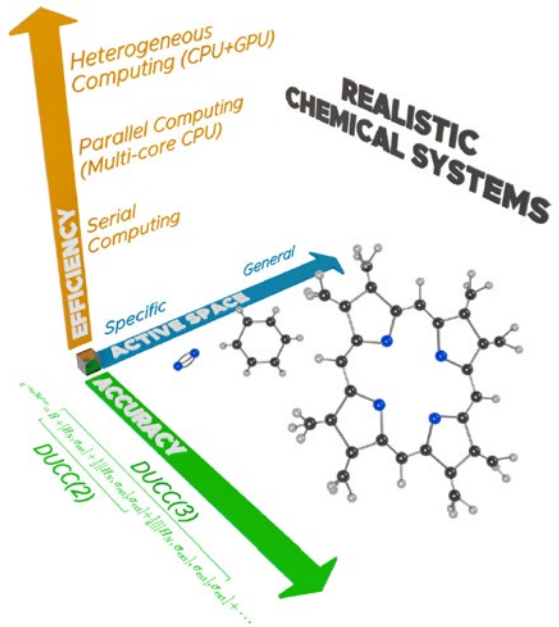
Coupled cluster downfolding theory in simulations of correlated systems on quantum hardware



Overview of the evolution of the couple cluster downfolding approximations and software based on the double-unitary coupled cluster Ansatz

Scientific Achievement

Developed HPC implementation of coupled cluster downfolding methods for chemistry applications

Significance and Impact

Provided hardware simulations for realistic systems in realistic basic sets using active-space representation of downfolded Hamiltonians

Research Details

- We performed ground-state simulations of benzene and free-base porphyrin (FBP) molecules in 6-orbital active spaces using downfolded Hamiltonians.
- We recovered 98% of total correlations using downfolded Hamiltonians. At the same time, the bare-Hamiltonian-based simulations in 6-orbital active space recover 3% (benzene) and 1% (FBP) of the total correlation energy.
- After applying error mitigation algorithm, IBM and Quantinuum hardware simulations provided similar level of accuracy.

N. P. Bauman, M. Zheng, C. Liu, N. Meyes, A. Panyala, B. Peng, A. Li, and K. Kowalski, “Coupled cluster downfolding theory in simulaitons of correlated systems on quantum hardware,” Phys. Rev. Res. 8, 013072 (2026).

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- **NQISRC Intellectual Role:** Collaborator
- **NQISRC Funding Role:** Minority
- **Explanation of Funding Institution Contributions**
  - DOE Office of Science, Quantum Science Center (NQISRC)
  - DOE Office of Science, Office of Basic Energy Sciences (Embedding QC into Many-body Frameworks)
  - DOE Office of Science, Office of Basic Energy Sciences (TEC4)
  - DOE Office of Science Early Career Research Program
  - PNNL's Quantum Algorithms and Architecture for Domain Science (QuAADS) Laboratory Directed Research and Development (LDRD) Initiative
  - Oak Ridge Leadership Computing Facility (OLCF)
  - National Energy Research Scientific Computing Center (NERSC)