Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

IBM-TCD PhD Fellowship in Quantum Computing

Error Mitigation & Circuit optimisation for Quantum Time Evolution: theory and algorithms

The School of Mathematics at Trinity College Dublin and IBM Research Dublin invite applications for a jointly supervised, fully funded PhD position. The PhD project will concern applying techniques from numerical analysis and numerical PDEs to address numerical challenges arising in quantum computing, namely estimation and optimization of errors arising in quantum time evolution.

Quantum computers have huge potential to simulate quantum many-body systems relevant for chemistry or material science. The evolution in time of the associated wave function is governed by the Schrödinger equation. A common technique used to evolve the Schrödinger equation in time is based on Trotter-Kato semigroups. The advantage of such methods is that they have rigorous error bounds when applied numerically. However, classical approaches in this direction become intractable due to the growth in dimension of the computation we need to perform.

Overcoming the curse of dimensionality in such approaches is one of the potential advantages of quantum computers. Near-term processors could potentially propagate wave functions forward in time in much higher dimension than classically possible. However, relying on Trotter formulas to solve the time-dependent Schrodinger equation on a quantum computer presents a challenge. Quantum circuits resulting from these methods quickly become very "deep". This presents a new computational challenge, since quantum computations introduce noise into the calculations, and this noise increases with the depth of the quantum circuit. We contrast this with the fact that shallow circuits lack “expressibility”.

We seek a PhD student to apply the tools of numerical analysis and scientific computing to overcome these issues. To avoid deep circuits, it is suggested that physics-informed Galerkin projection schemes offer a way to reduce the size of the problem to one that does not require prohibitively deep quantum circuits. Some such schemes have been proposed recently in the literature, but appropriate rigorous analysis of the error of these projection methods does not yet exist. This analysis would yield good estimates of the error incurred when projected with full equations onto a smaller subspace for apriori prediction of the performance of the methods. Additionally, a representation of the error can be fed back into the method to make refinements of the solution. A further challenge is that some of these projection schemes lead to linear systems with uncertain coefficients.

This PhD project offers a great opportunity to make advances in numerical methods in quantum computing, with challenges in numerical analysis and uncertainty quantification. The goal is to leverage classical optimization techniques to inform quantum error analysis and correction. Fault-tolerant methods developed in the setting of high-performance parallel computing may also be repurposed here. The overarching question we will be trying to address is how can we use physics of the problem to optimize circuit design? Can we go beyond classical computing limits for the simulation of specific Hamiltonians (e.g. chemistry, material science, drug discovery) using physics-informed circuits?

A successful candidate should have a strong background in numerical analysis and numerical PDEs (e.g., coursework and/or project work from an internship, independent study or the completion of a bachelor/masters degree), with an emphasis on the on-paper analysis aspects of that field. In addition, experience in uncertainty quantification, quantum computing, or quantum information theory would also be helpful but is not required. On top of having outstanding records of accomplishments at undergraduate or Master level, the candidate will be expected to be self-motivated and a self-starter with a passion for scientific research and advanced technology development. The successful candidate will be required to relocate to Dublin, Ireland and remain there throughout the duration of PhD studies.

The PhD student will be a full-time registered student at Trinity College Dublin and will complete the required coursework and progress reports for the award of a PhD while supported as an employee of IBM Research. The student will join the active internationally-recognised Computational and Applied Mathematics group at TCD and will make significant contributions to numerical methods in quantum computing. Through joint supervision the successful candidate will gain experience of numerical simulation on quantum computers, numerical error optimisation and analysis, uncertainty quantification, and fault-tolerant methods. The student will be expected to make significant contributions to the analysis, reduction, and mitigation of errors arising in numerical algorithms implemented on quantum and hybrid classical/quantum computing devices.

This selected student will have the following benefits:

- Access to resources both at IBM and TCD
- Research experience in both private and public sectors
- Employment opportunities after graduation
- **A substantial PhD Salary (>35,000) euro**

Further information and application

For further information please contact **Kirk M. Soodhalter** (ksoodha@maths.tcd.ie) at Trinity College Dublin or **Sergiy Zhuk** (sergiy.zhuk@ie.ibm.com) at IBM Research Dublin.

For consideration for the position please submit a full CV including the names of 3 potential referees to **Kirk M. Soodhalter** (ksoodha@maths.tcd.ie).

Please note that a separate application will be required at IBM for shortlisted candidates.