"Taking a quantum leap in time to solution for simulations of high-Tc superconductors."

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Abstract:

For over three decades, the high Tc-cuprates have been a gigantic challenge for condensed matter theory. Even the simplest representation of these materials, i.e. the single band Hubbard model, can not be solved quantitatively and its phase-diagram is therefore elusive. With the recent algorithmic advances in the Dynamical Cluster Approximation (DCA) [1] and a very efficient GPU-implementation of the latter [2], we were able to speed up the calculations with a factor of 10^9, while at the same time reduce the energy to solution with a factor of 6. These radical improvements allow us to determine the superconducting transition temperature accurately and show that the Cooper-pairs have indeed a d-wave structure, as was predicted by Zhang and Rice. These achievements were honored with an INCITE Award, the equivalent of 2 million dollars' worth of computing time on the supercomputer "Titan". This might finally open the door to resolve the phase-diagram of the single band Hubbard model and give us a better understanding of the physics that governs the high Tc-cuprates.

[1] Peter Staar, Thomas A. Maier and Thomas C. Schulthess (Phys. Rev. B 88, 115101 (2013))
[2] Peter Staar, Thomas A. Maier, Michael S. Summers, Gilles Fourestey, Raffaele Solca, and Thomas C. Schulthess. "Taking a quantum leap in time to solution for simulations of high-Tc superconductors." (In Proceedings of SC13: International Conference for High Performance Computing, Networking, Storage and Analysis, SC '13, pages 1:1–1:11, New York, NY, USA, 2013. ACM.)

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