THE UNIVERSITY OF CHICAGO | THE COMMITTEE ON COMPUTATIONAL AND APPLIED MATHEMATICS

JASON KAYE

Center for Computational Mathematics
Flatiron Institute

Efficient Numerical Algorithms for Simulating Quantum Dynamics

THURSDAY, November 18, 2021 at 4:15pm
Jones 303, 5747 S. Ellis Ave. Chicago, IL 60637
OR
via Zoom

I will describe a few new algorithms which reduce computational bottlenecks in simulations of quantum many-body dynamics.

In time-dependent density functional theory (TDDFT), the many-body wavefunction is approximated using a collection of single-particle wavefunctions, which independently satisfy the Schrodinger equation and are coupled through an effective potential. I will introduce a high-order, FFT-based solver for free space (nonperiodic) problems in TDDFT which sidesteps the usual requirement of imposing artificial boundary conditions.

Many-body Green's functions, which describe correlations between quantum observables, enable practical simulations beyond the effective one-body picture of TDDFT. The Green's functions satisfy history dependent Volterra integro-differential equations with kernel nonlinearities. I will outline efficient history integration algorithms which significantly extend feasible propagation times in both equilibrium and nonequilibrium calculations.

Organizer:

Jeremy Hoskins, Department of Statistics, jeremyhoskins@statistics.uchicago.edu
CAM Colloquium URL: https://cam.uchicago.edu/events/cam-colloquium/

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