Parallel Evaluation of Quantum Algorithms for Computational Fluid Dynamics

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Abstract

The development and evaluation of quantum computing algorithms for computational fluid dynamics is described along with a detailed analysis of the parallel performance of a quantum computer simulator developed as part of the present work. The quantum computer simulator is used in the evaluation of the quantum algorithms on a conventional parallel computer, and is applied to quantum lattice-based algorithms as well as the Poisson equation. A key result is a demonstration of how the Poisson equation can be solved effeciently on a quantum computer, while its use within a larger algorithm representing a full CFD solver poses a number of significant challenges.

Keywords: Quantum Computing, Quantum Computer Simulator, MPI

1. Introduction

Accurate simulations of many flows of scientific and engineering interest are among the most computationally demanding applications in scientific computing. Quantum computers along with carefully designed algorithms for such computing platforms could offer a significant potential for future scientific computing applications. Quantum computer applications aim to achieve a computational speed-up relative to classical computers by using unique quantum effects not available to other computing platforms. The first and most important for the algorithm considered here is quantum parallelism. This parallelism is based on the use of qubits representing a superposition of infinitely many possible states of a binary system. Quantum entanglement and quantum teleportation are the other main quantum effects used to create computational capabilities not available to classical computers.

In recent years the field of quantum computing has grown into a rich and diverse body of knowledge and significant progress has been made with building functional quantum computers. At the same time, research into applications of quantum computers has been more limited and two decades after their invention, Schor's algorithm for factoring composite integers and

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Grover's algorithm for quantum search are still among the main applications. Further applications have been developed which take advantage of the unique capabilities of quantum computing platforms, e.g. methods for the solution of linear systems of equations[1], numerical gradient estimation[2] and the Poisson equation[3].

2. Quantum CFD algorithms and Quantum Computer simulator

In the present work, the emphasis is on the development and evaluation of quantum computing algorithms for Computational Fluid Dynamics applications. In the algorithms considered in the present work, the flow state is defined through a multi-qubit register and the circuit-model approach to quantum computing is followed, i.e. single- and multi-qubit gates are acting to mofidy the state of the quantum system. For an n-qubit system, a 2^n state-vector of complex numbers results when modelled on a conventional computer. This exponential growth of the required memory to store the state vector has motivated the development of a quantum computer simulator suitable for parallel computation on distributed-memory computers, such that algorithms with a significant number of qubits (e.g. ≥ 30) can be solved without memory limitations.

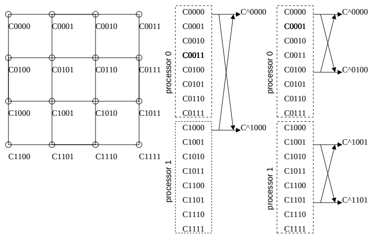

Fig. 1 – Numbering of complex state variables for example 2D mesh (left). For a state vector distributed over two processors, the one-qubit operator requires message passing for the 1st qubit (middle), while the one-qubit operators acting on the 2nd qubit in the multi-qubit register only require data on same processor.

Figure 1 shows an illustration of how the complex state variables on a two-dimensional mesh could be numbered for an example problem with 4 qubits. The storage on two processors is shown on the right. In the quantum algorithms considered, one-qubit operators are widely used. Using the current numbering, large strides occur for the most significant bits (on the left-hand side of the register in the example shown), while for other qubits the operations may only involve data on the present processor. Gate operations on multi-qubit registers result in relatively complex message-passing data exchanges. However, in the full paper it will be demonstrated that this feature of the qubit register can also be used for efficient evaluation of operations on multi-dimensional meshes, including Fourier transforms. In the full paper, the parallel performance of the quantum computer simulator will be assessed in detail along with a detailed analysis of quantum-lattice and Poisson solution methods for CFD solvers.

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