VISTA Seminar

Seminar 59

November 8, 2023

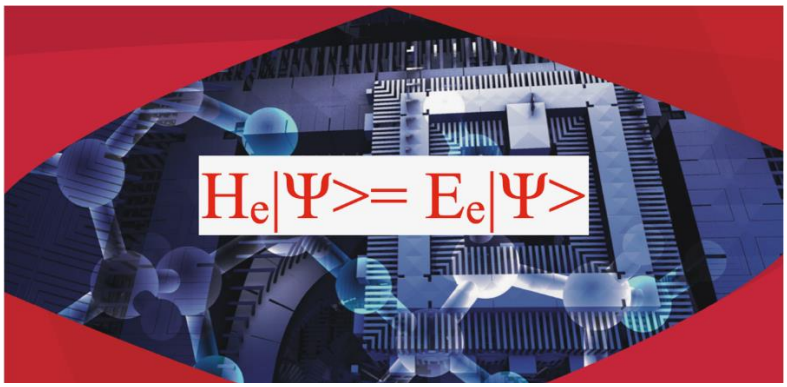
10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT London / 4:00 pm – 5:30 pm CET Paris / 10 pm CST Beijing

TOC:

Quantum Chemistry on a Quantum Computer

Artur Izmaylov

Department of Physical and Environmental Sciences, Department of Chemistry, University of Toronto
Web: http://www.utsc.utoronto.ca/~aizmaylov/ *Email:* artur.izmaylov@utoronto.ca

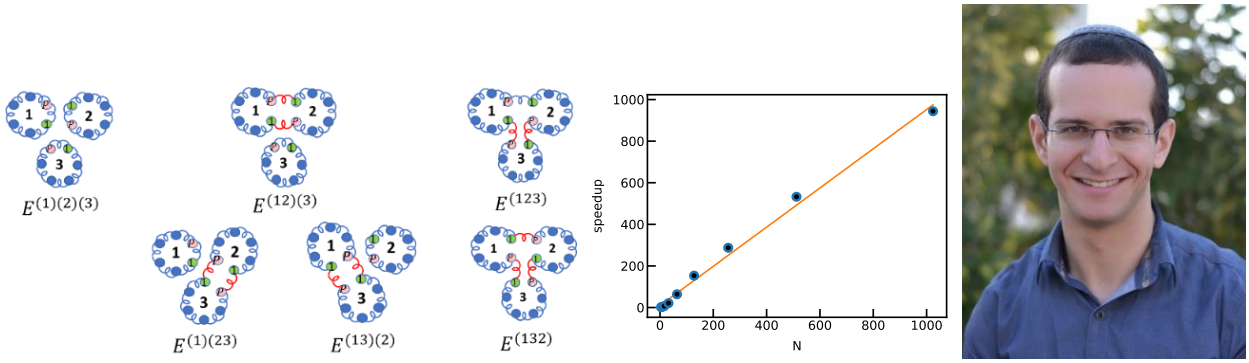


Quantum chemistry problem is one of the attractive targets for demonstrating quantum advantage of quantum computing technology. Having strongly correlated systems as the main target, I would like to discuss what new classical computing techniques need to be developed to help quantum computing algorithms to solve the electronic structure problem. Encoding the electronic Hamiltonian in the second quantized form on a quantum computer is not a trivial problem, and its efficiency can become a bottleneck for the entire quantum solution. Dealing with this Hamiltonian can be facilitated by partitioning it into a sum of fragments diagonalizable using rotations from either small Lie groups or the Clifford group. These fragments are convenient for performing various algebraic manipulations required in circuit compiling and quantum measurement. I will illustrate how the Hamiltonian partitioning can be used to improve performance of several quantum algorithms for quantum chemistry (e.g. Variational Quantum Eigensolver and Quantum Phase Estimation).

Quadratic Scaling Bosonic Path Integral Molecular Dynamics

Yotam Feldman, Barak Hirshberg

School of Chemistry, Tel Aviv University, Israel
Email: yotam.feldman@gmail.com



Bosonic exchange symmetry leads to fascinating quantum phenomena, from exciton condensation in quantum materials to the superfluidity of liquid ^{4}He. Unfortunately, path integral molecular dynamics (PIMD) simulations of bosons are computationally prohibitive beyond ~100 particles, due to a cubic scaling with the system size. We present an algorithm that reduces the complexity from cubic to quadratic, allowing the first simulations of thousands of bosons using PIMD. Our method is orders of magnitude faster, with a speedup that scales linearly with the number of particles and the number of imaginary time slices (beads). Simulations that would have otherwise taken decades can now be done in days. In practice, the new algorithm eliminates most of the added computational cost of including bosonic exchange effects, making them almost as accessible as PIMD simulations of distinguishable particles.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 59
Time: Nov 8, 2023 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/95588116073?pwd=VDlxTm9OQk85L3RIK1BVNlA1bFpidz09

Meeting ID: 955 8811 6073
Passcode: 168029