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Quantum Implementation of Numerical Methods for Convection-Diffusion Equations: Toward Computational Fluid Dynamics

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Abstract. We present quantum numerical methods for the typical initial boundary value problems (IBVPs) of convection-diffusion equations in fluid dynamics. The IBVP is discretized into a series of linear systems via finite difference methods and explicit time marching schemes. To solve these discrete systems in quantum computers, we design a series of quantum circuits, including four stages of encoding, amplification, adding source terms, and incorporating boundary conditions. In the encoding stage, the initial condition is encoded in the amplitudes of quantum registers as a state vector to take advantage of quantum algorithms in space complexity. In the following three stages, the discrete differential operators in classical computing are converted into unitary evolutions to satisfy the postulate in quantum systems. The related arithmetic calculations in quantum amplitudes are also realized to sum up the increments from these stages. The proposed quantum algorithm is implemented within the open-source quantum computing framework Qiskit [2]. By simulating one-dimensional transient problems, including the Helmholtz equation, the Burgers' equation, and Navier-Stokes equations, we demonstrate the capability of quantum computers in fluid dynamics.

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1 Introduction

Fluid mechanics is one of the earliest disciplines that widely bring in numerical simulations. Von Neumann and Charney [24] were beginning to use the first programmable digital computer ENIAC for meteorology as early as the 1940s. Nevertheless, the scales of simulation in computational fluid dynamics (CFD) without any modeling are still far away from industrial-strength problems, since the computational cost exponentially dependents on the Reynolds number (Re) [48]. Slotnick et al. [41] suggested that a potential paradigm shift driven by cutting-edge computing technologies, including quantum computing, may fundamentally change the situation. Motivated by the reaching point of quantum supremacy [37] in experimental quantum computing [3], we observe a flourishing development of quantum numerical methods or quantum simulations in researches and engineering practices with various physical contexts, including fluid dynamics. In the present work, our focus is the realization of the numerical methods for partial differential equations (PDEs) governing the fluid dynamics system.

The following introduction of the previous efforts on quantum solvers of PDEs inevitably involves some discussions on the categories of quantum computing hardware since some of the quantum numerical procedures are better considered as different architectures rather than algorithms, as suggested by Kendon et al. [25]. One category of quantum computing hardware is the so-called quantum analog computing [25] or analog quantum simulator [19], which uses a controllable quantum system to investigate another much more complex system. Although it is relatively feasible for implementation, the universality of quantum simulators relies on finding a corresponding Hamiltonian, which is nontrivial for fluid dynamics or other classical systems. Specific analog quantum hardware based on quantum annealing (QA) [23] is most likely to become commercially available [33] amongst many prototypes of quantum computing systems. QA algorithm utilizes the quantum-mechanical fluctuation to tunnel through the cost barrier between local minima, and thus it is suitable for optimization problems. Ray et al. [39] converted a one-dimensional (1D) laminar channel flow problem into a quadratic unconstrained binary optimization problem via the least square method. Srivastava and Sundararaghavan [42] constructed a graph representation of the functional of a 1D elastic bar via Ising Hamiltonian on a D-Wave machine. Both attempts [39, 42] directly adopted steady-state elliptical differential equations to an discretely equivalent form that is admitted to D-Wave hardware [8]. However, the PDEs in fluid dynamics are most often non-elliptic, as our discussion later on in Section 2.1. Therefore, the QA machines are very likely to be merely used for certain sub-process rather than for the entire solution process. Zanger et al. [50] proposed a QA-based integrator for ordinary differential equations (ODE), where a heuristic minor-embedding algorithm proposed by Cai et al. [9] is employed to make the connection locally condensed. Knudsen and Mendl [26] constructed a variational continuous-variable quantum algorithm [5] to integrate an ODE. An adiabatic quantum algorithm for solving a Hermitian linear system is proposed by Subasi et al. [45], and this algorithm is experimentally implemented and tested by Wen et al. [46].