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Quantum-HPC Hybrid Simulation for Quantum Chemistry.

Thursday, 28 August 2025 11:00 (1 hour)

Abstract:

Quantum chemistry has long been considered one of the most promising applications of quantum computing. However, due to the limitations of current NISQ (Noisy Intermediate-Scale Quantum) devices—particularly in terms of circuit depth and noise—these devices have only been applied to systems of around 20 qubits, where classical computers can still provide exact solutions.
In this talk, I will introduce one of the recent efforts led by IBM and collaborators to overcome these limitations: the Sample-based Quantum Diagonalization approach [1], which enables quantum chemistry simulations for systems with more than 50 qubits. The key features of this method include:
(1) incorporating the idea of efficiently estimating a suitable basis using sample data from quantum circuits [2],
(2) selecting shallow circuits executable on current NISQ devices,
(3) introducing a configuration recovery scheme to mitigate noise-induced degradation, and
(4) scaling up the diagonalization process through hybrid integration with classical supercomputers.
By combining these techniques, this approach has enabled quantum chemistry calculations for 50-qubit-scale systems—beyond the reach of classical exact methods.

[1] J. Robledo-Moreno et al., Sci. Adv. 11, adu9991 (2025).
[2] K. Kanno et al., arXiv:2302.11320 (2023).

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