

CCP-QC Quantum Algorithms Day Flash Talk and Poster Abstracts:



Quantum Simulation of False Vacuum Decay on Current Quantum Hardware

Presenter: James Ingoldby (IPPP, Durham)

Co-authors: Joana Fraxanet, Michael Spannowsky, Simon Williams, Matthew Wingate

I will present work in progress on the quantum simulation of false vacuum decay in the O'Brien–Fendley lattice spin chain. This process describes the decay of a higher-energy phase via quantum tunnelling, leading to the formation and expansion of “bubbles” of a lower-energy phase. We simulate these dynamics using Suzuki–Trotter decompositions of the time evolution operator, implemented on current IBM quantum hardware at the 100+ qubit scale. The decay is tracked through the time evolution of a simple observable (magnetisation), and benchmarked against tensor network simulations using the time-dependent variational principle (TDVP), providing a direct comparison between quantum hardware and classical methods. Beyond serving as a technical benchmark, this setup explores false vacuum decay in a model with a well-defined continuum limit, allowing current quantum devices to be assessed on a physically meaningful phase transition in quantum field theory.

High-order splitting of non-unitary operators on quantum computers

Presenter: Peter Brearley (presenter, University of Manchester)

Co-author: Philipp Pfeffer (TU Ilmenau, Germany)

Dissipation and irreversibility are central to most physical processes, yet they lead to non-unitary dynamics that are challenging to realise on quantum processors. High-order operator splitting is an attractive approach for simulating unitary dynamics, yet conventional product formulas introduce negative time steps at high orders that are numerically unstable for dissipative dynamics. We show how complex-coefficient product formulas can decompose dissipative dynamics into a sequence of simple Hamiltonian evolutions in real and imaginary time with high-order accuracy. The unitary substages use positive real coefficients, while the dissipative substages use complex coefficients with positive real parts, where the real parts preserve the contractive evolution and the imaginary parts are additional unitary evolutions. We demonstrate the approach by simulating the classical problem of lossy mechanical wave propagation on a trapped-ion quantum processor. A step of order 4 achieves greater accuracy than the steps with low orders 1 and 2, despite the increased circuit depth on noisy hardware. The results suggest that high-order operator splitting is an accurate and practical approach for simulating dissipative dynamics on near-term quantum processors.

Quantum Algorithms for Plasma and Fusion Physics

Authors: Matthew Christensen, Tom Goffrey, Animesh Datta (University of Warwick)

Quantum computing presents a novel method for tackling the computational challenges inherent in kinetic plasma physics. Perhaps one of the most challenging systems is that of the Vlasov-Poisson system due to its high dimensional phase space. We employ a Fourier-Hermite expansion of the distribution function [1] to obtain a nonlinear ODE in terms of the coefficients of expansion, and examine the viability of Carleman embedding [2] to produce a quantum algorithm. We reformulate the convergence conditions of the embedding process in terms of the physical plasma properties, and show the regimes of convergence with respect to the collision frequency of the plasma.

[1] Frederick C. Grant and Marc R. Feix. "Fourier-Hermite Solutions of the Vlasov Equations in the Linearized Limit". In: *The Physics of Fluids* 10.4 (Apr. 1, 1967), pp. 696–702. issn: 0031-9171. doi: 10.1063/1.1762177. url: <https://doi.org/10.1063/1.1762177>

[2] Jin-Peng Liu et al. "Efficient quantum algorithm for dissipative nonlinear differential equations". In: *Proceedings of the National Academy of Sciences* 118.35 (Aug. 31, 2021), e2026805118. doi: 10.1073/pnas.2026805118. url: <https://www.pnas.org/doi/10.1073/pnas.2026805118>

Fourier extensions for block encoding matrix functions with exponential convergence

Presenter: Thomas Howarth (Loughborough University, UK)

Co-authors: Peter Brearley (The University of Manchester, UK), Ben Adcock (Simon Fraser University, Canada)

We show how Fourier extensions, which approximate non-periodic functions as a Fourier series on an interval of a periodic domain, decompose functions of Hermitian matrices into an exponentially convergent linear combination of unitaries. By Hermitian dilations, the approach extends to odd singular-value transforms of general matrices, producing exponentially convergent block encodings of general matrices and general matrix inversions. For a given error, regularisation of the Fourier coefficients exploits redundancy in the Fourier extension basis, resulting in block encodings with near-optimal subnormalisation, minimising reliance on amplitude amplification. Fourier extensions therefore offer an accurate and versatile approach to non-unitary quantum computing.

Molecular property simulations on quantum computers

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Molecular simulation has been identified as one of the first practical applications where quantum computers could demonstrate utility, prompting extensive research into quantum algorithms for chemistry. Here, we go beyond ground state energy simulation and present various works related to obtaining molecular properties on quantum computers[1-7].

Crucially, we present first proof-of-concept hardware experiments of our algorithms on real quantum devices made possible by our quantum error mitigation research[8].

We present quantum linear response, a quantum algorithms for modelling spectroscopic properties by studying the response of matter to light. This allows among others accessing excited states, absorption and electronic circular dichroism spectra, and response function such as polarizabilities, optical rotations, and NMR coupling constants[1-6]. Spin-adapted orbital-optimised multistate contracted VQE is showcased as alternative route to excited states and their properties. Introducing unrestricted oo-VQE, we are able to simulate hyperfine coupling constant on real hardware[7].

[1] Ziems, Kjellgren, Reinholdt, Jensen, Sauer, Kongsted, Coriani, *J. Chem. Theory Comput.* **2024**, 20, 3551

[2] Buchwald, Ziems, Kjellgren, Sauer, Kongsted, Coriani, *J. Chem. Theory Comput.* **2024**, 20, 7093

[3] Reinholdt, Kjellgren, Fuglsbjerg, Ziems, Coriani, Sauer, Kongsted, *J. Chem. Theory Comput.* **2024**, 20, 3729

[4] Reinholdt, Kjellgren, Ziems, Coriani, Sauer, Kongsted, *J. Phys. Chem. A* **2025**, 129, 1504

- [5] Kjellgren and Ziemis. SlowQuant, <https://github.com/erikkjellgren/SlowQuant>
[6] Ziemis, Kjellgren, Sauer, Kongsted, Coriani, Chem. Sci., **2025**, 16, 4456
[7] Jensen, Hedemark, Ziemis, Kjellgren, Reinholdt, Knecht, Coriani, Kongsted, Sauer, J. Chem. Theory Comput. **2025**, 21, 16, 7878
[8] Rasmussen, Kjellgren, Reinholdt, Sauer, Coriani, Ziemis, Kongsted, arXiv:2511.21236

ATP Hydrolysis on a Quantum Computer

Presenter: Ryan LaRose (Michigan State University)

Co-authors: Brenda Rubenstein (Brown), Troy Van Voorhis (MIT), Sophia Economou (Virginia Tech), Norm Tubman (NASA), Grant Rotskoff (MIT)

We will describe our truly quantum molecular dynamics pipeline to compute the reaction mechanism of ATP hydrolysis. In particular, we will discuss our hardware-tailored ansatz design [1] and iterative modifications to sample-based quantum diagonalization [2] to improve the accuracy of energy estimates. These energies are then used to train state-of-the-art neural networks to compute force fields and enable molecular dynamics driven by accurate and scalable quantum computation [3]. We will show results for metaphosphate hydrolysis on IBM quantum computers, then discuss the scaling towards full ATP hydrolysis. Additionally, we will discuss the resources required for fault-tolerant quantum computation of molecular energies, in particular using quantum Krylov and quantum phase estimation [4]. (The talk will be based on our work from the [Wellcome Leap Quantum for Bio challenge](#) where we were one of six finalist teams.)

- [1] Ramôa et al., [<https://arxiv.org/abs/2601.20681>]
[2] Rowland et al., In preparation
[3] Khan et al., [<https://arxiv.org/abs/2406.08554>]
[4] LaRose et al., [<https://arxiv.org/abs/2601.19059>]

Markov Chain Monte Carlo for Quantum Portfolio Optimisation

Presenter: Shruti Jain(1)

Co-authors: Tobias Hartung(1), Karl Jansen(2), Hernan Leövey(3)

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(2) Deutsches Elektronen-Synchrotron DESY, Zeuthen, Germany

(3) Quantitative Trading (CEMT), Axpo AG, Baden, Switzerland

Portfolio optimisation is a fundamental problem in finance that involves allocating capital across assets to balance expected returns and risk. This problem can be formulated as the minimisation of a cost function subject to constraints such as asset selection limits, budget bounds, and discrete allocations. The combinatorial nature of these constraints results in an exponentially growing search space, making exact solutions computationally challenging to find. In this work, we propose a Variational Quantum Algorithm (VQA) approach to optimise a real-world cost function subject to constraints. We construct a parameterised quantum circuit to approximate Imaginary Time Evolution (ITE), as exact ITE follows a strictly downhill path in the cost-function landscape, causing the cost to decrease monotonically toward a minimum. But since exact ITE is non-unitary, an effective approximation is required for implementation on quantum hardware. We also propose Markov Chain Monte Carlo (MCMC) based optimiser, containing energy gradient information to accelerate convergence and approach the optimal value more reliably. We present convergence plot comparisons against some standard optimisers. Additionally, we provide a priori estimates of resource requirements and hyper-parameter selection, thus enabling the choice of ideal hyper-parameters that could lead to better

optimised values based on intuitive metrics like final resolution, global search space exploration, and acceptance rates.

Quantum Speed-up of PDEs arising in Option pricing

Presenter: Sofia Moliner (Imperial College London)

Co-authors: Jack Jacquier, Eyal Neuman (Imperial College London)

We present a novel quantum algorithm for option pricing based on an extension of Quantum Fast Forwarding [1] to heat equations with time-dependent Dirichlet boundary conditions. Our approach combines a discrete method of images with a forcing-term reformulation, transforming the original discrete-time evolution of the PDE into a symmetric Markov chain compatible with the QFF framework. This provides the first application of QFF to option pricing [2] and, more broadly, extends QFF beyond the class of PDEs with periodic boundary conditions [3,4]. We establish complexity bounds for the resulting algorithm and identify conditions under which it achieves a polynomial quantum advantage over classical finite-difference methods.

[1] Apers, Simon and Alain Sarlette (2018). “Quantum Fast-Forwarding: Markov Chains and Graph Property Testing”. In: arXiv preprint arXiv:1804.02321. Team SECRET, INRIA Paris, France; QUANTIC lab, INRIA Paris, France; Department of Electronics and Information Systems, Ghent University, Belgium. url: <https://arxiv.org/pdf/1804.02321>

[2] Herman, Dylan et al. (2026). Quantum Speedups for Derivative Pricing Beyond Black-Scholes. arXiv: 2602.03725 [quant-ph]. url: <https://arxiv.org/abs/2602.03725>.

[3] Linden, Noah, Ashley Montanaro, and Changpeng Shao (2022). “Quantum vs. Classical Algorithms for Solving the Heat Equation”. In: Communications in Mathematical Physics 395, pp. 601–641. doi: 10.1007/s00220-022-04442-6. url: <https://doi.org/10.1007/s00220-022-04442-6>.

[4] Devereux, Ellen and Animesh Datta (2025). “Quantum algorithms for solving a drift–diffusion equation”. In: arXiv preprint. arXiv: 2505.21221 [quant-ph]. url: <https://arxiv.org/abs/2505.21221>.

Hybrid HPC and quantum computing framework for multiscale modelling of chemical systems

Presenter: Joseph Thacker[†]

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We present a multiscale workflow that couples quantum computing algorithms for quantum chemical calculations with conventional High-Performance Computing (HPC) software. The resulting embedding framework, implemented in the multiscale computational chemistry environment ChemShell, combines a generic N-layer subtractive Quantum Mechanics/Molecular Mechanics (QM/MM) scheme and active orbital space embedding for the quantum computing region. We have benchmarked the embedding models for gas phase and solvated molecules to understand the performance, benefits and current limitations of embedding quantum computing algorithms within a QM/MM model. We compare the performance of simulated Quantum Phase Estimation (QPE) calculations on an HPC cluster using Graphical Processing Units (GPUs) and Central Processing Units (CPUs).]