SAND2017-0164C

Co-design strategies for quantum simulators

Jonathan E. Moussa*, Andrew D. Baczewski†, and Mohan Sarovar‡

Sandia National Laboratories, Albuquerque, NM 87185, USA

Abstract

At this stage in the development of quantum simulation, collaborative relationships are essential. We must bring together stakeholders working to simulate quantum systems on analog quantum simulators, digital quantum computers, and digital classical computers. Targeted strategies for co-design between abundant classical computing resources and limited quantum hardware will have the most impact in the near-term. We outline possible directions for such co-design and present recommendations pertinent to near-term quantum testbeds.

Analog and digital quantum simulation have the potential to elucidate the electronic structure of chemical and material systems governed by equations recognized as "much too complicated to be soluble" by classical means as early as 1929 [1]. Quantum hardware promises to address this through an exponential reduction in resources relative to classical hardware. However, current quantum hardware is restricted to small numbers of physical qubits and the "best" qubit technology remains an open question. Analog quantum simulation is possible using noisy physical qubits, though the influence of this noise on results is an open research question [2, 3]. General-purpose digital quantum simulation requires many error-corrected logical qubits, but the construction of a single logical qubit is yet to be achieved. Even though digital classical computers are at an exponential disadvantage, their maturity and abundance have led generations of electronic structure theorists to develop many practical approaches, from exact but inefficient direct diagonalization to approximate but efficient mean field theories. Further, inspiration from these approaches is evident in virtually all of the literature on quantum simulation with quantum hardware. While we are not optimistic that quantum hardware will revolutionize quantum simulation in the near-term (e.g., five years), collaboration between these communities is critical if such a revolution is ever to take place. A quantum testbed program will have the most impact if it encourages strong interactions between stakeholders in the quantum information science community and the computational physics and chemistry communities, in order to develop *strategies for co-design combining abundant classical computing resources with limited quantum hardware*. Such an effort will focus on the development of hybrid classical-quantum algorithms and methodologies to get the most utility out of all available computing resources and push the boundaries of large-scale quantum simulation. In the following we outline the most promising directions for co-design strategies and conclude with recommendations for how near-term quantum testbeds could address these issues.

We should expect quantum resources in the foreseeable future to be tightly integrated with much larger classical computers. On such a hybrid classical-quantum simulator it is not clear how to distribute the work of a quantum simulation, even for specific tasks such as electronic structure calculations. The classical computer is expected to form the basis functions and matrix elements that define a quantum system being simulated, by co-opting and refining established electronic structure methods and software. Ground state preparation might require the classical optimization of a variational quantum state [4] or follow a predetermined process such as the quantum Metropolis algorithm [5]. The atomic coordinates and high-energy electronic orbitals in an atomistic simulation are effectively classical and can probably be tracked by classical computers. However, there is no available methodology

*jemouss@sandia.gov
†adbacze@sandia.gov
‡mnsarov@sandia.gov

for hybrid classical-quantum simulations on hybrid hardware and no established criteria for reliable classical-quantum partitioning. Whereas traditional embedding methods determine whether a classical or quantum description is appropriate for each subsystem, we now must also determine whether classical or quantum computing resources should be used to simulate it. This is a critical co-design issue that requires further study.

Even with significant approximations (e.g. density functional theory (DFT)) and abundant resources, simulating quantum systems on classical computers is still expensive. DFT simulations are typically limited to thousands of atoms, while cheaper simulations of classical molecular dynamics can be pushed to millions of atoms to reduce finite-size artifacts. This drives the development of classical-quantum embedding methods [9] and parameterization of classical interatomic potentials using large amounts of DFT reference data [10]. More accurate but more scarce quantum computing resources will inevitably add a layer of quantum-quantum embedding [11] and contribute to the large body of reference data used to develop new classical approximations of quantum systems.

The development of one reliable logical qubit will involve more physical qubits (> 100) than can be directly simulated on foreseeable classical computers. Such a quantum device will be trivial to simulate when operated as a reliable digital quantum computer within a two-dimensional Hilbert space but difficult to simulate when the underlying noisy physical qubits are operated more generally on an intractably large Hilbert space. We expect *quantum supremacy* to be established along this development path, when noisy qubits are operated to produce a distribution of measurement outcomes that cannot be approximated efficiently on a classical computer [6, 7, 8]. This is a worst-case separation between classical and quantum computational complexity. Of more relevance to practical quantum simulation is a typical-case separation when devices are operated to mimic real materials. We do not yet know how to distinguish robust quantum supremacy from quantum simulations where noise enables efficient classical approximations. Resolving this issue is critical to understanding the quantum information processing advantage over classical algorithms when simulating real materials.

Even at this early stage, a testbed program will make vital connections between quantum hardware engineers and quantum simulation end users. While size, noise, and reconfigurability are all key dimensions along which testbed hardware will be assessed, we specifically recommend that reconfigurability be an early focus for quantum hardware engineers. This will ensure that a wide array of applications can be accommodated to attract a diverse pool of users (e.g., computational chemists and materials scientists), rather than focusing on the most natural applications (e.g., 1D/2D quantum spin systems) that will attract smaller niche communities.

Whether they are integrated with conventional supercomputing centers or housed in their own facilities, future quantum hardware could have as large an impact as existing DOE user facilities. Emerging quantum testbeds herald this future and serve to gauge the relative progress of classical and quantum computing resources in performing quantum simulation tasks from proof-of-principle experiments to the inevitable future of quantum supremacy. We summarize our narrative as a list of recommendations for co-design oriented scientific priorities of a quantum testbed:

1. Develop a methodology for reliable classical-quantum partitioning and hybrid simulation.
2. Adapt existing electronic structure software to utilize both classical and quantum computers.
3. Generate quantum reference data with quantified uncertainties to validate classical methods.
4. Study the effects of noise on quantum simulation complexity to guide classical approximations.
5. Focus efforts on reconfigurability of quantum hardware to address the needs of many users.

Addressing these priorities will guide a smooth transition from the simulation of quantum systems on today's classical computers to the hybrid classical-quantum simulators of the near future.

References

[1] P.A.M. Dirac, *Quantum Mechanics of Many-Electron Systems*, Proc. Roy. Soc. A **123**, 792 (1929).

[2] P. Hauke, F. M. Cucchietti, L. Tagliacozzo, I. Deutsch, and M. Lewenstein, *Can one trust quantum simulators?*, Rep. Prog. Phys. **75**, 082401 (2012).

[3] M. Sarovar, J. Zhang, and L. Zeng, *Reliability of analog quantum simulation*, EPJ Quantum Tech. **4**, 1 (2017).

[4] J. R. McClean, J. Romero, R. Babbush, and A. Aspuru-Guzik, *The theory of variational hybrid quantum-classical algorithms*, New J. Phys. **18**, 023023 (2016).

[5] K. Temme, T. J. Osborne, K. G. Vollbrecht, D. Poulin, and F. Verstraete, *Quantum Metropolis sampling*, Nature **471**, 87 (2011).

[6] S. Boixo, S. V. Isakov, V. N. Smelyanskiy, R. Babbush, N. Ding, Z. Jiang, J. M. Martinis, and H. Neven, *Characterizing Quantum Supremacy in Near-Term Devices*, arXiv:1608.00263 (2016).

[7] K. Fujii, *Noise Threshold of Quantum Supremacy*, arXiv:1610.03632 (2016).

[8] S. Aaronson and L. Chen, *Complexity-Theoretic Foundations of Quantum Supremacy Experiments*, arXiv:1612.05903 (2016).

[9] M. J. Field, P. A. Bash, and M. Karplus, *A combined quantum mechanical and molecular mechanical potential for molecular dynamics simulations*, J. Comput. Chem. **11**, 700 (1990).

[10] A. P. Bartók, M. C. Payne, R. Kondor, and G. Csányi, *Gaussian Approximation Potentials: The Accuracy of Quantum Mechanics, without the Electrons*, Phys. Rev. Lett. **104**, 136403 (2010).

[11] S. R. White, *Numerical canonical transformation approach to quantum many-body problems*, J. Chem. Phys. **117**, 7472 (2002).