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Abstract

Quantum simulation of chemistry and materials is recognized as one of the most practical and promising applications of quantum information processors. The simulation of local Hamiltonians such as those describing molecular systems is known to be efficient with quantum devices and inefficient with classical devices.

We will develop a family of quantum algorithms for the simulation of chemistry and materials to be employed in quantum simulators of different stages of development. The target quantum simulation platforms range from analog quantum simulators and early digital simulators to fully error corrected platforms. The quantum algorithms developed will belong to at least three different families of algorithms: gate-model simulation, variational quantum eigensolvers, and universal adiabatic simulators. We will seek collaboration with several experimental groups that employ different computing platforms (superconducting quantum bits, ion traps, quantum optics devices, etc.) for the experimental implementation of the proposed algorithms.

Led by the principal investigator, an interdisciplinary team will develop the algorithms. A practical deliverable will be a quantum simulation software compiler platform that will provide specifications for simulations of arbitrary molecules and one-, two- and three-dimensional materials based on the output of tractable classical computer programs. The output of the platform will include universal gate sequences with error correction, control sequences for variational quantum eigensolvers, and Hamiltonians specified with wiring patterns for superconducting adiabatic quantum devices.

The outcome of this research project should be a practical toolset and roadmap for the numerically *exact* simulation of matter. The results from this work, together with the development of large-enough quantum devices will be disruptive for the DOD materials design capability by accelerating the materials design cycle: computers will enter the realm of routine quantitative predictive power, in contrast to the unreliable, qualitative classical methods used nowadays.