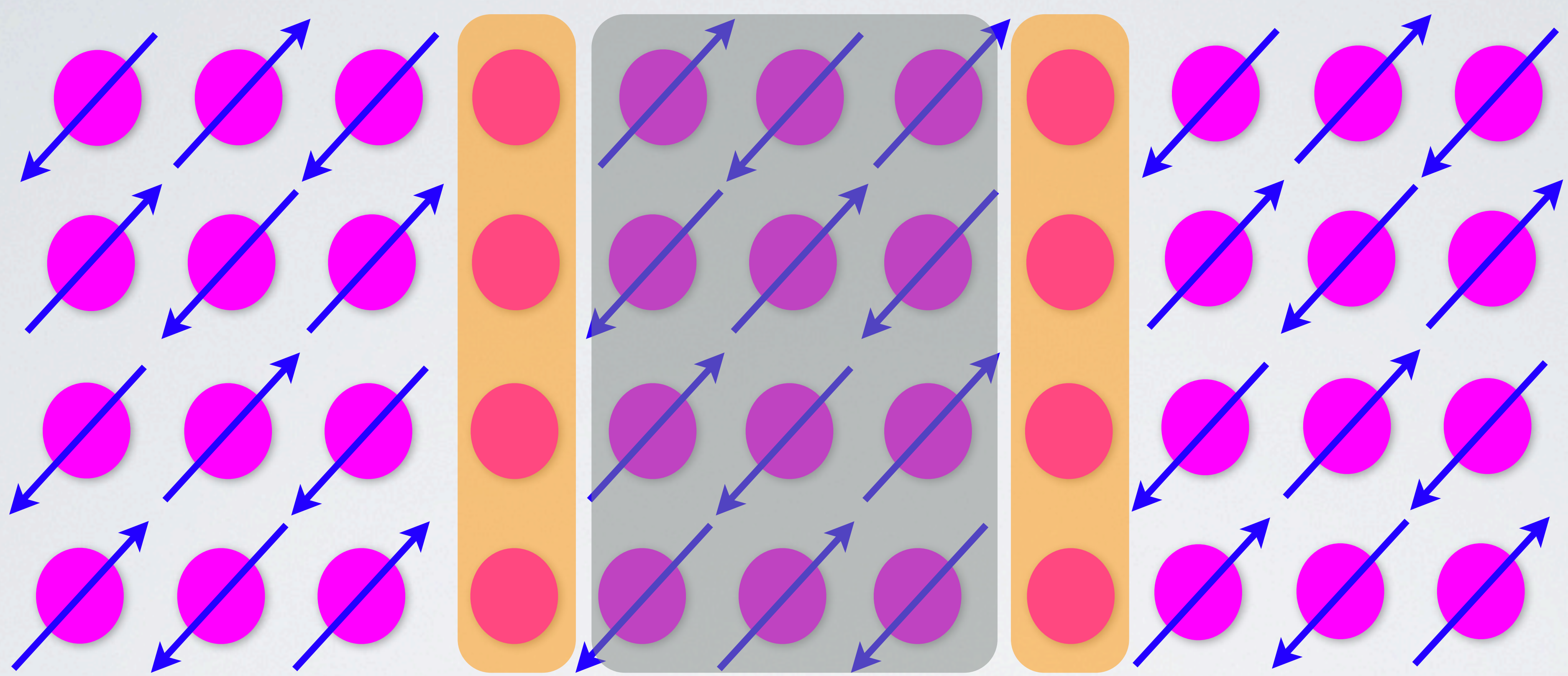
STRIPED STATE IN 1/8 DOPED LBCO

Good hole mobility

Tranquada et al., Nature 375, 561(1995)



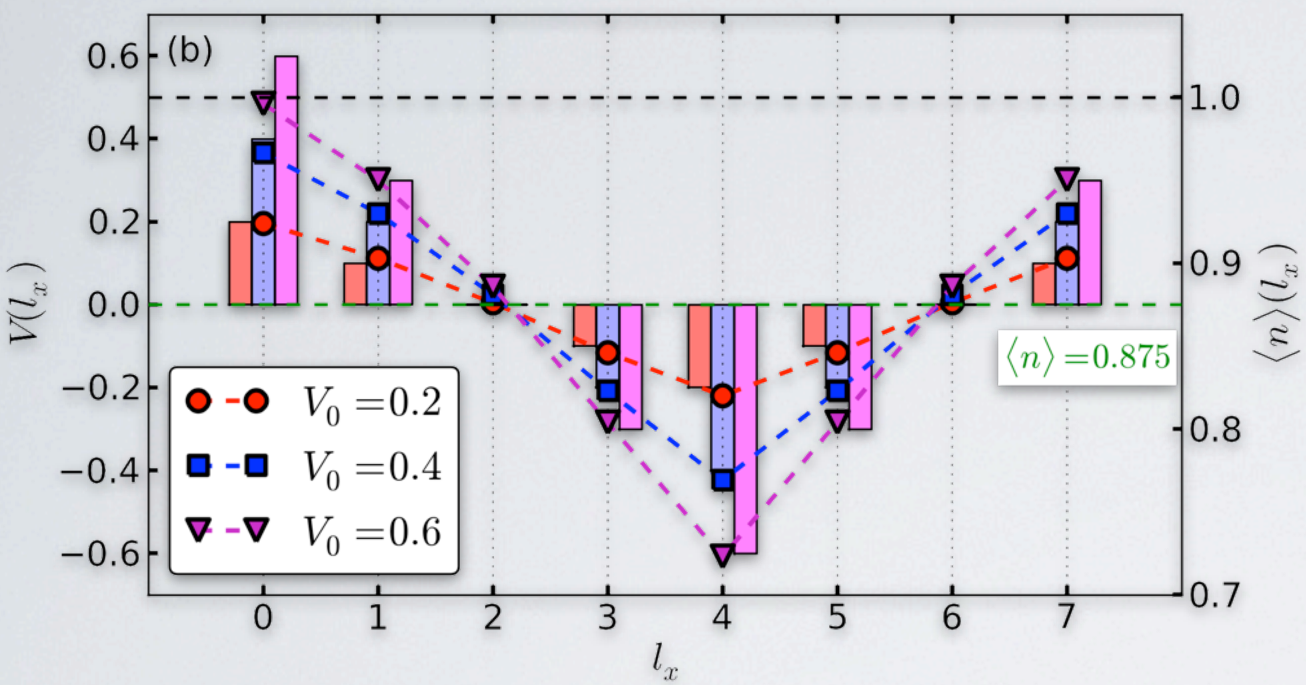
Strong pairing region

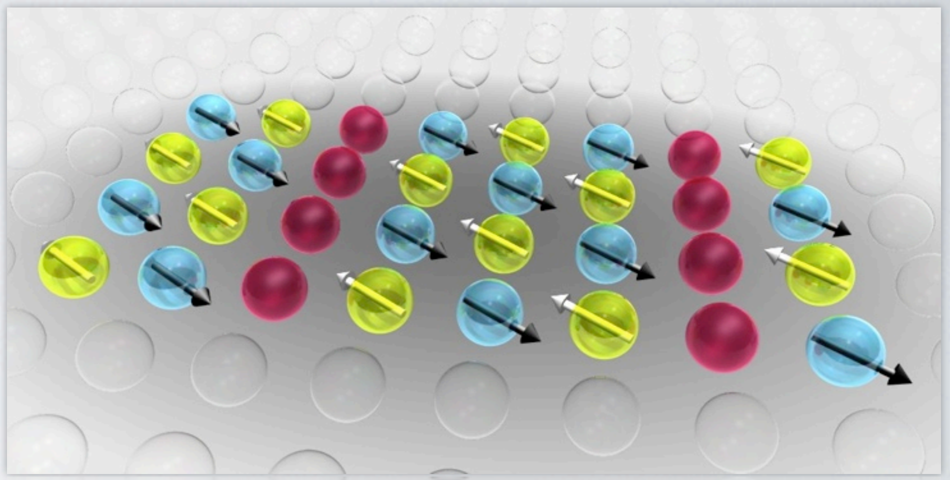
– Experimental evidence for optimization of SC in striped state

Valla et al., Science 314, 1914 (2006)
Li *et al.*, PRL 99, 067001 (2007)

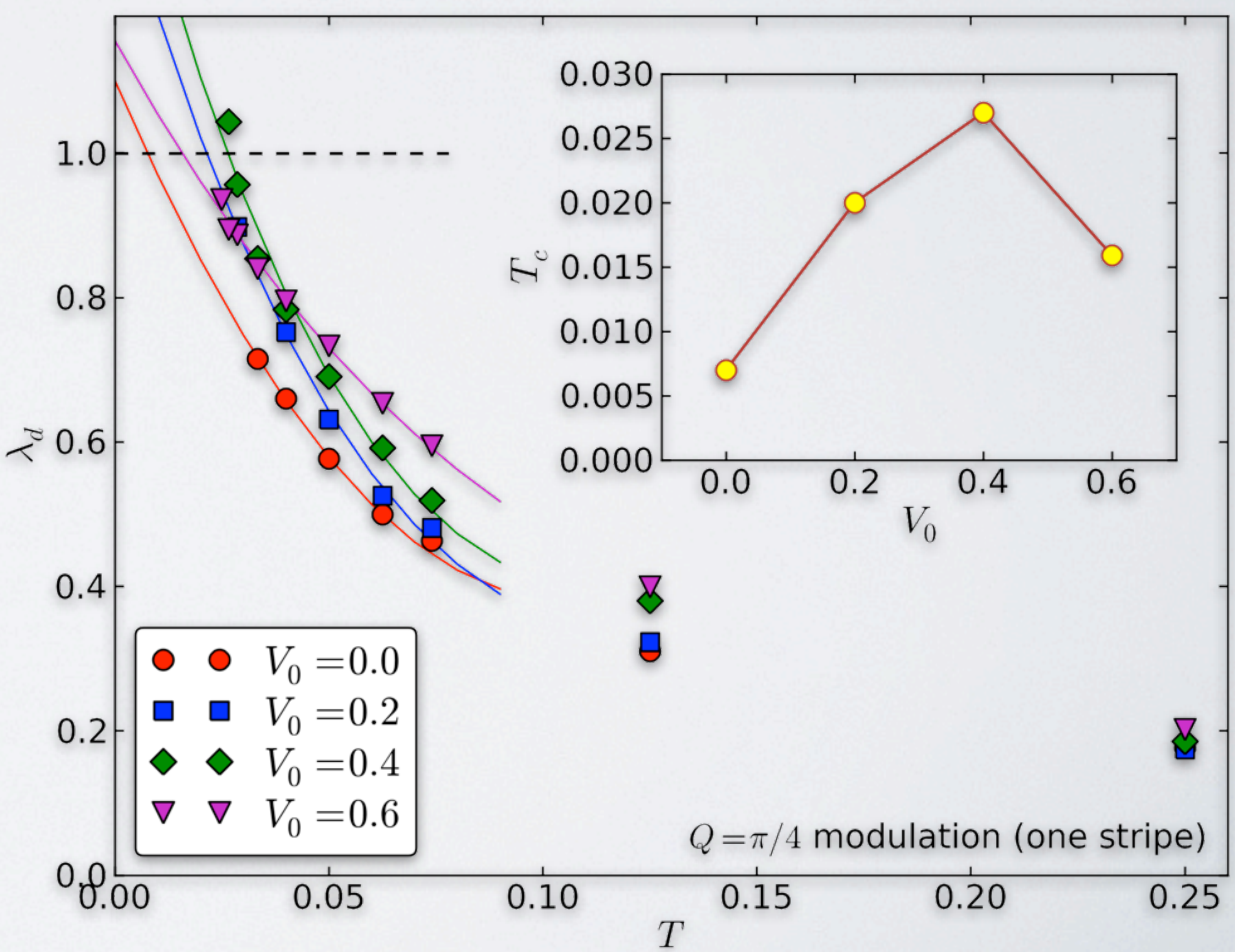
STRIPES OPTIMIZE T_c

Imposed potential and charge modulation





Leading eigenvalue of BSE in pp-channel



– ***Stripes can significantly enhance superconductivity***

Maier et al., PRL **104**, 247001 (2010)

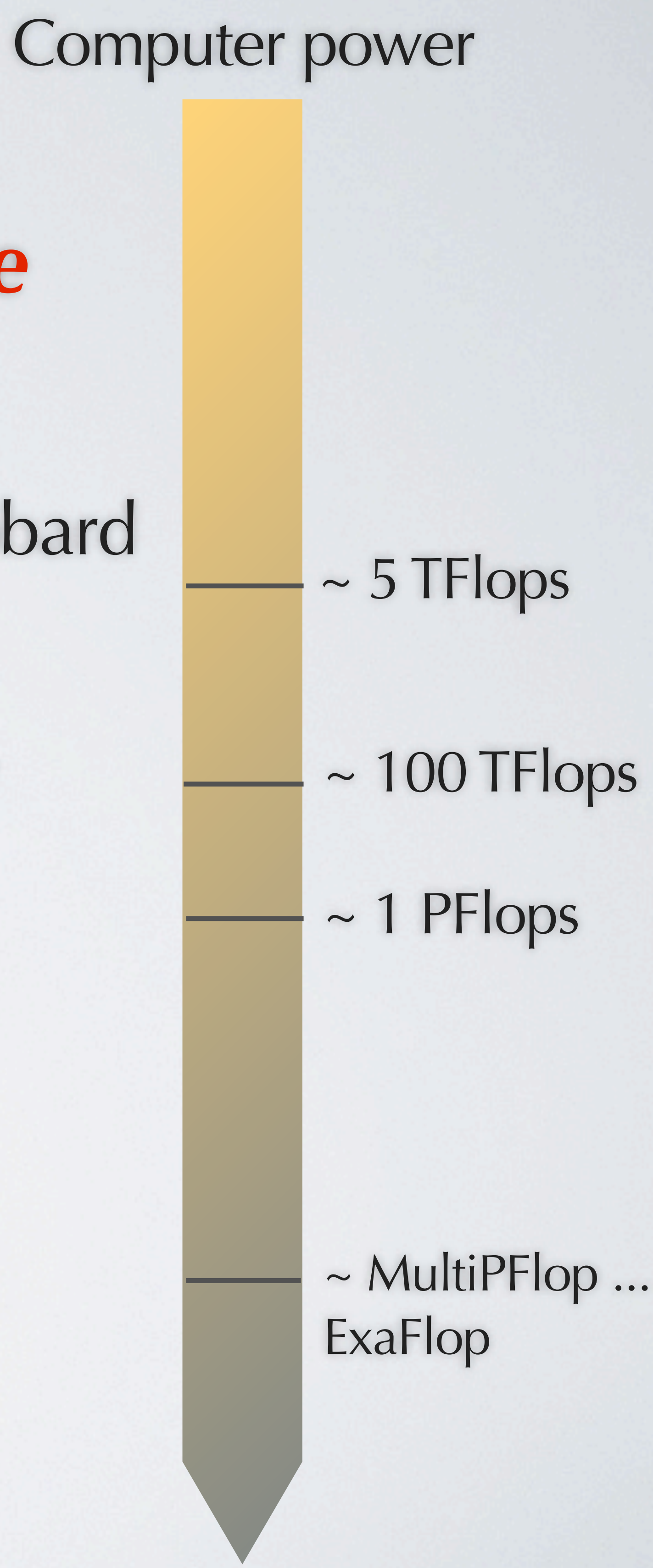
SUMMARY

– ***Advances in algorithms and computers have increased our ability to answer more and more complex questions***

- Evidence for superconductivity in coarse-grained Hubbard model of cuprate high-temperature superconductors
- Mechanism for pairing that leads to superconductivity
- Effect of nanoscale electronic inhomogeneities

– ***Future?***

- Predictive materials-specific simulations of correlated electron systems



EXASCALE: MATERIAL SPECIFICITY

– ***Why is there a factor 5 difference in the transition temperature between different cuprates?***

- Multi-orbital Hubbard models
- Energy-dependent Coulomb interactions
- Parameters systematically determined from DFT