Daley, A. J., Bloch, I., Kokail, C., Flannigan, S., Pearson, N., Troyer, M., & Zoller, P. (2022).
Practical quantum advantage in quantum simulation. Nature, 607(7920), 667-676.
https://doi.org/10.1038/s41586-022-04940-6

Practical Quantum Advantage in Quantum Simulation

Andrew J. Daley,[1,*] Immanuel Bloch,[2,3,4] Christian Kokail,[5,6] Stuart Flannigan,[1] Natalie Pearson,[1] Matthias Troyer,[7] and Peter Zoller[5,6]

[1] *Department of Physics and SUPA, University of Strathclyde, Glasgow G4 0NG, UK*
[2] *Max Planck Institute of Quantum Optics, 85748 Garching, Germany*
[3] *Ludwig Maximilians University, 80799 Munich, Germany*
[4] *Munich Center for Quantum Science and Technology, 80799 Munich, Germany*
[5] *Universität Innsbruck, 6020 Innsbruck, Austria*
[6] *Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, 6020 Innsbruck, Austria*
[7] *Microsoft Corporation, Redmond, WA, USA*

(Dated: August 31, 2022)

The development of quantum computing across several technologies and platforms has reached the point of having an advantage over classical computers for an artificial problem, a point known as "quantum advantage". As a next step along the development of this technology, it is now important to discuss *practical quantum advantage***, the point at which quantum devices will solve problems of practical interest that are not tractable for traditional supercomputers. Many of the most promising short-term applications of quantum computers fall under the umbrella of quantum simulation: modelling the quantum properties of microscopic particles that are directly relevant to modern materials science, high energy physics, and quantum chemistry. This would impact several important real-world applications, such as developing materials for batteries, industrial catalysis or nitrogen fixing. Much as aerodynamics can be studied either through simulations on a digital computer, or in a wind tunnel, quantum simulation can be performed not only on future fault-tolerant digital quantum computers, but already today through special-purpose analogue quantum simulators. Here we overview the state-of-the-art and future perspectives for quantum simulation, arguing that a first practical quantum advantage already exists in the case of specialised applications of analogue devices, while fully digital devices open a full range of applications but require further development of fault-tolerant hardware. Hybrid digital-analogue devices that exist today already promise substantial flexibility in near-term applications.**

* andrew.daley@strath.ac.uk

I. INTRODUCTION

Quantum computers have potential for medium to long-term wide-ranging impact on demanding computing tasks in many areas of modern society and industry – with proposed applications that range from materials science and chemistry to logistics and optimisation, encryption and information security, as well as artificial intelligence [1–3]. The power of quantum computers arises from the physical properties of the microscopic building blocks of nature, which are described by quantum mechanics, and for which the complexity of classically simulating a system can grow exponentially with the system size [4, 5]. However, determining how to take advantage of these properties in order to solve complex computational tasks is often very challenging. This is not "business as usual" for algorithm design [6], and often involves a completely different approach to solving a computing task than what was traditionally applied on a classical computer. Indeed, so-called quantum-inspired algorithms have been developed in recent years, allowing faster calculations on existing classical computers by taking different approaches to computing challenges, motivated by quantum algorithms (see, e.g. [7]). Recent demonstrations of the potential advantage of quantum computers over classical computing have generally been for artificial problems tailored to the specific setup [8–10]. Establishing a *practical quantum advantage* over classical computers, which we understand as involving *relevant* academic or commercial problems that are useful beyond testing the quantum hardware, is widely acknowledged to be a difficult step.

In looking for an early practical quantum advantage in near-term quantum computing, it is best to consider the simulation of quantum mechanical systems [11, 12]. This is the "native" and most natural application of quantum computers, where we aim to use a quantum computer to mimic the rules that describe physical microscopic quantum systems. These problems are computationally challenging for the same underpinning reason that quantum computers can be powerful. While systems in classical physics exist in just one configuration, in quantum mechanics different configurations can coexist at the same time in a *superposition* of all of the possible states in

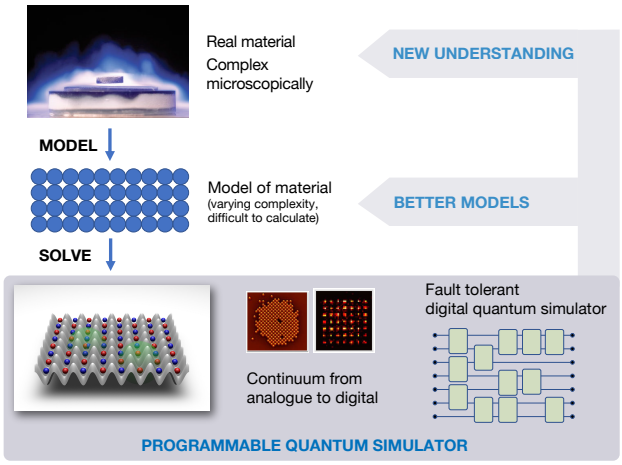


FIG. 1. **Overview of quantum simulators**. Understanding the physical properties of real and promising materials (depicted is a magnet, floating above a superconductor when this is sufficiently cold) often requires theoretical models that simplify the material enough to make it treatable. Such models could treat a material as a rigid lattice of interacting particles (depicted in blue in the figure), but even these models may be too complex to be calculated exactly. A range of these computational tasks could be mapped onto programmable quantum simulators, with digital and analogue means to approach these problems - much in the same way as classical aerodynamics uses wind tunnels in combination with digital computing. Problems could be solved on a fault-tolerant digital quantum computer (shown bottom right in the form of a circuit, where lines correspond to single qubits and boxes represent operations between qubits) or we can build a scale model of the problem in an analogue quantum simulator (depicted bottom left as an array of atoms, blue and red for different species, trapped in an optical lattice represented in grey). A range of programmable quantum simulators are now under development, looking to increase the programmability of analogue devices, and combine these with variational digital algorithms. Through the insights gathered from quantum simulators we can build better models or obtain new understanding of the modelled materials.

the system [4]. In this way, the complexity of classically simulating the problem can grow exponentially with the number of particles. This is particularly important when we start to look at problems describing the behaviour of electrons in materials, or in large molecules, as we encounter in quantum chemistry. Beyond the initial difficulty of writing a model that captures the full complexity of the real physical system, any model we construct to describe these real-world scenarios needs to deal with a large number of interacting particles. The direct solution of these models typically goes beyond the capabilities of classical supercomputers. In some cases, such as in quantum chemistry good existing approximate methods mean that we need many digits of precision to gain a practical advantage over existing approximate classical solutions [13]. But there are many puzzles in describing solid state materials where even the qualitative behaviour is not decided by classical computation, and accurately solving simplified models can provide significant insight [14] – both directly for the materials, and for validating and calibrating approximate classical calculation methods.

As depicted in Fig. 1, there are two ways to approach such problems via quantum simulation [12], the first of which is to use a digital quantum computer [32, 33], designed in analogy to modern classical computers. There, the computation is divided into a series of discrete "gate" operations that are used to manipulate information stored on quantum mechanical systems [4, 6]. This form of *digital* quantum computing provides the possibility to perform error correction [34] on imperfect implementations of the gates, with the potential for fault-tolerant operations enabling large scale quantum computations. Up to now, only certain aspects of error correction have been demonstrated for very small numbers of qubits and for a limited set of errors, and in order to make progress, most devices operate without any quantum error correction. This current situation is sometimes referred to as "Noisy intermediate-scale quantum (NISQ) computing" [35]. As noise severely limits the number of operations that can be carried out on such a device, the early demonstrations of the power of a quantum computer have worked closer to the native hardware, such as randomised sequences of native gate operations, as first shown by the result in 2019 from Google [9]. This also extends to specialised non-programmable devices built to demonstrate the complexity of quantum dynamics, such as Boson Samplers in the form demonstrated by several groups, including recently by USTC [10]. Going beyond these demonstrations, which we often refer to as showing *quantum primacy* for specific problems, the difficulty in looking for practical quantum advantage in near-term quantum computing, is that many of the algorithms developed require a large number of gate operations, far beyond the ability of NISQ devices without error correction.

While fault-tolerant digital quantum computers are still under development, we can already build "analogue quantum simulators" that allow us to compute quantum dynamics in a similar sense to how wind tunnels allow us to understand aerodynamics [5, 11, 12, 36]. They are special purpose analogue computers, which come with the restriction that you have to be able to realise a model to study directly in the laboratory. The major advantage is that these can readily scale to large system sizes, making them a natural frontier to search for a practical quantum advantage relative to classical simulations. There are a variety of experimental platforms allowing for the realisation of analogue quantum simulation, including but not limited to neutral atoms [20, 21], superconducting systems [19, 23], trapped ions [16, 17], and photons [18, 24]. In Box 1, we give more information on the state-of-the-art of these platforms with examples of physical models that they can simulate. We expand on one of these models, the Hubbard model, as a specific example in Box 2.

Already in the last years, these devices have been pro-

Box 1: Example Platforms for Analogue Quantum Simulation

Analogue Quantum Simulations are today performed on a variety of platforms [15–20], each of which offer distinct features that make them more suitable for specific simulation tasks.

Ultracold atoms in optical lattices – Currently up to 3000 atoms in optical potentials with single atom detection and control via so-called quantum gas microscopes. These uniquely implement models of interacting fermionic particles (such as the Hubbard model, see Box 2) or its bosonic variant using bosonic atoms. Spin models can also be engineered, with tailored

The model is deceptively simple in its construction, describing electrons of two spin components located in one orbital at each site, and involving tunneling of electrons between neighbouring sites (described in the Hamiltonian $H = -J\sum_{\langle i,j\rangle,\sigma} \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ by an annihilation operator removing a particle of spin $\sigma \in \uparrow,\downarrow$ from site i, $\hat{c}_{i\sigma}$, and a creation operator placing it on the neighbouring site j, $\hat{c}^\dagger_{\sigma i}$ with an amplitude J), and interactions when two particles of opposite spin are in the same orbital (represented by the operator for the number of particles on site i, $\hat{n}_{i\sigma} = c^\dagger_{\sigma i}c_{\sigma i}$ and an energy shift U).

The Hubbard model (and several of its generalisations) can be realised with cold atoms in optical lattices, where fermionic atoms represent the electrons, and are trapped in an interference pattern of light formed by overlapping many laser beams, with tunable interparticle interactions. Quantum gas microscopy has made it possible to take full spin and charge resolved photographs of such systems, revealing complex interplay of magnetic ordering and mobile dopants at a microscopic level [21]. The Hubbard model and its generalisations to multiple bands allow us to explore electronic systems close to a Mott transition, which is relevant for understanding a range of strongly-correlated materials, beginning with high-Tc superconductors [29]. Strong correlation in this form appears in many materials including heavy metals with electrons in d and f orbitals, which are important in a range of materials, including for batteries and catalysis [30]. For microscopically quantitatively accurate models we then need to include long-range hopping and exchange in addition to the terms present in the Hubbard model, but this could be explored in fault-tolerant digital quantum simulators [31].

viding insight into scientific problems, ranging from long-standing questions on the influence of disorder on quantum dynamics (see, e.g. [37]) and underlying physics that gives rise to high-temperature superconductors (see, e.g. [38]), to systems with topological properties [39, 40], and dynamics in spin systems with both short [41, 42] and long-range interactions [43–45]. Even today, these platforms are well-calibrated and provide quantitative measurements, e.g., of correlation functions, transport coefficients and dynamical exponents. As we will note below, the ultimate quantitative limitation of an analogue system without error correction is set by the calibration accuracy of the model that is implemented – this is where fault tolerant digital quantum simulation will eventually have an advantage in specified accuracy and in the broader programmability for more complex models, at the cost of substantial overhead in required hardware resources and computation time.

From a computational point of view, the dynamics of an analogue quantum simulator can be seen as a highly entangling operation on all of the particles/spins/qubits in the system, with time-dependent control. This can

also be combined for spin systems with operations from digital quantum computing, leading to a range of possible *programmable quantum simulators*[2, 17, 21, 46], which combine analogue elements with programmability. This provides a particular opportunity to scale to large sizes and to address problems of practical relevance, especially in variational approaches to quantum simulation problems.

In the remainder of this article, we will address the limitations of classical calculation of quantum dynamics, and the opportunities and challenges of quantum simulators. We will then analyse the potential for practical quantum advantage, again comparing state-of-the-art classical numerical methods to analogue and digital quantum simulators.

The first question is in which steps we go beyond **quantum primacy**, where we solve problems that are not accessible to classical computers primarily to demonstrate the abilities of quantum hardware. A first **practical quantum advantage** in this sense is offered by analogue quantum simulators, which can be quantitatively verified, with a precision that is ultimately dependent on the calibration of the hardware. These will be able to address the properties of models that can be natively realised within given hardware. The broader interest in solving these relevant problems (e.g., for the purposes of solid-state physics and materials science) takes us a step beyond quantum primacy, and can be further extended within programmable analogue quantum simulators. While these systems already allow us to explore qualitative elements of solid-state physics that underpin quantum materials science, with the addition of verification, these platforms have the potential to perform verified quantitative simulations of such models, both directly and through variational techniques (similar to NISQ hardware, but using the full analogue programmability of the system). In future, the realisation of **practical quantum advantage with digital quantum simulation on fault tolerant quantum computers** will remove restrictions on the models we can implement, and provide the potential for arbitrarily accurate calculations at a trade-off of increasing resources in terms of computation size and time.

We conclude below in broad terms that a first practical quantum advantage is already available with programmable analogue simulators for relevant problems – especially involving out-of-equilibrium dynamics in 2D. Going beyond this using a digital gate-based approach will most likely require development of fault-tolerant quantum hardware – which underlines the importance both of developing fault-tolerant hardware, and of understanding and utilising analogue devices in the era of NISQ Computing, where we stand at present. We give perspectives for analogue and digital devices, and emphasise the importance of combining existing digital and analogue techniques over the coming years.

II. CHALLENGES AND STATE-OF-THE-ART FOR SIMULATING QUANTUM DYNAMICS ON CLASSICAL COMPUTERS

In order to evaluate the opportunities and potential practical quantum advantage provided by quantum simulators, it is important to note the challenges in simulating many-body quantum dynamics on a classical computer. As mentioned above, this arises because of the huge number of configurations a system can take, which grow exponentially with its number of constituent particles (e.g., doubling every time we add another constituent building block). This makes even storing such a state on the most powerful existing supercomputers a challenging task in general once the system grows beyond a very small size (often of the scale of 50 quantum spins). To simulate a quantum system on a classical computer, we then in some sense need to either compress or sample from this exponentially large space. While this can be done efficiently for some systems in nature, for other relevant problems the time cost of the calculations grows exponentially with the system size for all known methods. We note that for some problems there are methods with uncontrolled approximations (including mean-field techniques) that can represent dynamics qualitatively and sometimes quantitatively for systems in some parameter regimes. But to be reliable in general these need to be benchmarked against simulations with controlled approximations. Indeed, one early application of quantum simulation will be to benchmark these methods. For this reason, we specifically consider general classical methods with controlled approximations.

A. Lowest energy state calculations

When calculating properties of a quantum system, we are typically interested either in calculation of the lowest energy states of a system (or specific excited states), or its time evolution. Both of these can be specified in terms of the total energy function, or Hamiltonian, H of the system. Typically, calculation of the lowest energy state is a simpler classical problem, because physical systems with local interactions between particles often lead to a much more limited range of possibilities than space of all possible solutions. It is therefore sometimes possible to sample the relevant states, or compress the number of parameters we store, rather than considering the whole exponentially large space. This can remove the exponential scaling, at least in terms of memory requirements. The last decades have seen many advances in classical methods for many-particle systems, and across Physics, Chemistry, and materials science there are large subfields dedicated to developing new computational methods. This also makes the bar for a practical quantum advantage a *constantly moving target*. Nonetheless, lowest energy state calculations remain elusive for many models, with the Hubbard model a particularly good example (see Box

2) [27, 28]. For example, while there has been tremendous progress made possible by Quantum Monte-Carlo methods over the past decades [47–49], path-integral monte-carlo calculations face the challenge of the so-called "sign problem" in sampling. This sampling problem has been shown to be NP-Hard, in the sense that a generally applicable solution to the specific issues encountered would be equivalent to proving that NP problems are solvable in polynomial time [50].

B. Quantum dynamics

In non-equilibrium dynamics (such as a quantum quench, when a parameter of the Hamiltonian is suddenly changed) we start from an initial state and observe how it evolves. An isolated quantum system then tends to explore a large part of the entire configuration space with its exponential-in-system-size growing number of quantum states, making such kinds of problems the most challenging and intractable for a classical computer. This is often connected with the notion of scrambling of information in quantum systems, where all degrees of freedom of the problem become important [51, 52], and we cannot apply classical methods that rely on compressing the state using a properly chosen basis. This also makes quantum dynamics a particularly good example for identifying the regimes of practical quantum advantage, as quantum information scrambling gives good arguments that the states cannot be compressed in the way that is often possible for lowest energy states. We will therefore focus on out-of-equilibrium dynamics in our analysis below.

To calculate the dynamics of a quantum system, we usually need to compute a time-evolution operation, which is expressed in terms of the Hamiltonian of the system, H. For Hamiltonians that are the sum of terms acting on different parts of the system H_l, the time evolution operator can be broken up via a Trotter decomposition as $\exp(-\mathrm{i}H\delta t/\hbar) = \prod_l \exp(-\mathrm{i}H_l\delta t/\hbar) + O(\delta t^2)$ with time-step δt. In practice, higher-order Suzuki-Trotter or other expansions are used [53]. The result is a time evolution with controlled error [54–57].

The ultimate constraint on classical methods for generic time evolution is that the state space occupied in quantum quench dynamics grows exponentially in time. State-of-the art methods for compressing the state in order to compute quantum dynamics with controlled approximations and errors are based on tensor network techniques (including time-dependent Density Matrix Renormalisation Group, Projected Entangled Pair States, and a variety of other configurations) [58–60]. These methods serve to compress the representation of the state from an exponentially large number of coefficients into a smaller, tractable representation. This works well when the time-evolving state has limited levels of quantum entanglement [61], and these methods are often excellent for computing low-energy states or near-equilibrium dynamics, especially in 1D systems with local interactions, where we expect the entanglement to be small [58–60]. They are also the best methods available for general non-equilibrium dynamics on classical computers. However, as noted above, for a general time evolution, rapidly growing entanglement still leads to an exponentially growing computational cost of the calculation.

III. QUANTUM SIMULATORS

Through direct implementation on quantum hardware, quantum simulators avoid the potential for exponential scaling in memory, and the time cost associated with manipulating or sampling this. The runtime cost of the computation could still be substantial (and even maybe exponential in some cases), especially for finding the lowest energy states, but for time evolution starting from a large class of initial states, the runtime cost can be reduced to a low order polynomial in the duration of the evolution, both on analogue and digital quantum simulators.

A. Analogue Quantum Simulators

In an analogue quantum simulator [11], the system is capable of implementing specific classes of models, and is engineered to implement a chosen model with well-calibrated parameters. The lowest energy state could then be found e.g., by starting from a simple, well controlled Hamiltonian and a well defined initial state of the system and then blending over very slowly to the more complex Hamiltonian. This approach is akin to the concept of an Adiabatic Quantum Computer (AQC) [62], but in a restricted sense, as one typically cannot control all degrees of freedom of the system to realise a universal AQC. We note that depending on the Hamiltonian, although a quantum simulator avoids exponential scaling for memory requirements, the runtime for producing lowest energy states adiabatically can still scale exponentially with the system size – in fact finding a ground state is at least as difficult as running an arbitrary quantum computation [63]. Simulation of dynamics out-of-equilibrium involve engineering the initial state, and then evolving the system under the Hamiltonian that has been engineered, with a linear cost in time because we directly observe the native time evolution.

The limitations of analogue quantum simulation can be grouped into two parts. Firstly, we only have access to models for which we can realise the Hamiltonian directly in the analogue simulator. Secondly, without error correction these systems are susceptible in general to calibration errors (including imperfectly implemented Hamiltonians, parameter calibration), as well as decoherence and noise. However, both the Hamiltonian and decoherence and noise processes can be determined from first principles, allowing us to diagnose errors in

current experiments either in terms of the many-body state, or on a practical level, in correlation functions that we would measure in experiments. Furthermore, one can estimate calibration errors directly from Hamiltonian learning techniques, which we will discuss below. One can similarly estimate errors due to initial state preparation and measurement techniques.

There are general arguments that especially for local models, the growth of errors due to imperfect calibration can be bounded, making analogue quantum simulation quantitatively reliable to an accuracy of a similar level as the calibration errors themselves [64]. The ultimate limit for analogue quantum simulation is then set by the decoherence timescale, which provides an upper bound on the timescale on which we can controllably observe coherent quantum dynamics. But this is generally well beyond the timescales accessible in classical calculations, allowing for regimes of practical quantum advantage to be achieved.

B. Fault-tolerant digital quantum simulators

Many of the algorithms used on a classical computer can be modified for use on a fault-tolerant digital quantum computer, and vice-versa [33]. This includes a range of methods calculating lowest energy states that can be adapted, as well as time evolution methods - including those based around Suzuki-Trotter decompositions of the time evolution, as described above [53]. The great strength of digital quantum simulators is the possibility to realise any desired Hamiltonian of the system [65, 66], providing opportunities to study wide-ranging models with no need to engineer this directly in the laboratory. While algorithms to prepare complex low-energy states could still scale exponentially in time, evolving a prepared initial state could be performed to arbitrary accuracy with a polynomially growing cost. Specifically, with decoherence, noise, and most calibration errors suppressed, the residual errors in computing time evolution would be model calibration errors from the non-zero Trotter timestep [32, 54, 55], which can be made arbitrarily small by increasing the length of the computation polynomially. There is a range of further methods beyond Trotter decompositions that provide more efficient convergence with the error tolerance, which can be implemented on fault tolerant digital quantum computers [67–70], giving fault-tolerant devices a clear advantage for the high-accuracy calculations needed, e.g., for many applications in quantum chemistry.

The catch is that in practice, algorithms to compute the time evolution would require a long calculation on a large fault-tolerant quantum computer. As with other fault-tolerant quantum computations, this comes with an overhead for error correction based on the gate fidelities, with a tremendous overhead in the number of required qubits and runtime to implement quantum error correction. We will give quantitative estimates of the number of gates required to reach the regime of quantum advantage in the next section.

IV. PRACTICAL QUANTUM ADVANTAGE IN ANALOGUE AND DIGITAL QUANTUM SIMULATION

We now address the question of quantum advantage and the present state-of-the-art. It is important to recognise that the threshold for quantum advantage remains moving target as classical algorithms continuously improve. Even for fully fault-tolerant digital quantum computing, where we have an exponential scaling advantage both for quantum simulation and other algorithms such as Shor's algorithm for factoring, there is no complexity proof that this advantage must hold for all future classical algorithms. However, we can make clear robust comparisons to well established classical algorithms, and have good general arguments, including both factoring and the simulation of general complex quantum dynamics, that it is an extraordinarily difficult task to produce an exponential improvement in the scaling of known classical algorithms. It is very unlikely that for general time evolution in quantum many-body systems, we will overcome the exponential scaling of classical calculations, as noted above.

Demonstrating a genuine practical quantum advantage then requires (A) showing that a quantum simulator can generate a reliable solution for a relevant problem beyond the bounds of classical simulation (with controlled errors), and (B) implementing techniques to verify or quantify the accuracy of a quantum simulation when it is operating beyond the capabilities of current classical simulations. This is the process undertaken in NISQ systems such as that of Google [9] and USTC [10], to demonstrate quantum primacy.

To illustrate this, we consider a dynamical evolution in which system parameters are abruptly adjusted (e.g., a quench) and the subsequent evolution of the system is tracked, which gives us the clearest comparison to state-of-the-art classical simulations as noted above. We take the example of a 2D Hubbard model with 10x10 lattice sites and 100 particles. We choose this size, as simulating dynamics for the time it would take particles to cross from one side of the system to the other is significantly beyond the capabilities of current classical simulators. We will compare the calibration requirements to reach errors below a few percent for analogue quantum simulators, and then identify the size requirements to match the accuracy of these analogue simulations on a fault-tolerant digital quantum computer. Finally, we will also consider the question of how to verify the solution in analogue hardware without fault-tolerance.

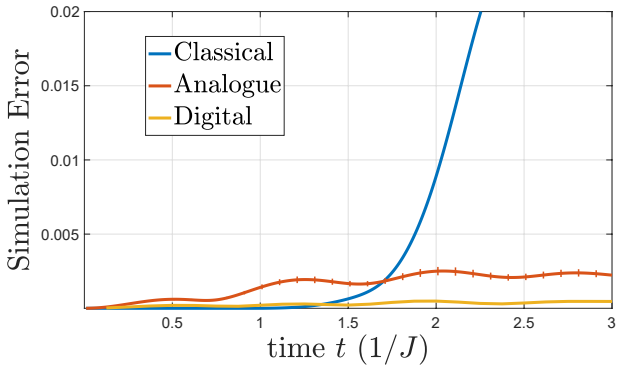


FIG. 2. **Quantum advantage of quantum simulators over classical simulation**. A future fault-tolerant digital quantum simulation will be able to compute dynamics with very small errors, controlled by the method for implementing the time evolution calculation (e.g. timestep errors in a Trotter decomposition). While analogue quantum simulation is affected over time by decoherence and propagation of calibration errors, these build up much more slowly than for the best available classical simulation, where once their limits are reached, errors will typically grow exponentially. To illustrate this, we use classical calculations for the errors in single-particle correlations $\sum_{n=1}^{20}\langle\hat{c}^\dagger_{10\uparrow}\hat{c}_{n\uparrow}\rangle/20$ arising for quench dynamics a 1D Hubbard model (see Box 2) for $U/J = 1$ and 20 sites, starting from half filling of each spin component, alternating on even and odd sites. (Blue) Single site time-dependent variational principle time-evolution using Matrix Product States with bond dimension D = 64 [58], as a demonstration of typical truncation errors from these classical methods relative to exact calculations, which are necessary for longer times and system sizes. (Red) Analogue simulation with calibration errors of 1% (error bars show the standard error from sampling a Gaussian distribution of Hamiltonian parameters). (Yellow) Digital simulation with a second order Trotter decomposition with a time-step $J\delta t = 1/8$.

A. Illustration of the regime of first practical quantum advantage for analogue and digital quantum simulators

Considering Hubbard model quench dynamics, we first identify the growth of errors based on comparison with classical simulations at short times. We give illustrative comparisons between classical simulations, and analogue and digital quantum simulators in Fig. 2. Once the capabilities of classical methods to represent the state of the quantum system reach the maximum computational capacity, errors in tracking the dynamics grow exponentially - measured either by the fidelity with which the state is represented, or the errors in estimates of measurable correlation functions. In contrast, for analogue quantum simulators we can determine an error budget, and find that errors are dominated by imperfect calibration and grow slowly and polynomially in time, as shown in Fig. 2. A 10x10 Hubbard model can be implemented in existing experiments [21], and the slow build-up of errors shown in Fig. 2 extends to 2D systems (see the supplementary material for further technical details of this comparison), so that calibration errors on the level of 1% provide reliable quantum simulation of dynamics (with errors below the percent level) [64, 71]. At longer times, the ultimate limit to the timescale for reliable calculation is decoherence, but for present experiments our example 10x10 lattice models with evolution times up to time $T = 10\hbar/J$ are clearly attainable.

In this sense, following the analysis of Ref. [71], we conclude that present experiments with cold atoms already operate in a regime of quantum advantage over state-of-the-art classical algorithms, for those models that can be natively implemented. We can make similar arguments for other quantum simulation platforms with well-controlled microscopic error and decoherence sources, including trapped ions [16, 17] and neutral atom arrays with Rydberg excitations [20, 72].

A truly fault-tolerant digital quantum computer would have only residual errors associated with Trotter timesteps, which are also shown in Fig. 2. The challenge is in building a large enough system of this kind. For our 10x10 Hubbard system evolving up to $T = 10\hbar/J$, we would require a minimum of 200 error-corrected logical qubits to store the system states, and over one million error corrected gate operations. To arrive at this number, we assume a Trotter decomposition for the time evolution, and allow timesteps as large as possible [54, 55] while matching the accuracy of the analogue quantum simulator for this problem, which is just below $1/J$ (so we take $1/J$ as our timestep for these estimates). This is extrapolated to keep the error in most observables to less than 1% over the time evolution. As described in the supplementary material, for these fixed, relatively large errors, Trotter decompositions are the most efficient available methods for systems with local interactions, and other methods that perform better in the limit of vanish error are less efficient here. The number of operations is then minimised by a 4th-order evolution [73], which we decompose into two-qubit gates with arbitrary connectivity (see the supplementary information for further details). We then require 2.6×10^5 2-qubit CNOT gates and 10^5 rotation gates to implement this time evolution, with the gate counts minimised by using ca. 20 further ancilla qubits [56, 57]. As the error budget is entirely used up in the Trotter error, we would then need to execute these gates to better than one part in 10^7, which is beyond all available NISQ hardware. To implement this on a fault-tolerant device we would need to decompose the rotations as ca. 30 fault tolerant T-gates per rotation, leading to the total of over 1 million gates (ca. 5 million for inhomogeneous systems).

The number of physical qubits required to implement this would depend on the fidelity of the physical digital gate operations, but near the threshold fidelity for digital quantum computing, would presently require several million physical qubits. In a digital NISQ machine, at the very least, many more gates operations would be re-

quired to trade off time-step errors in a simulation for gate errors, and obtaining errors of $< 1\%$ is beyond all presently available digital quantum computers.

For these quantum simulation problems, the hardware requirements for fault-tolerant digital systems are very demanding, and will require substantial further breakthroughs in development. But these systems bring a high pay-off in the flexibility of models that can be studied, and the applications, e.g., to broad classes of materials science and quantum chemistry problems once this is achieved, with the models unconstrained by what we can build physically in the laboratory.

B. Verification of quantum simulation

Based on an error budget above, we concluded that current analogue systems can already operate in a regime of quantum advantage. But the next step for experiments will be to verify the simulation being performed when it is beyond the bounds of classical simulation, i.e. in a regime where verification of the quantum device by direct comparison with classical computations is *a priori* not possible [74, 77]. Verification is also made difficult by the exponential scaling of the classical problem: direct verification on the level of the many-body quantum state, e.g. using techniques such as quantum state tomography, will similarly face the challenge of being exponentially costly.

A first method of verification in the regime of quantum advantage is cross-platform verification [74, 78]. This involves building two or more quantum devices, possibly on different platforms and employing different encodings of the many-body problem, but solving the same quantum task. By comparison we can gain confidence and build trust into the results predicted by the quantum devices. The situation is reminiscent of what we encounter when we want to verify the proper operation of atomic clocks operating today on the unprecedented level of 10^{-18} accuracy: we build several clocks, and we compare them. For two quantum simulators, such a comparison of predictions is readily performed by when we are interested in simple few-body expectation values that we can tabulate, e.g. properties of quantum materials. Cross-platform verification becomes challenging again when we wish to compare quantum simulation on the level of the full quantum many-body state, where – as remarked above – this comparison has an exponential overhead. There is an answer for this problem, although it is far from realisation with present technologies: instead of comparing the quantum states on a classical level, we employ quantum communication, i.e. teleportation of the quantum state [4] of the first simulator to the second to perform such a comparison.

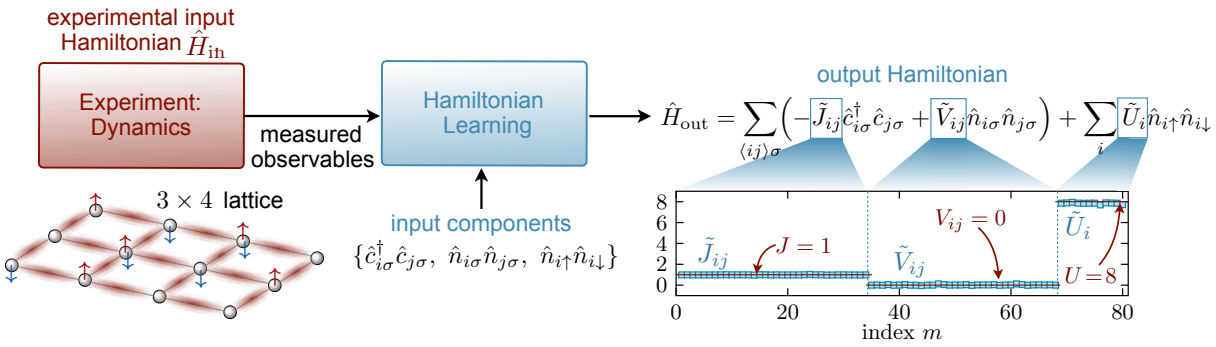
However, quantum simulation offers another intriguing route to ensure the proper functioning of a quantum device via the approach of Hamiltonian learning [74–76, 79–81]. In analogue simulation a Hamiltonian H is specified as the design goal to be implemented, and its implementation on the quantum device allows preparation of desired quantum states. Verification of quantum simulation via Hamiltonian learning takes the approach of "learning" the Hamiltonian back from the quantum device by making appropriate measurements on the quantum state stored in the quantum simulator. Comparing the design goal and reconstructed Hamiltonian provides an assessment of errors and functionality. Remarkably, this procedure is efficient, having only polynomial overhead, and thus also applies in the regime of quantum advantage. The key observation is that Hamiltonians of quantum many-body physics, and thus in quantum simulation only consists of a small number of terms. This is illustrated in Box 2 for the Hubbard model, where the parameter J characterises hopping of particles between adjacent sites, and U represents on-site interactions; and there is no other terms such as off-site interactions. Learning the Hamiltonian, instead of the quantum state, thus requires only determination of a small number of parameters in a tomographic reconstruction of the Hamiltonian. Hence the efficiency and potential scaling to the regime of quantum advantage. Box 3 provides an example of Hamiltonian learning and verification for the Hubbard model in non-equilibrium dynamics. The idea of Hamiltonian learning and verification is also readily applied to digital quantum simulation.

V. FUTURE PERSPECTIVES FOR PROGRAMMABLE QUANTUM SIMULATORS

We will now give a brief perspective on the development of programmable quantum simulators. In the case of analogue simulators, by the term "programmable", we highlight that the level of control is now such that in a variety of platforms we can realise a class of Hamiltonians with local control over parameters, as well as single-site resolved measurement, and typically local spin rotations. These are not universal, but already scale to large particle numbers for models that can be realised natively. In the future, we expect that fault-tolerant digital quantum simulators will give access to an even broader class of problems, but this requires further investment and hardware development. In the medium term, an exciting direction is to combine ideas from analogue and digital simulation, using the full programmability of analogue devices to implement NISQ algorithms, especially with variational approaches.

A. Analogue Quantum Simulators

In recent years, analogue quantum simulation has already begun to shed light on a wide range of scientific problems with lattice and spin models, across all of the platforms noted in Box 1. Some very recent examples include the exploration of out-of-equilibrium dynam-



The fact that quantum simulation is governed by a local Hamiltonian enables efficient verification via Hamiltonian learning in a regime inaccessible to classical simulations [74]. We illustrate this idea for non-equilibrium dynamics in a Hubbard model as introduced in Box 2 [21]. In our numerical simulations, fermionic atoms are placed in an antiferromagnetic configuration on the boundary of 3×4 lattice, and a quench with the input Hamiltonian $\hat{H}_{\rm in} = -J\sum_{\langle ij\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}$ $(U/J = 8)$ generates highly entangled states after about 4 hopping times $t \sim 4\,[1/J]$. In practice, the experiment has to be repeated several times for different time instances and local observables are measured at the end of each experimental run. Verification protocols based on Hamiltonian learning aim to reconstruct $\hat{H}_{\rm in}$ that governs the non-equilibrium dynamics [75, 76]. The starting point is an Ansatz consisting of polynomially many spatially local input components from which the output Hamiltonian $\hat{H}_{\rm out}$ is assembled and which determine the observables to be measured on the quantum system. The procedure infers the coefficients $\tilde{J}_{ij}$, $\tilde{V}_{ij}$ and $\tilde{U}_i$ of the input components from measurement data taken on the quantum simulator. As can be seen in the example above, terms not present in the input Hamiltonian like offsite density-density interactions $\hat{n}_{i\sigma}\hat{n}_{j\sigma}$ turn out to be zero. Here, the number of measurements required to estimate the coefficients up to a given error bar scales polynomially with the system size [76].

ics of the Hubbard model [38], disordered, interacting many-particle systems [82], topological phases of matter [39, 40, 83], robust features of out of equilibrium dynamics such as quantum many-body scars [41, 84], and Boson sampling as noted earlier [10]. In each case, analogue quantum simulators have allowed experiments to explore new dynamical features, and address previously inaccessible questions. One example of addressing existing questions is being able to directly investigate the interplay between disorder and interaction in 2D systems [37, 82], especially in determining the transition between localised and delocalised particles by observing expansion dynamics of particles on a lattice with controllable parameters in a quantum gas microscope. In terms of providing a new perspective on low-temperature behaviour in interacting systems of fermions, recent work has focussed on directly local measurements of correlations between particles and holes in the Hubbard model [38]. A wide range of controllability suggests possibilities to apply analogue quantum simulators to open problems in high energy physics [85], and the scrambling of information in black holes, including models connected with the holographic principle [86, 87], and there are also proposals in future for addressing quantum chemistry problems [88] as well as connecting to broader computations though universal hamiltonians [89, 90]. Beyond basic science, one of the areas of greatest potential is the application of these systems as programmable quantum sensors [91]. As noted below, a great opportunity also exists in hybridising these systems with digital operations to access a much wider range of physical models and problems beyond basic science.

B. Digital Quantum Simulators

Despite their resource cost, fault-tolerant Digital Quantum Simulators will open an even broader range of possibilities because we can implement any desired Hamiltonian without needing to engineer this in the laboratory. This will open the possibility to simulate processes in quantum chemistry [13, 92] and materials science [93, 94], where the effective models are often complex and involve long-range couplings. A lot of excitement around the potential to simulate the quantum chemistry of large molecules, for example, presupposes the potential to implement highly complex Hamiltonians. This is also especially important for the encoding of broader computational challenges (including, e.g., optimisation) on quantum dynamics, where the resulting Hamiltonians again generally involve long-range interactions [95, 96]. This underlines the importance for the area of quantum simulator of continuing work developing future fault-tolerant quantum computers.

C. Hybrid analogue-digital quantum simulators

A very exciting opportunity in the near-term, however, is the potential for programmable quantum simulators that begin with the capabilities of an analogue

system, and add the control from digital systems in different forms [97–102]. This is already progressing, [98] with random operations applied digitally being used for platform verification in analogue simulators [78], or the measurement of many-body entanglement in quench dynamics [98, 102, 103]. Hybridisation of analogue systems with classical digital computing is also underway, with recent small-scale demonstrations of variational quantum emulation, using a quantum system controlled by a classical optimiser to explore the lowest energy state of a many-body problem [99].

In these programmable hybrid quantum simulators, the dynamics governed by the system Hamiltonian essentially act as a many-particle operation as described in the introduction. This need not be restricted to simple evolution under one native Hamiltonian, as the time-dependent control over these systems allows for stroboscopic engineering of the dynamics, or indeed engineering of different models with rapid time-dependent processes (so-called Floquet engineering). We are also clearly not restricted to scientifically relevant models - as a simple starting point, several groups have shown, e.g., how industrially relevant optimisation problems can be mapped onto Hamiltonians that can be engineered in cold atom quantum simulators (see, e.g. [104]).

We can then go beyond directly simulating these models by using the large-scale entangling operations implied by many-body dynamics as a variational circuit that can form the basis for methods such as Variational Quantum Eigensolver [105], Quantum Approximate Optimisation [106], and Quantum Machine Learning [107, 108] on these programmable systems. This again opens access to a range of problems well beyond basic science. In many of these systems, we can still use some of the same operations we are familiar with in digital quantum computing. But we no longer restrict to the gate sets that are required for fault-tolerant digital computing, and instead, in the NISQ era when we do not yet have fault-tolerance, make best use of the native capabilities of our analogue hardware.

VI. CONCLUSIONS

In summary, addressing quantum problems in quantum many-body physics has a long history, and also many practical applications - both directly to quantum systems in physics, chemistry and materials science, and to calculations from other fields that can be rewritten in this form. These problems are both difficult to solve, and are relevant and important beyond testing quantum hardware, making them excellent candidates for demonstrating a practical quantum advantage. Though on a formal level, there are no complexity proofs that the time cost for classical algorithms must scale exponentially, the same is true for most hard problems in classical computing, including factoring and NP-complete problems such as the Travelling Salesperson. However, many decades of progress and understanding underline (as for factoring and NP-hard problems) that this is a difficult problem, which is very unlikely to find a general solution. Analogue and Digital Quantum simulators provide an answer to this challenge, avoiding exponential scaling arising in memory resources, and at least for time evolution starting from a known state, also in time cost of the calculation.

Analogue quantum simulators are now moving from providing qualitative demonstrations of physical phenomena to providing well-calibrated, quantitative solutions for native problems. A key element of this is the further development of verification techniques, and one way of achieving this would be via Hamiltonian learning. We understand from controlled error budgets that analogue quantum simulators are already operating quantitatively reliably in regimes that are intractable classically, with opportunities for efficient verification of this in experiments. In table I we summarise the state-of-the-art for simulation of quantum systems via classical, analogue and digital methods.

Analogue quantum simulators are already having a significant impact today on basic science. There is further excitement over the range of models, as well as scalability and accuracy that fault-tolerant digital quantum simulation will make available in the future, with cautious optimism regarding the timescales to achieve the necessary hardware. A particularly exciting way forwards in the near term is development of a range of programmable quantum simulators hybridising digital and analogue techniques. This holds great potential as the best way forward in the NISQ era, as – rather than restricting to a limited gate set that is only required for fault-tolerant machines – it combines the best advantages of both sides by making use of the native analogue operations to produce highly entangled states.

In computing history, classical analogue and digital computing coexisted for more than half a century, with a gradual transition towards digital computing. We expect the same thing to happen in quantum simulation, where over the coming decades, we anticipate that larger-scale, verified, and quantitatively controlled simulations on analogue and hybrid devices will continue to play an important role, while scalable fault-tolerant quantum simulators will be developed in the future to provide access to freely programmable models and specified accuracy.

ACKNOWLEDGMENTS

We acknowledge helpful discussions with Barbara Kraus and Guang Hao Low. This work was supported by the European Union's Horizon 2020 research and innovation program under grant agreement No. 817482 PASQuanS. Work at the University of Strathclyde was supported by the EPSRC Programme Grant DesOEQ (EP/P009565/1), the EPSRC Hub in Quantum Comput-

	Classical Simulation	Analogue Quantum Simulation	Digital Quantum Computing
Platforms	Classical supercomputers	Neutral atoms (optical lattices or tweezer arrays), Ions, Superconducting systems, Quantum Dots, Photons,...	Neutral atoms (optical lattices or tweezer arrays), Ions, Superconducting systems, Quantum Dots, Photons,...
Universality	Yes (up to restricted system sizes or timescales) due to exponential scaling in time (and potentially memory)	Limited to available physical models	Yes (with error correction, requiring substantial scaling up from current systems)
Quantum advantage	No, and the cost grows exponentially with system size or simulation time	Regimes of practical quantum advantage now for real scientific problems, with potential opportunities for industrial problems	Quantum primacy for specialised tasks, awaiting practical quantum advantage and eventually fault tolerance
Solvable models	Unrestricted models through best available classical algorithms	Specific particle (Fermion or Boson) Hamiltonian, Spin Models (Qubits). Potentially, other mathematical problems that can be mapped onto these models	Wide classes of models, solved through algorithms for Quantum Simulation on a general purpose quantum computer
System Size (Today)	$<$ 50 spins computed exactly, or specialised short-time calculations for larger systems	Platform dependent up to 50-1000 particles or spins	Around 50 noisy qubits are presently available, but no fault-tolerant digital qubits yet
Scalability (Near term)	Exponentially difficult to scale to larger system sizes and longer times, except for specialised problems	Direct path to $10^3 - 10^4$ particles within the next 2-3 years	Few hundred in NISQ devices, next step is to bring error corrected qubits online

TABLE I. **Summary of the state of the art in simulation of quantum systems**. In this table, we summarise the state of the art and near-term prospects for simulation of quantum systems by classical, analogue quantum, and digital quantum simulators.

ing and simulation (EP/T001062/1), and AFOSR grant number FA9550-18-1-0064.

Author contributions: All authors discussed the topics addressed in this perspective, wrote the article and agreed on the final text. The example of Figure. 2 was produced by SF and AD, the digital gate count example by NP and MT, and the Box 3 example by CK and PZ, in discussion with all authors.

Competing interests: The authors declare no competing financial interests.

[1] Ladd, T. D. *et al.* Quantum computers. *Nature* **464**, 45–53 (2010).

[2] of Sciences, N. A., Engineering & Medicine. *Quantum Computing: Progress and Prospects* (The National Academies Press, Washington, DC, 2019).

[3] Deutsch, I. H. Harnessing the Power of the Second Quantum Revolution. *PRX Quantum* **1**, 020101 (2020).

[4] Nielsen, M. & Chuang, I. *Quantum Computation and Quantum Information: 10th Anniversary Edition* (Cambridge University Press, 2010).

[5] Feynman, R. P. Simulating physics with computers. *International Journal of Theoretical Physics* **21**, 467–488 (1982).

[6] Montanaro, A. Quantum algorithms: An overview. *npj Quantum Information* **2**, 1–8 (2016).

[7] Aramon, M. *et al.* Physics-Inspired Optimization for Quadratic Unconstrained Problems Using a Digital Annealer. *Frontiers in Physics* **7** (2019).

[8] Gibney, E. Hello quantum world! Google publishes landmark quantum supremacy claim. *Nature* **574**, 461–462 (2019).

[9] Arute, F. *et al.* Quantum supremacy using a programmable superconducting processor. *Nature* **574**, 505–510 (2019).
This article was the first demonstration of a quantum advantage with verification for a mathematical problem designed to test the quantum hardware.

[10] Zhong, H.-S. *et al.* Quantum computational advantage using photons. *Science* **370**, 1460–1463 (2020).

[11] Cirac, J. I. & Zoller, P. Goals and opportunities in quantum simulation. *Nature Physics* **8**, 264–266 (2012).

[12] Georgescu, I. M., Ashhab, S. & Nori, F. Quantum simulation. *Reviews of Modern Physics* **86**, 153–185 (2014).

[13] Reiher, M., Wiebe, N., Svore, K. M., Wecker, D. & Troyer, M. Elucidating reaction mechanisms on quantum computers. *Proceedings of the National Academy of Sciences* **114**, 7555–7560 (2017).

[14] Quintanilla, J. & Hooley, C. The strong-correlations puzzle. *Physics World* **22**, 32–37 (2009).

[15] Bloch, I., Dalibard, J. & Nascimbène, S. Quantum simulations with ultracold quantum gases. *Nature Physics*

8, 267–276 (2012).

[16] Blatt, R. & Roos, C. F. Quantum simulations with trapped ions. *Nature Physics* **8**, 277–284 (2012).

[17] Monroe, C. *et al.* Programmable quantum simulations of spin systems with trapped ions. *Reviews of Modern Physics* **93**, 025001 (2021).

[18] Aspuru-Guzik, A. & Walther, P. Photonic quantum simulators. *Nature Physics* **8**, 285–291 (2012).

[19] Houck, A. A., Türeci, H. E. & Koch, J. On-chip quantum simulation with superconducting circuits. *Nature Physics* **8**, 292–299 (2012).

[20] Browaeys, A. & Lahaye, T. Many-body physics with individually controlled Rydberg atoms. *Nature Physics* **16**, 132–142 (2020).

[21] Gross, C. & Bloch, I. Quantum simulations with ultracold atoms in optical lattices. *Science* **357**, 995–1001 (2017).

[22] Schäfer, F., Fukuhara, T., Sugawa, S., Takasu, Y. & Takahashi, Y. Tools for quantum simulation with ultracold atoms in optical lattices. *Nature Reviews Physics* **2**, 411–425 (2020).

[23] Hartmann, M. J. Quantum simulation with interacting photons. *Journal of Optics* **18**, 104005 (2016).

[24] White, A. G. Photonic quantum simulation. In *2014 OptoElectronics and Communication Conference and Australian Conference on Optical Fibre Technology*, 660–661 (2014).

[25] The Hubbard model at half a century. *Nature Physics* **9**, 523–523 (2013).

[26] Essler, F. H. L., Frahm, H., Göhmann, F., Klümper, A. & Korepin, V. E. *The One-Dimensional Hubbard Model* (Cambridge University Press, Cambridge, 2005).

[27] Zheng, B.-X. *et al.* Stripe order in the underdoped region of the two-dimensional Hubbard model. *Science* **358**, 1155–1160 (2017).

[28] LeBlanc, J. P. F. *et al.* Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms. *Physical Review X* **5**, 041041 (2015).

[29] Lee, P. A., Nagaosa, N. & Wen, X.-G. Doping a mott insulator: Physics of high-temperature superconductivity. *Rev. Mod. Phys.* **78**, 17–85 (2006).

[30] von Burg, V. *et al.* Quantum computing enhanced computational catalysis. *Phys. Rev. Research* **3**, 033055 (2021).

[31] Bauer, B., Bravyi, S., Motta, M. & Chan, G. K.-L. Quantum algorithms for quantum chemistry and quantum materials science. *Chemical Reviews* **120**, 12685–12717 (2020). URL `https://doi.org/10.1021/acs.chemrev.9b00829`.

[32] Childs, A. M., Maslov, D., Nam, Y., Ross, N. J. & Su, Y. Toward the first quantum simulation with quantum speedup. *Proceedings of the National Academy of Sciences* **115**, 9456–9461 (2018).

[33] Lloyd, S. Universal Quantum Simulators. *Science* **273**, 1073–1078 (1996).
This was the first article to discuss in detail how digital quantum simulation could be implemented on quantum computers, and forms the basis for the fault tolerant quantum simulation protocols discussed here.

[34] Roffe, J. Quantum error correction: An introductory guide. *Contemporary Physics* **60**, 226–245 (2019).

[35] Preskill, J. Quantum computing in the nisq era and beyond. *Quantum* **2**, 79 (2018).

[36] Buluta, I. & Nori, F. Quantum Simulators. *Science* **326**, 108–111 (2009).

[37] Choi, J.-y. *et al.* Exploring the many-body localization transition in two dimensions. *Science* **352**, 1547–1552 (2016).
This paper gives an important recent demonstration of the use of analogue quantum simulators with cold atoms in optical lattices in order to explore dynamics of interacting particles in a disordered system, which is intractable to classical computation.

[38] Chiu, C. S. *et al.* String patterns in the doped Hubbard model. *Science* **365**, 251–256 (2019).

[39] Semeghini, G. *et al.* Probing Topological Spin Liquids on a Programmable Quantum Simulator. *arXiv:2104.04119 [cond-mat, physics:physics, physics:quant-ph]* (2021). 2104.04119.

[40] Satzinger, K. J. *et al.* Realizing topologically ordered states on a quantum processor. *arXiv:2104.01180 [cond-mat, physics:quant-ph]* (2021). 2104.01180.

[41] Bluvstein, D. *et al.* Controlling quantum many-body dynamics in driven Rydberg atom arrays. *Science* **371**, 1355–1359 (2021).
This article demonstrates the state of the art for observing many-body dynamics in an analogue quantum simulator with neutral atom arrays and Rydberg excitations.

[42] Scholl, P. *et al.* Quantum simulation of 2d antiferromagnets with hundreds of rydberg atoms. *Nature* **595**, 233–238 (2021).
This article demonstrates analogue quantum simulation of dynamics with 196 spins using neutral atoms in tweezer arrays.

[43] Zhang, J. *et al.* Observation of a many-body dynamical phase transition with a 53-qubit quantum simulator. *Nature* **551**, 601–604 (2017).

[44] Zhang, J. *et al.* Observation of a discrete time crystal. *Nature* **543**, 217–220 (2017).

[45] Barreiro, J. T. *et al.* An open-system quantum simulator with trapped ions. *Nature* **470**, 486–491 (2011).

[46] Altman, E. *et al.* Quantum simulators: Architectures and opportunities. *PRX Quantum* **2**, 017003 (2021).

[47] Bauer, B. *et al.* The ALPS project release 2.0: Open source software for strongly correlated systems. *Journal of Statistical Mechanics: Theory and Experiment* **2011**, P05001 (2011).

[48] Becca, F. & Sorella, S. *Quantum Monte Carlo Approaches for Correlated Systems* (Cambridge University Press, Cambridge, 2017).

[49] Werner, P., Oka, T. & Millis, A. J. Diagrammatic Monte Carlo simulation of nonequilibrium systems. *Physical Review B* **79**, 035320 (2009).

[50] Troyer, M. & Wiese, U.-J. Computational Complexity and Fundamental Limitations to Fermionic Quantum Monte Carlo Simulations. *Physical Review Letters* **94**, 170201 (2005).

[51] Eisert, J. Entangling power and quantum circuit complexity. *arXiv:2104.03332 [cond-mat, physics:hep-th, physics:quant-ph]* (2021). 2104.03332.

[52] Swingle, B., Bentsen, G., Schleier-Smith, M. & Hayden, P. Measuring the scrambling of quantum information. *Physical Review A* **94**, 040302 (2016).

[53] Hatano, N. & Suzuki, M. Finding Exponential Prod-

uct Formulas of Higher Orders. In Das, A. & K. Chakrabarti, B. (eds.) *Quantum Annealing and Other Optimization Methods*, Lecture Notes in Physics, 37–68 (Springer, Berlin, Heidelberg, 2005).

[54] Childs, A. M., Su, Y., Tran, M. C., Wiebe, N. & Zhu, S. Theory of Trotter Error with Commutator Scaling. *Physical Review X* **11**, 011020 (2021).

[55] Heyl, M., Hauke, P. & Zoller, P. Quantum localization bounds trotter errors in digital quantum simulation. *Science advances* **5**, eaau8342 (2019).

[56] Wecker, D., Bauer, B., Clark, B. K., Hastings, M. B. & Troyer, M. Gate-count estimates for performing quantum chemistry on small quantum computers. *Physical Review A* **90**, 022305 (2014).

[57] Wecker, D. *et al.* Solving strongly correlated electron models on a quantum computer. *Physical Review A* **92**, 062318 (2015).

[58] Schollwöck, U. The density-matrix renormalization group in the age of matrix product states. *Annals of Physics* **326**, 96–192 (2011).

[59] Verstraete, F., Murg, V. & Cirac, J. I. Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems. *Advances in Physics* **57**, 143–224 (2008).

[60] Vidal, G. Efficient Simulation of One-Dimensional Quantum Many-Body Systems. *Physical Review Letters* **93**, 040502 (2004).
This article introduced classical simulation of 1D many-body systems using matrix product states, which provide the present state-of-the-art in classical simulation of quench dynamics in strongly interacting systems.

[61] Amico, L., Fazio, R., Osterloh, A. & Vedral, V. Entanglement in many-body systems. *Reviews of Modern Physics* **80**, 517–576 (2008).

[62] Albash, T. & Lidar, D. A. Adiabatic quantum computation. *Reviews of Modern Physics* **90**, 015002 (2018).

[63] Kempe, J., Kitaev, A. & Regev, O. The complexity of the local hamiltonian problem. *SIAM Journal on Computing* **35**, 1070–1097 (2006). https://doi.org/10.1137/S0097539704445226.

[64] Poggi, P. M., Lysne, N. K., Kuper, K. W., Deutsch, I. H. & Jessen, P. S. Quantifying the Sensitivity to Errors in Analog Quantum Simulation. *PRX Quantum* **1**, 020308 (2020).

[65] Lanyon, B. P. *et al.* Universal digital quantum simulation with trapped ions. *Science* **334**, 57–61 (2011).

[66] Martinez, E. A. *et al.* Real-time dynamics of lattice gauge theories with a few-qubit quantum computer. *Nature* **534**, 516–519 (2016).

[67] Berry, D. W., Childs, A. M., Cleve, R., Kothari, R. & Somma, R. D. Simulating hamiltonian dynamics with a truncated taylor series. *Phys. Rev. Lett.* **114**, 090502 (2015).

[68] Haah, J., Hastings, M. B., Kothari, R. & Low, G. H. Quantum algorithm for simulating real time evolution of lattice hamiltonians. *SIAM Journal on Computing* FOCS18–250–FOCS18–284 (2021).

[69] Aharonov, D. & Ta-Shma, A. Adiabatic quantum state generation and statistical zero knowledge. In *Proceedings of the Thirty-Fifth Annual ACM Symposium on Theory of Computing*, STOC '03, 20–29 (Association for Computing Machinery, New York, NY, USA, 2003).

[70] Low, G. H. & Chuang, I. L. Hamiltonian Simulation by Qubitization. *Quantum* **3**, 163 (2019).

[71] Flannigan, S. *et al.* Propagation of errors and quantitative quantum simulation with quantum advantage (2022). URL `https://arxiv.org/abs/2204.13644`.

[72] Morgado, M. & Whitlock, S. Quantum simulation and computing with rydberg-interacting qubits. *AVS Quantum Science* **3**, 023501 (2021).

[73] Sornborger, A. T. & Stewart, E. D. Higher-order methods for simulations on quantum computers. *Physical Review A* **60**, 1956–1965 (1999).

[74] Carrasco, J., Elben, A., Kokail, C., Kraus, B. & Zoller, P. Theoretical and Experimental Perspectives of Quantum Verification. *PRX Quantum* **2**, 010102 (2021).

[75] Li, Z., Zou, L. & Hsieh, T. H. Hamiltonian tomography via quantum quench. *Physical review letters* **124**, 160502 (2020).

[76] Bairey, E., Arad, I. & Lindner, N. H. Learning a Local Hamiltonian from Local Measurements. *Physical Review Letters* **122**, 020504 (2019).

[77] Eisert, J. *et al.* Quantum certification and benchmarking. *Nature Reviews Physics* **2**, 382–390 (2020).

[78] Elben, A. *et al.* Cross-Platform Verification of Intermediate Scale Quantum Devices. *Physical Review Letters* **124**, 010504 (2020).

[79] Evans, T. J., Harper, R. & Flammia, S. T. Scalable Bayesian Hamiltonian learning. *arXiv:1912.07636 [cond-mat, physics:quant-ph]* (2019). 1912.07636.

[80] Valenti, A., van Nieuwenburg, E., Huber, S. & Greplova, E. Hamiltonian learning for quantum error correction. *Physical Review Research* **1**, 033092 (2019).

[81] Wang, J. *et al.* Experimental quantum Hamiltonian learning. *Nature Physics* **13**, 551–555 (2017).

[82] Abanin, D. A., Altman, E., Bloch, I. & Serbyn, M. Colloquium: Many-body localization, thermalization, and entanglement. *Reviews of Modern Physics* **91**, 021001 (2019).

[83] Ozawa, T. *et al.* Topological photonics. *Reviews of Modern Physics* **91**, 015006 (2019).

[84] Turner, C. J., Michailidis, A. A., Abanin, D. A., Serbyn, M. & Papić, Z. Weak ergodicity breaking from quantum many-body scars. *Nature Physics* **14**, 745–749 (2018).

[85] Bañuls, M. C. *et al.* Simulating lattice gauge theories within quantum technologies. *The European Physical Journal D* **74**, 165 (2020).

[86] Bentsen, G. *et al.* Treelike Interactions and Fast Scrambling with Cold Atoms. *Physical Review Letters* **123**, 130601 (2019).

[87] Periwal, A. *et al.* Programmable Interactions and Emergent Geometry in an Atomic Array. *arXiv:2106.04070 [cond-mat, physics:quant-ph]* (2021). 2106.04070.

[88] Argüello-Luengo, J., González-Tudela, A., Shi, T., Zoller, P. & Cirac, J. I. Analogue quantum chemistry simulation. *Nature* **574**, 215–218 (2019).

[89] Cubitt, T., Montanaro, A. & Piddock, S. Universal quantum hamiltonians. *Proc. Natl. Acad. Sci. 115:38 p9497-9502 (2018)* (2017). 1701.05182.

[90] Zhou, L. & Aharonov, D. Strongly universal hamiltonian simulators (2021). 2102.02991.

[91] Kaubruegger, R. *et al.* Variational Spin-Squeezing Algorithms on Programmable Quantum Sensors. *Physical Review Letters* **123**, 260505 (2019).

[92] Liu, H. *et al.* Prospects of Quantum Computing for Molecular Sciences. *arXiv:2102.10081 [quant-ph]* (2021). 2102.10081.

[93] Bassman, L. *et al.* Simulating Quantum Materials with Digital Quantum Computers. *arXiv:2101.08836 [quant-ph]* (2021). 2101.08836.

[94] Ma, H., Govoni, M. & Galli, G. Quantum simulations of materials on near-term quantum computers. *npj Computational Materials* **6**, 1–8 (2020).

[95] Rieger, H. Combinatorial Optimization and the Physics of Disordered Systems. In Das, A. & K. Chakrabarti, B. (eds.) *Quantum Annealing and Other Optimization Methods*, Lecture Notes in Physics, 299–324 (Springer, Berlin, Heidelberg, 2005).

[96] Hauke, P., Katzgraber, H. G., Lechner, W., Nishimori, H. & Oliver, W. D. Perspectives of quantum annealing: Methods and implementations. *Reports on Progress in Physics* **83**, 054401 (2020).

[97] Lamata, L., Parra-Rodriguez, A., Sanz, M. & Solano, E. Digital-analog quantum simulations with superconducting circuits. *Advances in Physics: X* **3**, 1457981 (2018).

[98] Brydges, T. *et al.* Probing Rényi entanglement entropy via randomized measurements. *Science* **364**, 260–263 (2019).

[99] Kokail, C. *et al.* Self-verifying variational quantum simulation of lattice models. *Nature* **569**, 355–360 (2019). **This article presented the first demonstration of an analogue quantum simulator being used for variational quantum simulation, demonstrating a self-verified solution to a model from high-energy physics.**

[100] Babukhin, D. V., Zhukov, A. A. & Pogosov, W. V. Hybrid digital-analog simulation of many-body dynamics with superconducting qubits. *Physical Review A* **101**, 052337 (2020).

[101] Arrazola, I., Pedernales, J. S., Lamata, L. & Solano, E. Digital-Analog Quantum Simulation of Spin Models in Trapped Ions. *Scientific Reports* **6**, 30534 (2016).

[102] Kokail, C., van Bijnen, R., Elben, A., Vermersch, B. & Zoller, P. Entanglement hamiltonian tomography in quantum simulation. *arXiv preprint arXiv:2009.09000* (2020).

[103] Joshi, M. K. *et al.* Quantum information scrambling in a trapped-ion quantum simulator with tunable range interactions. *Physical Review Letters* **124**, 240505 (2020).

[104] Henriet, L. *et al.* Quantum computing with neutral atoms. *Quantum* **4**, 327 (2020).

[105] Cerezo, M. *et al.* Variational quantum algorithms. *arXiv:2012.09265* (2020).

[106] Zhou, L., Wang, S.-T., Choi, S., Pichler, H. & Lukin, M. D. Quantum Approximate Optimization Algorithm: Performance, Mechanism, and Implementation on Near-Term Devices. *Physical Review X* **10**, 021067 (2020).

[107] Biamonte, J. *et al.* Quantum machine learning. *Nature* **549**, 195–202 (2017).

[108] Huang, H.-Y. *et al.* Power of data in quantum machine learning. *arXiv preprint arXiv:2011.01938* (2020).

[109] Hartke, T., Oreg, B., Jia, N. & Zwierlein, M. Quantum register of fermion pairs. *arXiv:2103.13992* (2021).

[110] Mazurenko, A. *et al.* A cold-atom fermi–hubbard antiferromagnet. *Nature* **545**, 462–466 (2017).

[111] Jaksch, D. & Zoller, P. The cold atom hubbard toolbox. *Annals of Physics* **315**, 52 – 79 (2005).

[112] Gerbier, F. & Castin, Y. Heating rates for an atom in a far-detuned optical lattice. *Phys. Rev. A* **82**, 013615 (2010).

[113] Pichler, H., Schachenmayer, J., Daley, A. J. & Zoller, P. Heating dynamics of bosonic atoms in a noisy optical lattice. *Phys. Rev. A* **87**, 033606 (2013).

[114] Poulin, D. *et al.* The trotter step size required for accurate quantum simulation of quantum chemistry. *Quantum Inf. Comput.* **15**, 361–384 (2015).

[115] Kliesch, M., Gogolin, C. & Eisert, J. *Lieb-Robinson Bounds and the Simulation of Time-Evolution of Local Observables in Lattice Systems*, 301–318 (Springer International Publishing, Cham, 2014).

[116] Childs, A. M., Su, Y., Tran, M. C., Wiebe, N. & Zhu, S. A theory of trotter error (2019).

[117] Amato-Grill, J., Jepsen, N., Dimitrova, I., Lunden, W. & Ketterle, W. Interaction spectroscopy of a two-component mott insulator. *Phys. Rev. A* **99**, 033612 (2019).

[118] Wei, D. *et al.* Quantum gas microscopy of kardar-parisi-zhang superdiffusion (2021). 2107.00038.

[119] Wecker, D., Bauer, B., Clark, B. K., Hastings, M. B. & Troyer, M. Gate-count estimates for performing quantum chemistry on small quantum computers. *Phys. Rev. A* **90**, 022305 (2014).

[120] Wecker, D. *et al.* Solving strongly correlated electron models on a quantum computer. *Phys. Rev. A* **92**, 062318 (2015).

[121] Hastings, M. B., Wecker, D., Bauer, B. & Troyer, M. Improving quantum algorithms for quantum chemistry. *Quantum Info. Comput.* **15**, 1–21 (2015).

[122] Bocharov, A., Roetteler, M. & Svore, K. M. Efficient synthesis of universal repeat-until-success quantum circuits. *Phys. Rev. Lett.* **114**, 080502 (2015).

[123] Gidney, C. Halving the cost of quantum addition. *Quantum* **2**, 74 (2018).