Excited-State Dynamics: Linking Classical and Quantum Approaches

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Utilizing quantum computers for scientific discovery presents many challenges driven by the currently still-experimental nature of quantum hardware and the absence of the essential software needed to "program" this hardware in the near term. Software for quantum computing is in its infancy, and therefore the development of executable code for quantum hardware using current strategies is arduous. In this context, in the first part of the talk, I will discuss our recent demonstration of a new allocation algorithm that combines the simulated annealing method with local search of the solution space using Dijkstra's algorithm. Our algorithm takes into account the weighted connectivity constraints of both the quantum hardware and the quantum program being compiled. Using this novel approach, we are able to optimally reduce the error rates of quantum programs on various quantum devices. In the second part of my talk, I will present a strategy to compute excited-states and reaction dynamics on NISQs. Finally, I will discuss a pathway to computing "complex" molecules, both energies and dynamics, leveraging a combination of quantum chemistry and quantum computer science approaches.