Quantum computing of nonlinear reacting flows with the probability density function method

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Quantum computing offers the promise of exponential speedups in scientific computing tasks, particularly those involving large-scale linear systems[1]. However, its application to reacting flows, particularly in combustion, remains challenging due to the nonlinear source terms and the need for time-dependent solutions[2]. In this work, we address these issues by employing a probability density function (PDF)[3] formulation to transform the nonlinear reacting-flow partial differential equations (PDEs) into linear ones. The evolution process is then solved by the space-time coupling history state, in which all time steps are stored as a superposition state[4]. This approach avoids repeated quantum state measurement and preparation at intermediate steps, fully leveraging the advantage of the quantum linear systems algorithm (see Figure 1a). By encoding the distributions in a quantum state, we can efficiently measure the PDF's statistical moments through carefully designed quantum algorithms. This advances the practical value of the algorithm, allowing for an end-to-end application of quantum computing on nonlinear reacting flows. Our computational complexity analysis indicates a near-exponential speedup over classical algorithms. To validate the proposed framework, we perform a series of test cases simulating reacting flows with various conditions (see Figure 1b). The results highlight the potential of quantum computing for solving reacting flows with nonlinear source terms and extracting statistics efficiently.

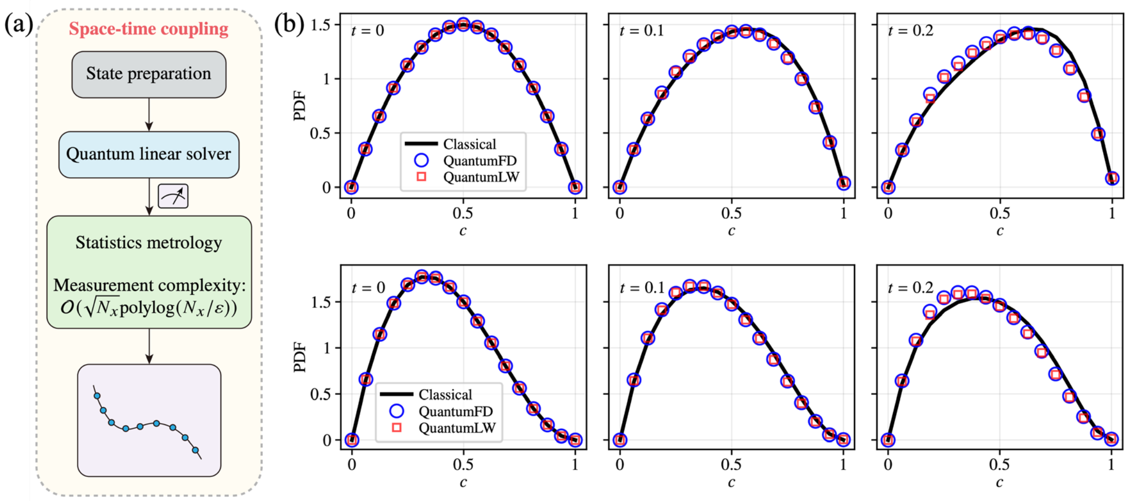

Figure 1: (a) Schematic of the space-time coupling scheme for solving the PDF evolution. The initial state is first encoded into the wave function, after which the history state for all time steps is computed via the quantum linear systems algorithm[4]. Quantum metrology is then used to extract the PDF's statistical moments from the quantum state. (b) Evolution of the PDF distribution for reacting flows at various time steps, compared between quantum computing (with different finite difference schemes) and classical results.

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