

Title: Quantum algorithms and architectures for the NISQ era: Can they really work?

Abstract:

In this talk I will offer an overview of my Oxford group's recent work targetting NISQ (noisy intermediate scale quantum) devices. This is an area of tremendous interest at the moment as we are starting to see quantum devices at, or beyond, the practical limits of simulation power of today's supercomputers. But of course the ability to build a machine that a conventional computer cannot simulate may be a long way from building something useful! Whether or not this can be done in the era before true fault tolerant quantum computers emerge is still an open question. For the answer to be affirmative we will need progress in harnessing the power of shallow circuits with, e.g., better quantum variational algorithms, as well as novel techniques to efficiently mitigate errors, and optimised architectures that recognise the needs of hybrid classical-quantum software. I will discuss these themes and indicate the key challenges.

My group have recently studied and reported a variety of NISQ applications ranging from simulation of general open systems [1] to specific novel uses in quantum chemistry [2]. These approaches involve seeking a ground state, and can be adapted to a yet-more diverse range of problems including the optimal compilation of quantum circuits [3]. Can approaches of this kind be impactful on real-world problems? Efficient exploration of the space spanned by the variational circuit, or ansatz, is crucial and I will describe our work using imaginary time a.k.a. Natural Gradient as a one of the most effective options [4]. Achieving results of practical significance beyond the QIP field will also require using 'every trick' to control errors; our group is among those that pioneered quantum error mitigation techniques [5], which can now be extended to incorporate concepts such as automatic learning and adaption to cancel noise [6]. The question of optimal architectures then arises, and 'multicore NISQ' has emerged as an idea from the work of group member Zhenyu Cai [7]. I will also describe QuEST, the Quantum Exact Simulation Toolkit [8], an open source tool which our group has developed to explore all these ideas through numerical simulation.

[1] Theory of variational quantum simulation, Xiao Yuan, Suguru Endo, Qi Zhao, SCB, Ying Li, available as arXiv:1812.08767 published in Quantum 3, 191 (2019), and Variational quantum simulation of general processes, Suguru Endo, Ying Li, SCB, Xiao Yuan, arXiv:1812.08778 published as Phys. Rev. Lett. 125, 010501 (2020).

[2] Variational

quantum algorithms for discovering Hamiltonian spectra, Suguru Endo, Tyson Jones, Sam McArdle, Xiao Yuan, SCB, available as arXiv:1806.05707 and published in Phys. Rev. A 99, 062304 (2019), and

Quantum computation of molecular vibrations, Sam McArdle, Alex Mayorov, Xiao Shan, SCB, Xiao Yuan, To appear in Chemical Science, available as arXiv:1811.04069 and published as Chem. Sci., 2019, 10, 5725.

[3] Quantum compilation and circuit optimisation via energy dissipation, Tyson Jones and SCB, arXiv:1811.03147

[4] Variational ansatz-based quantum simulation of imaginary time evolution, Authors: Sam McArdle, Tyson Jones, Suguru Endo, Ying Li, SCB, Xiao Yuan, available as arXiv:1804.03023 and published in npj Quantum Information 5, 75 (2019), and Quantum natural gradient generalised to non-unitary circuits, Bálint Koczor, Simon C. Benjamin, arXiv:1912.08660.

[5] Practical Quantum Error Mitigation for Near-Future Applications, Suguru Endo, Simon C. Benjamin, Ying Li available as arXiv:1712.09271 and published in Phys. Rev. X 8, 031027 (2018).

[6] Learning-based quantum error mitigation, Armands Strikis, Dayue Qin, Yanzhu Chen, Simon C. Benjamin, Ying Li, arXiv:2005.07601.

[7] Resource Estimation for Quantum Variational Simulations of the Hubbard Model, Zhenyu Cai, available as arXiv:1910.02719 and published in Phys. Rev. Applied 14, 014059 (2020). (This paper introduces the ‘multicore NISQ’ concept as an enabler for practical quantum advantage).

[8] QuESTlink -- Mathematica embiggened by a hardware-optimised quantum emulator, Tyson Jones, Simon C Benjamin, available as arXiv:1912.07904 and published in Quantum Sci. Technol. (2020) doi.org/10.1088/2058-9565/ab850

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