New high-performance-computing capabilities bring decisive change in understanding high-temperature superconductivity

Despite years of active research, the understanding of superconductivity in the high-temperature "cuprate" superconductors remains one of the most important outstanding problems in materials science. A complete theoretical understanding of cuprate superconductors could lead to the ability to design and synthesize room-temperature superconductors, which would have tremendous technological implications.

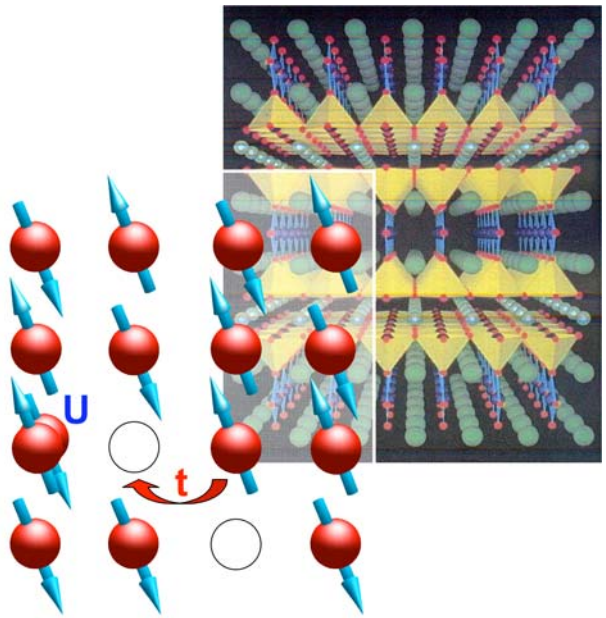

Figure 1: Crystal structure of $YBa_2Cu_3O_5$ and two-dimensional Hubbard model of the hole doped CuO planes, with on-site Coulomb interaction "U" and hopping "t".

In the superconducting state of a material, electrons form so-called Cooper pairs, allowing them to condense into a coherent macroscopic quantum state in which they conduct electricity without resistance. In conventional superconductors, pairing results from an attractive interaction between electrons that is mediated by lattice vibrations (phonon-mediated pairing). The consensus today is that the pairing mechanism in high-temperature superconductors is of an entirely different nature and is probably related to strong non-local correlations between electrons, a feature that distinguishes these materials from conventional superconductors. To address the problem theoretically, one must solve the quantum many-body problem for a macroscopic number of electrons without being limited to the typical single-particle approximations, such as Hartree-Fock or the local density approximation to density functional theory. A recent concurrence of new algorithmic developments and significant improvements in computational capability has opened a clear path to solving the quantum many-body problem for high-temperature superconductors.

A new algorithm: Mark Jarrell and his collaborators have found a way to extend effective medium theories beyond the mean field to systematically account for strong non-local correlations in systems with a macroscopic number of electrons. The method is called the Dynamical Cluster Approximation (DCA) and is closely related to the Coherent Potential Approximation (CPA), which has been used in alloy theory since the late 1960s. The algorithmic advancement in the DCA is that clusters, rather than single atoms, are embedded coherently into an effective medium. The approximate many-body DCA-Green function then accounts for the physically relevant non-local correlations and maintains key mathematical properties of the exact many-body Green function.

Model and implementation: The cuprate superconductors are modeled with a two-dimensional single-band Hubbard model (Fig. 1), and auxiliary-field Quantum Monte Carlo (QMC) is used to solve the quantum many-body problem of the cluster. Runs with small, four-atom clusters on the IBM p690 at the Center for Computational Sciences (CCS) show that the model reproduces the superconducting and antiferromagnetic phases of the cuprates observed in experiment (Fig. 2). They further indicate that the pairing mechanism is kinetic-energy driven, which is in agreement with recent experimental observations [ref. H. Molegraaf *et al.*, *Science* 295, 2239 (2002)]. An apparent violation of the Mermin-Wagner theorem, according to which no ordered phases are allowed in the two-dimensional Hubbard model at finite temperatures, is a consequence of the small cluster size used in the simulations. In the real cuprates, the third dimension introduces a weak coupling between the CuO planes that recovers the ordered phases.

New computational capability: The runtime of the DCA/QMC algorithm is dominated by rank-one matrix updates, which require high memory bandwidth, Parallel scalability is limited by a significant fixed start-up cost for each process. Increasing the cluster size for simulations on cache-dependent computers results in a dramatic loss of efficiency and expansion of runtime, making such calculations infeasible. The high memory bandwidth of the Cray X1 provides well over an order of magnitude increase in capability per processor, enabling simulations of larger clusters (Fig. 3). Recent runs on the Cray X1 at the CCS show that the model does indeed capture the relevant non-local physics, and larger cluster sizes do indeed recover the Mermin-Wagner theorem for the two-dimensional Hubbard model in the infinite-cluster-size limit.

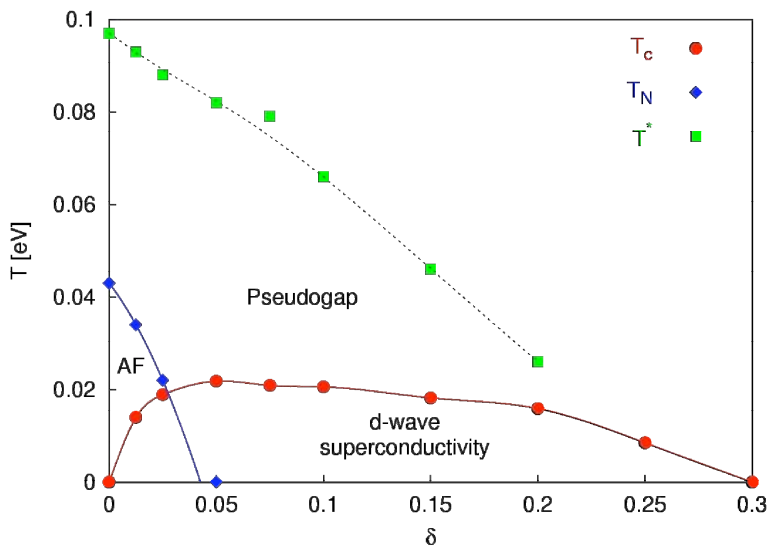

Figure 2: Phase diagram of two-dimensional Hubbard model as a function of doping.

Future plans: Since the coupling between CuO planes is weak, it can be introduced into the model as a perturbation without dramatically increasing the computational complexity. We expect to carry out full three-dimensional simulations of the phase diagram of the cuprate superconductors in the near future on the Cray X1. To extend the simulations to other classes of transition metal-oxide superconductors, and to eventually enable the design of new and optimized superconductors, we plan to parameterize the model with *ab-initio* electronic-structure calculations and generalize the method to include multiple bands. Since these plans amount to a polynomial increase in computational complexity, the initial simulations will require expansion of the Cray X1. The longer-term goal of designing new superconducting materials will require further dramatic increases in computational capability, through such efforts as the UltraScale Scientific Computing Capability recently proposed by the DOE Office of Science.

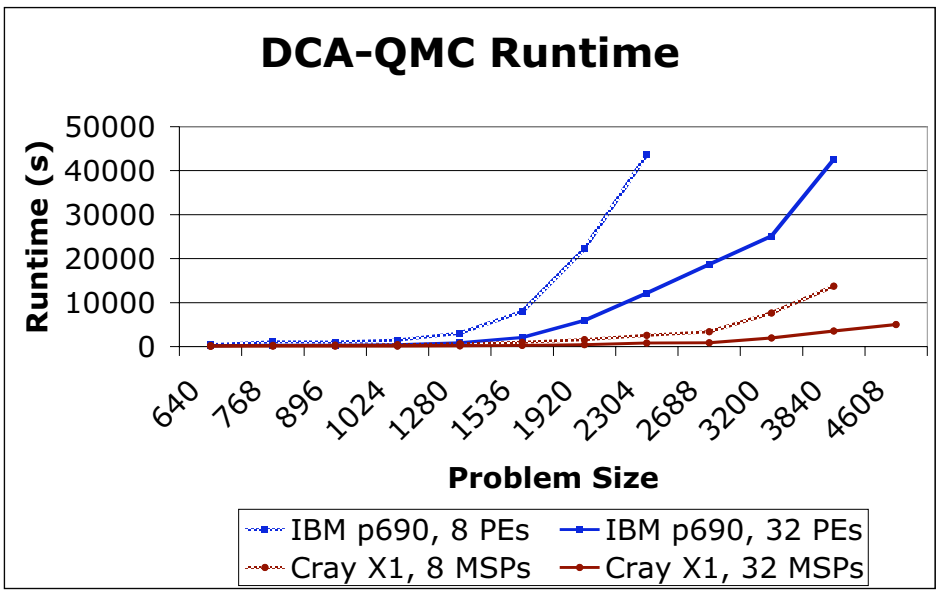

Figure 3: Runtimes for a series of initial production runs with a cluster size of 64. (Runs in the series generally get more expensive, but they vary multiple parameters. Lines connecting the points are for clarity.)

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