PROPOSITION DE SUJET DE THESE

Quantum computing for solving linear and nonlinear partial differential equations

Référence : **SNA-DAAA-2024-37**
(à rappeler dans toute correspondance / to be included in all correspondence)

Start of contract: September 2024	**Application deadline:** May 2024

Keywords: Quantum computing, partial differential equations, Schrödinger equation, linear algebra

Profile and required skills: A solid background in scientific computing, programming skills and motivation to learn are required. Background in quantum mechanics is welcome. Ideally with M.Sc. degree in applied mathematics, mechanics or a related discipline, with excellent academic records

Context: Quantum computers offer the possibility of technology exponentially more powerful than current classical computers, but the current state of the art is largely experimental with several obstacles to useful applications [Wiki]. We are here interested in evaluating quantum computing and associated algorithms for solving partial differential equations (PDEs) in the field of fluid dynamics.

The common approach to solve PDEs on a quantum computer consists in encoding the PDE solution as the amplitude of a quantum state (preparation step), then mapping the PDE to a problem for which efficient quantum algorithms exist. It can be the Schrödinger equation solved with Hamiltonian simulation (e.g. quantum Fourier transform), or a linear system solved with a quantum linear solver (e.g., HHL algorithm). The theoretical complexity analysis of those algorithms shows a potential exponential speedup compared to traditional algorithms in classical computing. Measurements are finally applied to get physical observables that can be compared with the classical solution. So we need a map either between the PDE and the Schrödinger equation, or between the PDE after discretization and a linear system. Likewise, challenges remain to obtain practical implementations on hardware such as the probabilistic nature of qubits making computations nondeterministic, the decoherence phenomenon introducing noise into calculations, the potentially prohibitive cost of the preparation and measurement steps, the difficulty to scale up in terms of qubit size, etc. Those aspects will be addressed during this PhD work.

Description of work: The objective of this PhD project is to review, design, analyze, implement, run and compare algorithms for solving linear and nonlinear PDEs. We will focus on the Schrödingerisation approach [Jin23a] that maps any linear PDE into a Schrödinger equation, thus allowing the application of efficient Hamiltonian simulation algorithms such as the Fourier spectral method. The level set method [Jin23b] can be used to further map some nonlinear PDEs (such as scalar nonlinear hyperbolic equations) into linear PDEs. This approach will be considered and compared to other approaches based on Carleman linearization procedure [Liu21], or based on quantum-classical hybrid algorithms using either variational quantum computing [Lub20], or quantum neural networks [Kyr21].

The research activities to be conducted include:

- Literature review of different approaches for solving linear and nonlinear PDEs. This will enable to evaluate the potential speedup compared to classical algorithms, the impact of noise on their accuracy, to identify bottlenecks, etc.
- Derive algorithms for solving PDEs of increasing complexity (linear transport equation, scalar nonlinear hyperbolic equations, gas dynamics equations). Both approaches using mappings either to the Schrödinger equation or to a linear system will be considered and compared.
- Consider different paradigms (gate-based paradigm, analog paradigm, tensor networks, etc.) for writing the quantum programs and evaluate their efficiency.

- Analyze the algorithms in terms of complexity (for the preparation, evolution and measurement steps) and accuracy when assuming ideal quantum programs neglecting the effect of noise (fault tolerant quantum computing – FTQC – perspective).
- Estimate errors due to decoherence and the probabilistic output of the measurement step.
- If time permits, consider error-correction algorithms that minimize error accumulation due to quantum decoherence.
- Run large scale quantum computations with tens of qubits on a high-performing quantum simulator (with and without noise models) to validate the theoretical analysis.

The candidate will implement and run experiments by using a quantum simulator's programming framework (e.g., myQLM from Atos, Qiskit from IBM [QS]). The results will be the subject of publications in journals and scientific conferences.

Bibliography:

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[Jin23b] S. Jin et al., Time complexity analysis of quantum algorithms via linear representations for nonlinear ordinary and partial differential equations. J. Comput. Phys., 487 (2023), https://doi.org/10.1016/j.jcp.2023.112149.

[Liu21] J.-P. Liu et al., Efficient quantum algorithm for dissipative nonlinear differential equations, PNAS, 118 (2021), https://doi.org/10.1073/pnas.2026805118.

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Collaborations: CERMICS - Ecole des Ponts ParisTech and Atos Quantum Lab.

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