TEQUILA: A platform for rapid development of quantum algorithms.

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Variational quantum algorithms are currently the most promising class of algorithms on near-term quantum computers. In contrast to classical algorithms, there are almost no standardized methods yet, and the field continues to evolve rapidly. Similar to classical methods, heuristics play a crucial role in the development of new quantum algorithms, resulting in a high demand for flexible and reliable ways to implement, test, and share new ideas. Inspired by this demand, we introduce TEQUILA, a development package for quantum algorithms in python, designed for fast and flexible implementation, prototyping and deployment of novel quantum algorithms in electronic structure and other fields. TEQUILA operates with abstract expectation values which can be combined, transformed, differentiated, and optimized. On evaluation, the abstract data structures are compiled to run on state of the art quantum simulators or interfaces.

I. INTRODUCTION

Quantum computing is currently in the Noisy Intermediate-Scale Quantum (NISQ) [1] era, in which devices of intermediate size can execute non-trivial quantum computation but must grapple with non-negligible noise and a lack of error correction. The algorithmic form set to dominate the NISQ field is that of hybrid quantum-classical algorithms, particularly variational quantum algorithms (VQAs). Such algorithms leverage classical coprocessors to iteratively improve the performance of parametrized quantum circuits with respect to a variety of objectives. VQAs exhibit generally shallow depth and are postulated to have greater resistance to noise, both of which are necessary to leverage the potential of near term devices. Algorithms like the Variational Quantum Eigensolver (VQE) [2] and the Quantum Approximate Optimization Algorithm (QAOA) [3] have shown great promise in solving difficult problems in a variety of fields, ranging from quantum chemistry and materials science to finance. Alongside the development of variational algorithms, classes of algorithms broadly categorized as Quantum Machine Learning (QML) [4] herald the extension of the power of machine learning to applications on quantum data.

The rapid expansion of VQAs and QML algorithms has been accompanied and assisted by an ever-expanding market of quantum information and simulation packages; to date, over 100 different quantum simulation packages have been released. [5] The most popular ‘full stack’ simulation packages are written in or are interoperable with python, and many of them are backed by leading companies in the quantum industry, such as Cirq [6], Qiskit [7], Q#. [8], PyQuil [9] and Strawberry Fields [10] respectively developed by or affiliated with Google, IBM, Microsoft, Rigetti, and Xanadu. Where applicable, these industrially developed packages also integrate the cloud quantum computing services made available by their respective organization.

However, the large variety of simulation software poses a challenge both for the validation of experiments and the adoption of new algorithms. As the NISQ era continues to progress, quantum scientists stand to benefit markedly from a unified development framework in which the strengths and resources of different software packages — both quantum and classical — can be easily coordinated, with minimal constriction of algorithmic design choices, to further accelerate the pace of development. To this end, we introduce TEQUILA.

We note that a number of software packages have...
been created to meet similar needs, such as PennyLane [11], which pioneered in introducing automatic differentiation to variational quantum algorithms, and classical quantum simulators with an extended interface, including some of the aforementioned packages as well as XACC [12], ProjectQ [13], Qibo [14], Yao [15] and Qulacs [16]. TEQUILA differs from the aforementioned either by a difference in functionality or through its application programming interface, which rests firmly in an object-oriented programming framework, much like Python itself. The benefits and strengths of individual packages largely depend on the intended applications and individual preferences of the user.

TEQUILA is an open-source Python 3 software package, which integrates diverse simulation software, classical optimization routines, and powerful tools for the manipulation and combination of quantum circuits and variational objectives thereof. Additionally, TEQUILA has a native interface for popular electronic structure packages like psi4 [17] or pyscf [18, 19]. Focused on variational algorithms, whose objectives may require classical transformations on the output of expectation values or circuit measurements, TEQUILA implements convenient tools for arithmetics on those structures, and interfaces the powerful autodifferentiation libraries JAX [20] and autograd to allow hassle-free analytic differentiation of user defined objective functions. TEQUILA maintains a firmly object-oriented user interface, with which circuits, Hamiltonians, expectation values, and user-defined objectives can be conveniently combined arithmetically, using code that represents the underlying mathematics in a blackboard fashion. Here, we detail with examples of how construction, compilation, manipulation, differentiation, and optimization of variational quantum objectives can be performed in TEQUILA, in order to illustrate the core of the application programming interface. Further tutorials and documentation are available on the TEQUILA Github repository [21].

II. HOW TEQUILA WORKS

The core intention of the design of TEQUILA is to provide an open-source environment for the rapid development and demonstration of new ideas in (variational) quantum computation through a high-level of abstraction, resembling the chalk-and-blackboard mathematics underlying the algorithm. This was inspired by the application programming interface of the MADNESS [22] package. The user is offered a choice, illustrated in Fig. 1, between treating quantum computers as black box samplers of abstract expectation values, and controlling the use of the quantum computer more directly. In the following, we will describe how TEQUILA can be used in both fashions.

A. Abstract data structures

TEQUILA allows users to treat quantum backends, which serve as interfaces to real hardware or simulators as abstract sampling devices, requiring little to no knowledge about the underlying technical details of simulation or execution. The user merely needs to be familiar with the physical principles behind quantum computation and have an idea of how the specific problems of interest could be solved with access to quantum computers. The core functionality of TEQUILA is provided by abstract data structures depicted in Fig. 2 where the user only deals directly with Objectives, Hamiltonians and Circuits. These last two objects define abstract Hamiltonians and unitaries (quantum circuits) which can be combined to create abstract expectation values. TEQUILA bundles these abstract expectation values into objectives which can then be transformed, combined or differentiated in a blackboard style fashion.

1. Objectives

Objectives are callable data structures that hold a list of abstract expectation values and variables as well as a
Figure 2. Abstract data structures in TEQUILA

transformation that defines how those structures shall be processed after evaluation. Formally, a TEQUILA objective can be written as

\[ O = f(E_0, E_1, \ldots, a_0, a_1, \ldots), \]

with variables \( a_k \) and expectation values \( E_k \), which can themselves depend on the variables:

\[ E_k = \langle 0 | U_k^\dagger (g(a, b, \ldots)) H_k U_k (g(a, b, \ldots)) | 0 \rangle, \]

with arbitrary transformations \( g \). Operations on objectives return objects of the same type, as illustrated in Fig. 5 rendering the combination and extension of objectives more convenient. For example, take the addition of the two objectives \( O_1 = E_1^2 \) and the more complicated \( O_2 = e^{-E_2^2} + c \). In this example, each of these objectives only carries one expectation value for simplicity and \( c \) can be a constant, a variable or a scalar function. The corresponding transformations in the data structures are \( f_1(x) = x^2 \) and \( f_2(x) = e^{-x^2} + c \). If both objectives are added together as \( O_3 = O_1 + O_2 \) the resulting data structure carries two abstract expectation values, and the transformation is \( f_3(x, y) = x^2 + e^{-y^2} + c \). See Fig. 5 for the explicit illustration of a similar example.

The objectives are fully differentiable. We make use of the shift-rule gradient technique developed by Schuld et al. [23], first implemented within PENNYLANE [11], alongside automatic differentiation of the transformation of the objective. For objectives whose expectation values contain quantum gates that do not fulfill the requirements of being directly differentiable, we employ a variety of decomposition techniques, similar in spirit to those proposed in Ref. [24]. Differentiation of an objective again gives back an objective, enabling convenient access to arbitrary order derivatives. An explicit illustration using automatic decomposition of controlled rotations and the resulting Objective data structure is shown in Figs. 6 and 3, where we illustrate blackboard style TEQUILA code for a small toy model.

TEQUILA objectives are abstract data structures that can be translated into various quantum backends which are interfaces to existing quantum hardware and/or simulators. The compile function allows the translation of an abstract objective into an objective that is tied to a specific backend. After compilation, the objective can be used as an abstract function with respect to its parameters. In the following, there is a small example of how the second derivative of a TEQUILA objective can be obtained as an abstract TEQUILA objective, which can then be translated to a quantum backend and later be used as an abstract function

where not setting the samples keyword will result in the exact simulation of all objectives, and the original objective could, for example, be the objective in Fig. 3. Note that the quantum backend was not specified in the example code above. If this is the case, TEQUILA will detect all supported and installed backends automatically and choose the one most appropriate for the given task, based on an intrinsically defined hierarchy of efficiency for said task. The compile function takes additional keywords like backend, samples, and noise in order to specify which backend to use if finite samples are simulated or if a noise model is used for a simulation. If finite samples are desired, those can be passed to the compile function, influencing the automatic selection of the available quantum backends. After compilation, the sample size can still be changed when calling the objective.

2. Hamiltonians

Hamiltonians in TEQUILA are represented as linear combinations of tensor products of Pauli matrices – so called Pauli strings – and by default use OPENFermion [25] as a backend for algebraic manipulations. Transformations into different data formats like the symplectic binary form are also possible for more in-depth tasks (see the next section). In principle,
import tequila as tq
from numpy import exp, pi
a = tq.Variable("a")
U = tq.gates.Ry(angle=(-a**2).apply(exp)*pi,
             target=0)
U += tq.gates.X(target=1, control=0)
H = tq.QubitHamiltonian.from_string("-1.0*X(0)*Y(1)
                                      + 0.5*Z(0) + Y(1)")
E = tq.ExpectationValue(H=H, U=U)
dE = tq.grad(E, "a")
objective = E + (-dE**2).apply(exp)
result = tq.minimize(method="phoenics",
                      objective=objective)

Figure 3. An illustrative toy model implemented and optimized within TEQUILA. The top panel illustrates the model system used, where defined loss function \( L \) was minimized. The middle panel depicts the implementation with TEQUILA. The lower panel depicts an example of optimization results using the PHOENICS optimizer.

within the abstract expectation values, the Hamiltonians represent averaged measurements. A measurement of a single qubit in the computational basis can, for example, be represented by the two projectors

\[
Q_+ = |0\rangle\langle 0| = \frac{1}{2}(1 + \sigma_z) \tag{3}
\]

\[
Q_- = |1\rangle\langle 1| = \frac{1}{2}(1 - \sigma_z). \tag{4}
\]

Hamiltonians can be initialized directly, through strings, or from OPENFERMION operators. Take for example the following Hamiltonian:

\[
H = \sigma_x(0)\sigma_y(1) + 3\sigma_y(3) \tag{5}
\]

which can be initialized by combining primitives,

\[
H = \text{tq.paulis.X}(0)\text{tq.paulis.Y}(1)
H = 3.0*\text{tq.paulis.Y}(3)
\]

or from strings.

\[
H = \text{tq.QubitHamiltonian.from_string("1.0*X(0)*Y}
    \quad \rightarrow (1) + 3.0*Y(3)")
\]

More complicated Hamiltonians, such as that of the Heisenberg model,

\[
H = \sum_k J_x\sigma_x(k)\sigma_x(k+1) + \sum_k J_y\sigma_y(k)\sigma_y(k+1) + \sum_k J_z\sigma_z(k)\sigma_z(k+1) + \sum_k h\sigma_z(k), \tag{6}
\]

can be initialized in a similar way:

\[
H = \text{tq.paulis.Zero()}
for k in range(n_qubits):
    H += Jx*tq.paulis.X([k,k+1])
H += Jy*tq.paulis.Y([k,k+1])
H += Jz*tq.paulis.Z([k])
H += h*tq.paulis.Z([k])
\]

where \( J_x, J_y, J_z \) and \( h \) are floating point numbers and the integer \( n_{qubits} \) determines the number of sites.

Hamiltonians can also be defined more indirectly by defining abstract qubit wave functions and forming operations on them in Dirac notation. Take for example the projector on a predefined wave function

\[
H = |\Psi\rangle\langle\Psi| \tag{7}
\]

which can be defined within TEQUILA as

\[
\text{rho_targ} = \text{tq.paulis.Projector(wfn=wfn_targ)}
\]

where \( wfn\_targ \) is the \( |\Psi\rangle \) wave function that itself can be initialized from strings or arrays of coefficients, where coefficients \( c_i \) corresponds to the computational basis state \( |i\rangle \) in binary notation. The internal representation of
of the projector after initialization is decomposed into
Pauli strings so that we end up with the same data
structure as before. For example, consider the Bell state
wavefunction
\[ |\Psi^+\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle). \]  
whose projector takes the form
\[ |\Psi^+\rangle \langle \Psi^+| = \frac{1}{2} \left( |00\rangle \langle 00| + |11\rangle \langle 11| \right). \]  
Each of the four individual terms is decomposed into
Pauli strings, similarly to Ref. [26]:
\[ \sigma^+ \equiv |0\rangle \langle 1| = \frac{1}{2} (\sigma_x + i\sigma_y), \]  
\[ \sigma^- \equiv |1\rangle \langle 0| = \frac{1}{2} (\sigma_x - i\sigma_y). \]  
and with Eqs. (3) and (4). Similar to Projector,
the KetBra function of TEQUILA decomposes the operator
\(|\Psi\rangle \langle \Phi|\) into a non-hermitian combination of Pauli
strings. An arbitrary matrix can then be decomposed
into a TEQUILA Hamiltonian with the help of the KetBra
function. By applying the split function, the anti-
hermitian and hermitian parts can be separated for in-
dividual treatment within abstract expectation values.

The decompositions above use wavefunction syntax for
convenience and are only feasible for problems that can be
encoded into small analytical wave functions. Projectors
on larger, potentially unknown, wavefunctions can be encoded as well, as long as the unitary circuit
that prepares them is known. The projector then looks like
\[ |\Psi\rangle \langle \Psi| = U_\Psi |0\rangle \langle 0| U_\Psi^\dagger \]  
where the unitary \(U_\Psi\) is a TEQUILA quantum circuit.
In Fig. 4 we illustrate both techniques for the evaluation
of fidelities \(F = |\langle \Psi|\Phi\rangle|^2\).

3. Quantum Circuits

Abstract quantum circuits can be defined over primitive
quantum gates, either from those in the TEQUILA
gate set, or by defining them over a generator which itself
is given by a TEQUILA Hamiltonian.

As an example, consider the Y-rotation around qubit 0
\[ R_y(a) = e^{-i\frac{a}{2}\sigma_y(0)} \]  
which can be initialized in the following fashion:
\[ U = \text{tq.gates.Ry}(|\text{angle}=1.0, \text{target}=0|) \]  
\[ U = \text{tq.gates.ExpPauli}(|\text{angle}=1.0, \text{paulistring}="Y") \]  
\[ = (0\rangle) \]  
\[ \text{g = tq.paulis.Y(|0\rangle) \]  
\[ U = \text{tq.gates.Trotterized}(|\text{angles}=[1.0], \]  
\[ \text{generators}=[\text{g}], \text{steps}=1) \]  
where the Trotterized function accepts arbitrary her-
mitian generators and follows the same conventions as
the one qubit rotations with the exponent being \(-i\theta/\)2.
Note that there is no approximation used in this exam-
ple, since a single step in the formal trotterization is

Figure 4. Example portraying how to obtain the fidelity
between two states using TEQUILA and different strategies.
One for states that are analytically known and one for states
encoded in quantum circuits. We use the same Bell state for
both illustrations. The fidelities are computed with respect
to a state encoded in circuit \(U\), that is assumed to be already
initialized.
exact here; however this is not the case for all generators. In general TEQUILA allows the definition of arbitrary gates over hermitian generators \( G = \sum_k c_k \sigma_k \), represented by a weighted sum over \( K \) Pauli strings \( \sigma_k \), as a formal Trotter expansion with \( N \) steps, 
\[
U(a) = e^{-i \frac{\pi}{4} G} = \prod_{n=1}^{N} \prod_{k=1}^{K} e^{-i \frac{\pi}{4} \sigma_k}.
\]

(14)

Parametrized gates like rotations can also be initialized by variables or transformations of variables. Take for example the parametrized rotation:
\[
R_y(f(a)) = e^{-i \frac{(f(a))}{2} \sigma_y}, \quad f(a) = e^{-a^2}.
\]

(15)

which can be initialized as
\[
a = \text{tq.Variable("a")}
\]
\[
a = (-0.25*a**2). \text{apply}(\exp)
\]
\[
U = \text{tq.gates.Ry}(\text{angle}=fa, \text{target}=0)
\]

where \( \exp \) is the exponential function, for example from NUMPY, and transformation of abstract variables uses the same data structures as the abstract objectives. The actual values of the variables are not tied to the circuit structures but are passed down when the objectives are evaluated (see previous sections). In this way, the objectives can be used like abstract functions.

Quantum circuits usually consist of more than one gate, and their construction can be achieved by simply adding individual gates together. The arithmetic is here implemented according to the quantum circuit model where addition is interpreted as concatenating two circuits, and the leftmost circuit is the one that acts first. Take for example, the following unitary operation consisting of four individual unitary operations
\[
U = U_6 + U_5 + U_4 + U_3
\]

which is written in the opposite order using the language of unitary matrices \( U = U_6 U_5 U_4 \). At the top level, TEQUILA does not distinguish between gates and circuits. The rotations initialized above are initialized as circuits containing a single gate. See, for example, Fig. 3, and the applications illustrated later. Circuits can be evaluated in the same way as objectives if one is interested in simulating the wave function or sampling from its distribution:
\[
\text{wfn} = \text{tq.simulate}(U, \text{variables}="a":1.0)
\]

and similarly with the compile function. The returned data type is the same for finite sampling (\texttt{samples=finite\_value} and explicit simulation (\texttt{samples=None}) where the former contains the counts for the corresponding measurements and the latter the simulated amplitudes.

Figure 5. Top: Abstract data structure for objectives in TEQUILA. Arithmetic operations, transformations or derivatives give back objects of the same type. Bottom: Example of arithmetic operations on TEQUILA objectives and their resulting data structures. The right hand side shows the full objective defined as \( O_3 = (E_0 + E_1)^2 \).

Figure 6. Gradient compiling in TEQUILA: (Top) TEQUILA Top level code. (Middle) The abstract circuit and the internally compiled circuit. (Bottom) The objective structure representing the gradient \( dO \) in the code. \( E_{\pm} \) denote the left and right shifted expectation values with respect to the \( i \)th occurrence of the variable \( a \) in the compiled circuit. In this specific examples the transformations \( g \) and \( \tilde{g} \) are rescaling by \( \pm \frac{1}{\sqrt{2}} \).
B. Simulation and execution

Some improvements in algorithmic quantum computing concern more technical details in its implementation such as efficient unitary gate compilation, error mitigation or optimizing measurement protocols. In these cases, it is not sufficient to treat the quantum computer as a black box, and more details about the device are necessary. TEQULA, due to its modular design, offers the platform to implement and incorporate these technical improvements quickly and easily, making them available, accessible, and easy to use for a broad user base. For instance, a feature already included in TEQULA is the automatic compilation of abstract multi-qubit gates (like multi-Pauli rotations and controlled-rotations) into primitive quantum gates and the option to optimize measurement protocols by grouping the Hamiltonian into commuting cliques.

1. Optimized Measurement Protocols

The protocol for grouping a Hamiltonian into commuting and qubit-wise commuting cliques are described in detail in Refs. [27] and [28], respectively. The implementation thereof uses the binary-symplectic representation of the Hamiltonian, where each Pauli string is represented by two integer arrays (see [27] for more details). TEQULA can convert the standard Hamiltonians into binary-symplectic form and vice versa. The grouping algorithm transforms each expectation value of an objective into multiple expectation values of the form

$$\langle H \rangle_U = \sum_i \langle \tilde{H}_i \rangle_{U,U}$$

Equation (17)

where the individual Hamiltonians $\tilde{H}_i$ are built up solely from Pauli-Z and unit operators and the $U_i$ correspond to Clifford gates. Optimizing the measurement protocol for a TEQULA objective will return an Objective as well. After the optimization, all non-trivial operators in the Hamiltonians are Pauli-Z operators, necessitating only a single type of measurement to be performed for each of them. This type is automatically detected and applied if an evaluation with finite sample sizes is requested. TEQULA will then request measurements of the qubits supported in the Hamiltonian in the computational basis from the corresponding quantum backend. The counts $p_0(i)$, $p_1(i)$, when qubit $i$ was measured to be in state 0 and 1, are then used to estimate the individual expectation values in the objective. Take for example

$$E = \langle aZ(1) + cZ(1)Z(2) \rangle_U$$

$$= a \langle Z(1) \rangle_U + c \langle Z(1)Z(2) \rangle_U$$

$$= a(p_0(1) - p_1(1))$$

$$+ c((p_0(1) - p_1(1))(p_0(2) - p_1(2)))$$

Equation (18)

where $Z = |0\rangle \langle 0| - |1\rangle \langle 1|$. Note that strict equality holds only for an infinite number of samples where $p_x = |\langle x|U|0\rangle|^2$ is the exact measurement probability. Comprehension of the details of the implementation of the measurement optimization requires in-depth technical knowledge about measurement on quantum computers, but the user of does not. This optimization is available to all TEQULA users by the inclusion of a simple optimize_measurements=true keyword statement when initializing an expectation value (see the online tutorials [21] for an explicit example).

2. Gate Compilation and Translation

In order to simulate or execute abstract circuits and Objectives, the structures must first be translated into the appropriate backend at the gate level. In TEQULA this can be accomplished either at time of execution, or by compilation in advance through the tq.compile function. In its base version, TEQULA offers compilation for gradients and backends for (controlled) rotations, (controlled) exponentiated Pauli gates (power gates) and arbitrary quantum gates defined over generators as in Eq. (14). For the future, we anticipate further improvement by the integration of specialized compiler packages such as TKET [29].

Evaluation of a quantum circuit requires two protocols: compilation, followed by translation. In compilation, abstract TEQULA gates are mapped to a more restricted set of gates by a TEQULA Compiler object. The said object is generally deployed within a predefined TEQULA function, though Compilers may also be constructed by the user. The said compiler then, according to a series of boolean arguments received upon initialization, sequentially performs a number of compilations, such as the translation of multicontrol or multitarget gates into a sequence of single control or single target gates, compilation of controlled rotations into CNOT and single qubit gates, the compilation of power gates into rotation gates, etc. This compiler is also required when automatic differentiation of Objectives is performed, and is handled automatically as a subroutine of tq.grad.

After an abstract circuit (or Objective containing several abstract circuits) is compiled to a reduced
gate set, it may then be translated into the language of a specific quantum backend, like QULACS, QIBO, QISKIT, CIRQ or PYQUIL. This is accomplished through the BackendCircuit object, more specifically through backend-specific inheritors of this class, such as BackendCircuitCirq or BackendCircuitQulacs, etc. These classes create the respective circuits in their target packages from TEQUILA QCircuit objects upon initialization, and handle all tasks of simulation, sampling, updating of variables, etc. for the target quantum backend. Because each backend supports only a subset of the available TEQUILA abstract gates directly, each BackendCircuit inheritor class contains the hard-coded list of compilation instructions required to map an arbitrary TEQUILA QCircuit into one containing only operations which are individually translatable into operations supported in the target backend. After the necessary compilation is performed, the BackendCircuit inheritor then translates each operation, differentiating between parametrized gates, unparametrized gates, and measurement operations as it does so in order to map TEQUILA parameter arguments (Variables and Objectives thereof) into the variable placeholders used by the quantum backend.

Note that compiled objectives can still be combined in the same fashion as before. This allows having objectives with expectation values that are themselves evaluated on different quantum backends. Therefore applications where different parts of a variational algorithm are executed on different hardware or where part of an algorithm is simulated classically are naturally realizable within TEQUILA.

3. Optimizers

Iterative classical optimization is a core subroutine of any VQA, and TEQUILA is purposefully tailored toward simplifying this task. Any parametrized tequila Objective can be optimized, either through the use of the built-in TEQUILA gradient descent optimizer, or through a number of optimizer objects that provide an interface between TEQUILA and powerful optimization packages like SciPy, GPyOpt, or Phoenics. All optimizers in TEQUILA inherit from a shared base class, designed for ease of extension. Additionally, TEQUILA implements a class called History, which allows for easy manipulation and plotting of the trajectories followed Objectives and their parameters over the course of some optimization run. All the optimizers are callables, taking an Objective alongside a variety of keyword arguments, and return a NamedTuple specific to that optimizer. All supported methods are conveniently accessible through the minimize function, which can take the same keywords as compile and simulate in order to control the quantum backend and additional optimizer specific keywords like gradient, initial_values, or maxiter. Partial optimization of a specific set of variables can be achieved by passing them as a list with the variables keyword. We refer to Fig. 3, the application section below and the tutorials provided on Github [21] for explicit use cases and illustrations.

TEQUILA has its own gradient descent optimizer, capable of optimizing by a variety of popular optimization routines, such as Adam, RMS-prop, Nesterov Momentum, and more. In addition to the usual use through a function call, the TEQUILA gradient descent optimizer can be used as a step-wise optimizer, to give users a more fine-grained control over its use. Both the TEQUILA GDOPrimer and the SciPyOptimizer can accept custom gradients provided by the user over the gradient keyword. These optimizers can combine their classical update routines with the Quantum Natural Gradient (QNG) [30] a method of transforming the gradients of expectation values based on the Fubini-Study metric of said expectation value. Numerical gradients are also available for both optimizers. See for example the UpGCCSD optimization further down or the TEQUILA tutorials [21].

At present, TEQUILA has plugins to two Bayesian optimization packages: GPyOpt[31], and Phoenics[32]. These packages allow for robust global optimization and may serve well for Objectives that contain a small or intermediate number of parameters but whose gradients require a large array of expectation values. Bayesian optimization has shown promise in the optimization of quantum circuits. These optimizers can be accessed identically to the gradient descent optimizers, chiefly through the tq.minimize function. See, for example, Fig. 3.

4. Noise

Because of the noise-prone nature of near term quantum devices, the exploration of how a VQA behaves in the presence of quantum noise is crucial to evaluate the performance of the algorithm at hand. Because the formalism for the simulation of quantum noise varies considerably among quantum backends, TEQUILA attempts to abstract away more painstaking details of noisy simulation so as to allow comparison between multiple backends. A few assumptions are made in order to accomplish this task:

1. All operations can be affected by noise.

```python
result = tq.minimize(objective, method="bfgs")
```
2. Individual noise sources are independent of each other.

3. Each noise source affects all k-qubit gates equally.

4. Each noise source affects k-qubit gates independently from 1,...,k−1, k+1,...,n-qubit gates (i.e. 1-qubit gates are noised separately from 2-qubit gates, etc).

5. The effects of noise on a given operation are independent from its position in the circuit.

Among these assumptions, the third is perhaps most questionable, but from the perspective of implementation, it is currently necessary in order to make the quantum noise in TEQUILA backend independent. Future releases of TEQUILA may permit more fine-grained, backend-restricted control over quantum noise; only universally-supported operations have been incorporated in this first release.

In TEQUILA, noise is represented by a NoiseModel object, itself a container for various QuantumNoise objects. Six types of quantum noise are supported in TEQUILA, these being: bit flips, phase flips, amplitude damps, phase damps, simultaneous amplitude-phase damps, and symmetric depolarizations. Each QuantumNoise object holds a probability (or list thereof), and a level, designating the number of qubits in the operations it should act upon. The NoiseModel object contains (and wraps over) these QuantumNoises, and is passed to a quantum backend upon translation of a QCircuit or Objective. NoiseModel objects may be combined with each other through simple addition.

The manner in which a NoiseModel object is translated into the application of noise depends entirely on the quantum backend in question. NoiseModel objects may be passed to tq.simulate, tq.compile, and tq.minimize through the noise keyword argument of each function. Note that, because noise is probabilistic, the application of noise requires sampling; it can currently not be combined with wavefunction simulation. Shown below is a simple example of the construction of a NoiseModel and its application to the simulation of a simple quantum expectation value.

where the noise model instructs the quantum backend to apply BitFlip noise with probability $p = 0.1$ to all 1 qubit and $p = 0.3$ to all 2 qubit gates.

5. Real devices

TEQUILA is capable of executing and emulating circuits and Objectives on real quantum devices through their corresponding interfaces (quantum backends). To access or emulate a device, the user only needs to supply a keyword argument, device, to tq.compile, tq.simulate, or tq.minimize. The value of this keyword can be any of several types, depending on the quantum backend through which the device is accessed; in general, this may be a string, a dictionary, or some backend-specific instantiation of the device as an object in itself. In the case of device emulation, the user can include the specific properties and gate set of a real device in the simulation by setting the device-specific noise model in noise='device'. The quantum backend in question provides some means of access to this noise modeling, as do, for example, Qiskit and PyQuil. Similar to noise modeling, the use of a device requires sampling. Shown below is a small example of how a TEQUILA user with an IBMQ account may use TEQUILA to run a circuit on the IBMQ Vigo device

where more fine-grained device specifications (including IBMQ providers etc) can be specified by passing either a dictionary or an already initialized IBMQ device.

III. EXAMPLES AND APPLICATIONS

TEQUILA is a general purpose library and aims to simplify initial prototyping, testing, and deployment for quantum algorithm development. It currently provides extended features for quantum chemistry applications [34] and has also been used in the context of quantum optics [35] and VQE extensions [36]. In the following, we will illustrate how TEQUILA can be applied through explicit application examples. Further, more detailed illustrations can be found in tutorials provided on Github [21].
A. Quantum Chemistry

One of the proposed “killer applications” [37] for quantum computers, and the original application proposed for the quantum variational eigensolver [2, 38] is the electronic structure problem of quantum chemistry. The goal of this application is to find well-behaved approximations to the eigenvalues of the electronic Hamiltonian which describes the electronic energy of molecular systems within the Born-Oppenheimer approximation. The electronic Hamiltonian for a molecule with \( N_e \) electrons can be written as

\[
H \left( \vec{r}_1, \ldots, \vec{r}_{N_e} \right) = \sum_k h \left( \vec{r}_k \right) + \frac{1}{2} \sum_{k \neq l} g \left( \vec{r}_k, \vec{r}_l \right), \tag{19}
\]

where the one-electron potential \( h = T + V \) is the combination of the one-electron kinetic energy operator \( T \) and the summed Coulomb potentials \( V \) between a single electron and the nuclear point charges, and \( g \left( \vec{r}_k, \vec{r}_l \right) \) is the electron-electron Coulomb potential between two electrons at positions \( \vec{r}_k \) and \( \vec{r}_l \). Given a set of orthonormal one-electron basis-functions (spin-orbitals) the electronic Hamiltonian can be written in second-quantized form as

\[
H = \sum_{kl} h_{kl} a_k^\dagger a_l + \frac{1}{2} \sum_{klmn} g_{klmn} a_k^\dagger a_l^\dagger a_n^\dagger a_m, \tag{20}
\]

where \( a_k^\dagger \) (\( a_k \)) are anti-commuting operators that create (annihilate) electrons in the spin-orbital \( k \) and \( h, g \) denote the integrals of the corresponding operators and spin-orbitals in Dirac notation. If the set of spin-orbitals forms a complete orthonormal system, the second quantized Hamiltonian (20) is equivalent to the electronic Hamiltonian (19) restricted to the anti-symmetric wave functions obeyed by fermionic systems. The fermionic anti-symmetry of the electronic states is conveniently guaranteed through the anti-commutation relations of the second-quantized operators. Detailed introductions can be found in relevant literature [39–42], and in recent reviews [43–45]. The second-quantized Hamiltonian can be encoded into a qubit Hamiltonian by application of the Jordan-Wigner or Bravyi-Kitaev transformations [46, 47], or more recently developed encodings such as the Bravyi-Kitaev Superfast transformation [48]. TEQUILA provides a convenient interface to initialize qubit encoded electronic Hamiltonians by deploying the transformations implemented in OPENFERMION [25]. The molecular integrals can either be supplied as NUMPY arrays or may be calculated by interfacing electronic structure packages such as PSI4 [49]. TEQUILA initializes a MOLECULE object which can then initialize qubit encoded electronic Hamiltonians and qubit encoded excitation generators, and can serve as an interface to classical methods of PSI4. The MOLECULE object ensures that the use of encodings, active-spaces, basis-sets and molecular parameters stays consistent for all further initialization.

1. Molecules and Hamiltonians

Using only their high-level functionality, TEQUILA molecules can be initialized by providing the molecular geometry and the one- and two-electron integrals \( h \) and \( g \). The constant nuclear-repulsion can optionally be provided to be included in the results. If PSI4 is installed the molecular parameters and integrals can be computed automatically by providing a Gaussian basis set (see for example Ref. [45]). Molecular structure data can be initialized by passing a string that addresses a file in xyz format, or directly. The following short example instructs one upon how to initialize molecules with PSI4 or by providing the integrals as NUMPY arrays \( h \) and \( g \), which are assumed to be already initialized here. In order to comply with other quantum computing packages the electron repulsion integrals \( g \) are expected in the OPENFERMION convention. In the example below we illustrate how to construct a TEQUILA molecule from the PSI4 interface or manually from NUMPY arrays of molecular integrals.

```python
# Can be filename.xyz or explicit string
geomstring = "He 0.0 0.0 0.0"

# Molecule construction with Psi4
molecule = tq.chemistry.Molecule(
    geometry=geomstring,
    basis_set="6-31G",
    transformation="bravy_kitaev"
)

# Manual Molecule construction
# resort g integrals (given as numpy array) from Mulliken
# to openfermion convention
# g = g.elems
molecule = tq.chemistry.Molecule(
    backend="base",
    geometry=geomstring,
    one_body_integrals=h,
    two_body_integrals=g,
    nuclear_repulsion=0.0,
    transformation="bravy_kitaev"
)
```

where the two-body integrals \( g \) were assumed to be in Mulliken notation (\( g_{pqrs}^{\text{Mulliken}} \equiv \langle pq|g|rs \rangle \equiv \langle pr|g|qs \rangle \equiv g_{prqs}^{\text{Dirac}} \)), used for example, by PSI4. If installed, PSI4 is automatically detected by TEQUILA and used as a default. The backend keyword allows to demand specific backends if multiple supported backends are installed. Most functionalities are implemented backend independent, allowing convenient introduction of
novel ways to represent Hamiltonians as for example a basis-set-free approach [34] representing the Hamiltonian with directly determined pair-natural orbitals [50]. The transformation keyword specifies the qubit encoding that will be used for further operations, i.e. Jordan-Wigner, etc. Currently, all transformations within openfermion are supported. Alternatively, a callable object can be passed as transformation allowing easy integration of user defined transformations. Additional parameters for qubit encodings, as for example, as needed within the qubit-tapered [51] form of the Bravyi-Kitaev transformation can be passed down as keyword arguments using transformation as prefix. If not provided TEQUILA will try to guess them. We refer to the online tutorials [21] for explicit examples.

2. Active Spaces

If the psi4 interface is used, active spaces can be set through the active_orbitals keyword by selecting orbitals which are labeled by their irreducible representation for the underlying point group of the molecule. Additionally, the occupation of the reference determinant can be defined, where the default is the Hartree-Fock reference computed by psi4 (the determinant constructed by the first \( \frac{N}{2} \) spatial orbitals). Custom reference orbitals can be chosen with the reference keyword using the same input format as for the active_orbitals. Without psi4 as a backend, irreducible representations are not considered and active spaces are set by an array of indices representing the active orbitals. Active spaces are tied to the molecule objects and shouldn’t be changed after initialization. When the active space is set, all Hamiltonians, excitation generators, classical amplitudes and energies are computed within that active space. The following example illustrates the initialization of a benzene molecule, restricted to the active space of its 6 conjugated \( \pi \) orbitals (three occupied and three unoccupied).

3. Unitary Coupled-Cluster

Unitary coupled-cluster (UCC) has become a promising model for quantum chemistry on quantum computers [2, 38] and several promising extensions thereof have been developed in recent years. Examples include extended strategies [52–55] pair-excitation based [56] and adaptive strategies in the qubit [57–59] or fermionic [60, 61] representation. TEQUILA allows the user to combine unitary operators in the UCC framework to develop new approaches. The basic building blocks are unitary operators:

\[
U_{pq}(\theta) = e^{-i \frac{\theta}{2} G_{pq}}
\]

generated by the hermitian fermionic \( n \)-body excitation generators

\[
G_{pq} = i(a_p^\dagger a_q - a_q^\dagger a_p)
\]

\[
G_{pqrs} = i(a_p^\dagger a_q a_r^\dagger a_s - h.c.)
\]

\[
G_{pq} = i \prod_n a_{p_n}^\dagger a_{q_n} - h.c.
\]

where \( p, q, r, s \) are arbitrary spin-orbital indices. Qubit encoded generators of this form can be created from the Molecule object by passing a list of \((p_0, q_1)\) ... tuples to the function make_excitation_generator which will return a TEQUILA Hamiltonian representing the qubit encoded hermitian generators of Eq. (24). The generators can be used to define a Trotterized unitary quantum gate,

```python
idx = [(p0, q0), (p1, q1)]
G = molecule.make_excitation_generator(idx)
generators=[0],
angles=["theta"],
steps=1
```

where a single Trotter step suffices in this case due to the commutativity of the Pauli strings originating from a single excitation generator. [52] TEQUILA uses alternating enumeration for spin-orbitals, meaning that the spin-up orbital \( p_1 \) of spatial orbital \( p \) is enumerated with \( 2p \) and the corresponding spin-down orbital \( p_1 \) is enumerated as \( 2p + 1 \). Note that this enumeration is independent of the chosen qubit encoding.

4. Interface to Classical Methods

TEQUILA offers a convenient interface to psi4's various classical methods by calling the compute_energy method of the Molecule. Within unitary coupled-cluster the amplitudes of canonical coupled-cluster often come in handy as potential starting points for further optimization, or for screening purposes. These can

Note that psi4 does not support the full \( D_{6h} \) point-group and uses \( D_{3h} \) instead, leading to different irreducible representations for the degenerate \( \pi \) orbitals \((A_{2u} \rightarrow B_{1u}, E_{1g} \rightarrow B_{2g}, B_{3g}, E_{2u} \rightarrow B_{1u}, A_u, B_{2g} \rightarrow B_{3g})\).
be computed with the method `compute_amplitudes`. We refer to the online tutorials for explicit examples.

5. Example: 1-UpCCGSD

As an explicit example we illustrate how to implement the 1-UpCCGSD ansatz of Ref. [56] for a Hydrogen-Flouride (HF) molecule in an active space with TEQUILA. Other molecules and active spaces may be explored in the same fashion by simply replacing the corresponding lines of code. The UpCCGSD ansatz is built up from the single and double excitation generators of equations (22) and (23) where the doubles are restricted to pairs of doubly-occupied orbitals $G_{p,q,p',q'}$. This example employs a single Trotter step, and orders by orbital number, but note that other orderings are also possible. [62, 63] The ansatz herein is constructed explicitly, but note that the molecule structure already offers a convenient initialization of the $k$-UpCCGSD unitary through the `make_upccgsd_ansatz` function. The full code to optimize the UpCCGSD expectation value is as follows:

```python
import tequila as tq
# define the active orbitals
active = active = {"A1": [1,2,3,4,5,6],
                                  "B1": [0],
                                  "B2": [0]}
geomstring = "H 0.0 0.0 0.0

mol = tq.chemistry.Molecule(
    geomstring=geomstring,
    geometries=geomstring,
    geometry=geomstring,
    active_orbitals=active)

H = mol.make_hamiltonian()
EFCI = mol.compute_energy("fci")
# get some classical reference values

# initialize the hamiltonian
H = mol.make_hamiltonian()

# indices defining the UpCCGSD ansatz
idx = []
for i in range(mol.n_orbitals):
    for a in range(i+1, mol.n_orbitals):
        id.append(((2*i,2*a),(2*i+1,2*a+1)))
        id.append(((2*i,2*a)))
        id.append(((2*i+1,2*a+1)))

# initialize the circuit for the initial state
U = mol.prepare_reference()

# abstract generators which generate the gates
generators = [mol.make_excitation_generator(i)
                     for i in idx]

# create a trotterized unitary
U += tq.gates.Trotterized(generators=generators,
              k=1, angles=idx, steps=1)

# form the abstract expectation value
E = tq.ExpectationValue(H=H, U=U)

# bfgs with numerical gradients
result = tq.minimize(objective=E,
                       method="bfgs",
                       gradient="2-point",
                       method_options={"finite_diff_rel_step":1.e-4})

print("Final VQE Energy:", result.energy)
print("FCI Energy :", EFCI)
```

where the scipy implementation of the BFGS optimizer with numerical gradients is employed.

6. Example: Sequential Excited State Solver

One way for VQAs to optimize bound excited states of a given Hamiltonian is to solve for the ground state and project them out of the Hamiltonian repeating this procedure sequentially. [56, 64] After solving for $n$ states $|\Psi_i\rangle$, generated by the unitaries $U_i$, the expectation value of the ansatz $U$ and projected Hamiltonian is given by

$$\langle QHQ \rangle_U = \sum_{i=1}^{n} \langle 0 | U^\dagger (1 - |\Psi_i\rangle \langle \Psi_i|) H U | 0 \rangle$$

$$= \langle H \rangle - \sum_{i=1}^{n} E_i \langle 0 | U^\dagger U_i | 0 \rangle \langle 0 | U_i^\dagger U | 0 \rangle$$

$$= \langle H \rangle - \sum_{i=1}^{n} E_i \langle P_0 | U_i^\dagger U | P_0 \rangle$$

where we used the idempotency of the projector $Q = 1 - |\Psi_i\rangle \langle \Psi_i|$ and assumed $[H,Q] = 0$ which is true if the $|\Psi_i\rangle$ are true eigenstates of $H$ and will therefore only hold approximately within most VQAs. [56] The $P_0$ operator denotes the projector onto the all-zero qubit state $|0\ldots0\rangle$ and the second part expectation value is the squared overlap between the current ansatz and the previously found states. In Fig. 7 we illustrate how such a sequential strategy for excited states can be applied with TEQUILA. In this example we use a customized designed quantum circuit $U$ which could be replaced or combined with

```python
U = mol.make_upgccsd_ansatz(label=i)
```

to solve with the $k$-UpCCGSD as done in Ref. [56]. Note that the `label` is added to the variables of the circuit in order to keep the different runs in the sequential solver distinguishable.

B. Variational Quantum Classifier

As an example of a Quantum Machine Learning application, consider a Variational Quantum Classifier (VQC). Herein is presented a TEQUILA tutorial demonstrating the implementation a single-qubit classifier with data re-uploading [65].
This VQC model encodes data points into single-qubit rotational gates multiple times within the circuit. Each layer is defined as

$$L(\vec{x}, \vec{\theta}_i) = R_z(x^1 + \theta^1_1) R_y(x^0 + \theta^1_0),$$  (26)

where $\vec{x} = (x^0, x^1)$ are data points and $\vec{\theta}_i$ are the optimization parameters of layer $i$. The circuit is a concatenation of layers, similar to other VQAs:

$$U_{\text{class}}(\vec{x}, \vec{\theta}_1, ..., \vec{\theta}_L) = L(\vec{x}, \vec{\theta}_1) \cdots L(\vec{x}, \vec{\theta}_L).$$  (27)

This VQC model can be initialized using the following function, which depends on the number of layers and the data points:

```python
import tequila as tq
# define the geometry directly
geometry="be 0.0 0.0 0.0\nh 0.0 0.0 \{R\}nh
R = 1.0
# define the |00\rangle\rangle qubit projector
P0 = tq.paulis.Projector("|00\rangle\rangle")
# define an active space
active = {"b1u": [0], "b2u": [0]}
# initialize the current molecule
mol = tq.chemistry.Molecule(geometry=geometry,
                            active=active,
                            # specify the active orbitals
                            active_orbitals="active")
# get the hamiltonian
H = mol.make_hamiltonian()
# collect results
results = []
# for data, U2 in results:
for i in range(2):
    # toy circuit
    U = tq.QCircuit()
    # for i in range(1):
    th0 = tq.Variable((0, i))
    th1 = tq.Variable((1, i))
    U += tq.gates.Ry((i, "b1u"), th0, 0)
    U += tq.gates.Rx(x[0]+ th0, 0)
    U += tq.gates.Rx(x[1]+ th1, 1)
    return

def UClass(x, l):
    U = tq.QCircuit()
    for i in range(len(y)):
        th0 = tq.Variable((0, i))
        th1 = tq.Variable((1, i))
        U += tq.gates.Ry((i, "b1u"), th0, 0)
        U += tq.gates.Rx(x[0]+ th0, 0)
        U += tq.gates.Rx(x[1]+ th1, 1)
    return

panel shows the full implementation with TEQUILA. The results of a 2-D circle classification problem are shown in Fig. 8. Using a 3-layer single-qubit classifier, 400 training points and the rms-prop optimization algorithm, the accuracy achieved is in this case 90.5%.

The single-qubit classifier defines a target state on the Bloch sphere for each class. For a binary classification, the target states are simply the corresponding target states $|y_i\rangle\rangle \in \{|0\rangle\rangle, |1\rangle\rangle\}$ as

$$L = \sum_{i} (1 - F(\vec{x}_i, y_i))^2$$  (28)

with the fidelities between training points defined as

$$F(\vec{x}_i, y_i) = |\langle y_i | U_{\text{class}}(\vec{x}_i, \vec{\theta}) | 0 \rangle|^2$$

and $P_{y_i}$ as $|y_i\rangle\langle y_i|$. This is similar to the illustration in Fig. 4. The cost function for this VQC can be initialized as

```python
def cost(x, y, l):
    loss = 0.0
    for i in range(len(y)):
        th0 = tq.Variable((0, i))
        th1 = tq.Variable((1, i))
        U = tq.paulis.Projector(ystate)
        F = tq.ExpectationValue(H=P, U=U)
        loss += (1 - F)**2
    return loss / len(x)
```

and, after initialization, can be optimized with one of the optimizers provided by TEQUILA.
IV. CONCLUSION

Herein we have introduced TEQUILA, a full-stack open-source PYTHON package for the rapid development and deployment of variational quantum algorithms. Through the deployment of novel callable structures, the incorporation of automatic differentiation, and the inclusion of extensible plugins for numerical optimization, quantum chemistry, and more, TEQUILA is primed for the easy, intuitive transformation of ideas into code. We seek to continuously forge TEQUILA into a wide and robust platform, permitting the quantum community to work in a shared and accessible framework to further embolden the ever-accelerating pace of quantum information science and quantum learning, in the hope of enhancing collective mastery of the tools set to emerge in the coming era.

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[1] J. Preskill, Quantum computing in the nisq era and beyond, Quantum 2, 79 (2018).
[2] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O’brien, A variational eigenvalue solver on a photonic quantum processor, Nature communications 5, 4213 (2014).
[3] E. Farhi, J. Goldstone, and S. Gutmann, A quantum approximate optimization algorithm (2014), arXiv:1411.4028 [quant-ph].
[4] P. Wittek, Quantum Machine Learning: What Quantum Computing Means to Data Mining (Elsevier, 2014).
[5] Quantiki, List of qc simulators (2020).
[6] T. cirq developers, Cirq: A python framework for creating, editing, and invoking noisy intermediate scale quantum circuits (2018).
[7] H. Abraham et al., Qiskit: An open-source framework for quantum computing (2019).
[8] Microsoft, The Q# user guide - microsoft quantum.
[9] R. S. Smith, M. J. Curtis, and W. J. Zeng, A practical quantum instruction set architecture (2016), arXiv:1608.03355 [quant-ph].
[10] N. Killoran, J. Isaac, N. Quesada, V. Bergholm, M. Amy, and C. Weedbrook, Strawberry Fields: A Software Platform for Photonic Quantum Computing, Quantum 3, 129 (2019).
[11] V. Bergholm, J. Isaac, M. Schuld, C. Gogolin, C. Blank, K. McKiernan, and N. Killoran, Pennylane: Automatic differentiation of hybrid quantum-classical computations, arXiv preprint arXiv:1811.04968 (2018).
[12] A. J. McCaskey, D. I. Lyakh, E. F. Dumitrescu, S. S. Powers, and T. S. Humble, Xacc: A system-level software infrastructure for heterogeneous quantum-classical computing (2019), arXiv:1911.02452 [quant-ph].
[13] D. S. Steiger, T. Hänner, and M. Troyer, ProjectQ: an open source software framework for quantum computing, Quantum 2, 49 (2018).
[14] S. Efthymiou, S. Ramos-Calderer, C. Bravo-Prieto, A. Pérez-Salinas, D. García-Martín, A. García-Saez, J. I. Latorre, and S. Carraza, Qibo: a framework for quantum simulation with hardware acceleration (2020), arXiv:2009.01845 [quant-ph].
[15] X.-Z. Luo, J.-G. Liu, P. Zhang, and L. Wang, Yao.jl: Extensible, efficient framework for quantum algorithm design, arXiv preprint arXiv:1912.10877 (2019).
[16] Quilacs (2018), https://github.com/quilacs/quilacs.

[17] R. M. Parrish, L. A. Burns, D. G. Smith, A. C. Simonetti, A. E. DePrince III, E. G. Hohenstein, U. Bozóky, A. Y. Sokolov, R. Di Remigio, R. M. Richard, et al., Psi4 1.1: An open-source electronic structure program emphasizing automation, advanced libraries, and interoperability, Journal of chemical theory and computation 13, 3185 (2017).

[18] Q. Sun, T. C. Berkelbach, N. S. Blunt, G. H. Booth, S. Guo, Z. Li, J. Liu, J. D. McClain, E. R. Sayfutyarova, S. Sharma, S. Wouters, and G. K.-L. Chan, PyCscf: the python-based simulations of chemistry framework, Wiley Interdisciplinary Reviews: Computational Molecular Science 8, e1340 (2018).

[19] Q. Sun, Libcint: An efficient general integral library for gaussian basis functions, Journal of Computational Chemistry 36, 1664 (2015).

[20] J. Bradbury, R. Frostig, P. Hawkins, M. J. Johnson, C. Leary, D. Maclaurin, and S. Wanderman-Milne, A multiresolution, adaptive numerical environment for quantum chemistry, ACS Central Science 4, 206 (2018).

[21] R. J. Harrison, G. Beylkin, F. A. Bischoff, J. A. Calvin, Q. Sun, Libcint: An efficient general integral library for novel quantum algorithms (2020), arXiv:1710.07629 [quant-ph].

[22] R. J. Harrison, G. Beylkin, F. A. Bischoff, J. A. Calvin, G. I. Fann, J. Fosso-Tande, D. Galindo, J. R. Hammond, R. Hartman-Baker, J. C. Hill, et al., Madness: A multiresolution, adaptive numerical environment for scientific simulation, SIAM Journal on Scientific Computing 38, S123 (2016).

[23] M. Schuld, V. Bergholm, C. Gogolin, J. Izaac, and N. Killoran, Evaluating analytic gradients on quantum hardware, Physical Review A 99, 032331 (2019).

[24] G. E. Crooks, Tequila: A generalized development library for novel quantum algorithms (2020), https://github.com/aspurom Guzik-group/tequila.

[25] J. R. McClean, K. J. Sung, I. D. Kivlichan, Y. Cao, C. Dai, E. S. Fried, C. Gidney, B. Gimby, P. Gokhale, T. Häner, T. Hardikar, V. Havlíček, O. Higgott, C. Huang, J. Izaac, Z. Jiang, X. Liu, S. McArdle, M. Neely, T. O’Brien, B. O’Gorman, I. Ozfidan, M. D. Radin, J. Romero, N. Rubin, N. P. D. Sawaya, K. Setia, S. Sim, D. S. Steiger, M. Steudler, Q. Sun, W. Sun, D. Wang, F. Zhang, and R. Babbush, Openfermion: The electronic structure package for quantum chemistry: an elementary introduction (Elsevier, 2012).

[26] J. S. Kottmann, M. Krenn, T. H. Kyaw, S. Alperin-Lea, and A. Aspuru-Guzik, Quantum computer-aided design of quantum optics hardware (2020), arXiv:2006.03075 [quant-ph].

[27] J. S. Kottmann, T.-C. Yen, and A. F. Izmaylov, The meta-variational quantum eigensolver (meta-vqe): Learning energy profiles of parameterized hamiltonians for quantum simulation (2020), arXiv:2009.13545 [quant-ph].

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

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

[30] T. Helgaker, P. Jorgensen, and J. Olsen, Molecular electronic-structure theory (John Wiley & Sons, 2014).

[31] I. Shavitt and R. J. Bartlett, Many-body methods in chemistry and physics: MBPT and coupled-cluster theory (Cambridge university press, 2009).

[32] R. Surján, Second quantization-based methods in quantum chemistry (Elsevier, 2012).

[33] R. Babbush, Openfermion: The electronic structure package for quantum computers, Proceedings of the National Academy of Sciences 114, 7555 (2017).

[34] J. R. McClean, J. Romero, R. Babbush, and A. Aspuru-Guzik, The meta-variational quantum eigensolver (meta-vqe): Learning energy profiles of parameterized hamiltonians for quantum simulation (2020), arXiv:2009.13545 [quant-ph].

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

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

[37] T. Helgaker, P. Jorgensen, and J. Olsen, Molecular electronic-structure theory (John Wiley & Sons, 2014).

[38] I. Shavitt and R. J. Bartlett, Many-body methods in chemistry and physics: MBPT and coupled-cluster theory (Cambridge university press, 2009).

[39] R. Surján, Second quantization-based methods in quantum chemistry (Elsevier, 2012).

[40] R. Babbush, Openfermion: The electronic structure package for quantum computers, Proceedings of the National Academy of Sciences 114, 7555 (2017).
[45] J. T. Ferminn and E. F. Valeev, Fundamentals of molecular integrals evaluation (2020), arXiv:2007.12057 [quant-ph].

[46] S. B. Bravyi and A. Y. Kitaev, Fermionic quantum computation, Annals of Physics 298, 210 (2002).

[47] J. T. Seeley, M. J. Richard, and P. J. Love, The Bravyi-Kitaev transformation for quantum computation of electronic structure, The Journal of Chemical Physics 137, 224109 (2012).

[48] K. Setia and J. D. Whitfield, Bravyi-Kitaev superfast simulation of electronic structure on a quantum computer, The Journal of Chemical Physics 148, 164104 (2018).

[49] D. Smith, L. Burns, A. Simmonett, R. Parrish, M. Schieber, R. Galvelis, P. Kraus, H. Kruse, R. Di Remigio, A. Alemenian, et al., Psi4 1.4: Open-source software for high-throughput quantum chemistry, (2020).

[50] J. S. Kottmann, F. A. Bischoff, and E. F. Valeev, Direct determination of optimal pair-natural orbitals in a real-space representation: The second-order Moller–Plesset energy, The Journal of Chemical Physics 152, 074105 (2020).

[51] S. Bravyi, J. M. Gambetta, A. Mezzacapo, and K. Temme, Tapering off qubits to simulate fermionic hamiltonians, arXiv preprint arXiv:1701.08213 (2017).

[52] J. Romero, J. Babbush, J. R. McClean, C. Hempel, P. J. Love, and A. Aspuru-Guzik, Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz, Quantum Science and Technology 4, 014008 (2018).

[53] B. T. Gard, L. Zhu, G. S. Barron, N. J. Mayhall, S. E. Economou, and E. Barnes, Efficient symmetry-preserving state preparation circuits for the variational quantum eigensolver algorithm, npj Quantum Information 6, 1 (2020).

[54] S. Yalouz, B. Senjean, J. Günther, F. Buda, T. E. O’Brien, and L. Visscher, A state-averaged orbital-optimized hybrid quantum-classical algorithm for a democratic description of ground and excited states (2020), arXiv:2009.11417 [quant-ph].

[55] I. O. Sokolov, P. K. Barkoutsos, P. J. Ollitrault, D. Greenberg, J. Rice, M. Pistoia, and I. Tavernelli, Quantum orbital-optimized unitary coupled cluster methods in the strongly correlated regime: Can quantum algorithms outperform their classical equivalents?, The Journal of Chemical Physics 152, 124107 (2020), https://doi.org/10.1063/1.5141835.

[56] J. Lee, W. J. Huggins, M. Head-Gordon, and K. B. Whaley, Generalized unitary coupled cluster wave functions for quantum computation, Journal of chemical theory and computation 15, 311 (2018).

[57] I. G. Ryabinkin, T.-C. Yen, S. N. Genin, and A. F. Izmaylov, Qubit coupled cluster method: a systematic approach to quantum chemistry on a quantum computer, Journal of chemical theory and computation 14, 6317 (2018).

[58] I. G. Ryabinkin, R. A. Lang, S. N. Genin, and A. F. Izmaylov, Iterative qubit coupled cluster approach with efficient screening of generators, Journal of Chemical Theory and Computation 16, 1055 (2020).

[59] R. A. Lang, I. G. Ryabinkin, and A. F. Izmaylov, Iterative qubit coupled cluster method with involutory linear combinations of pauli products, arXiv preprint arXiv:2002.05701 (2020).

[60] H. R. Grimsley, S. E. Economou, E. Barnes, and N. J. Mayhall, An adaptive variational algorithm for exact molecular simulations on a quantum computer, Nature communications 10, 1 (2019).

[61] H. L. Tang, E. Barnes, H. R. Grimsley, N. J. Mayhall, and S. E. Economou, qubit-adapt-vqe: An adaptive algorithm for constructing hardware-efficient ansatze on a quantum processor, arXiv preprint arXiv:1911.10205 (2019).

[62] H. R. Grimsley, D. Claudino, S. E. Economou, E. Barnes, and N. J. Mayhall, Is the trotterized uccsd ansatz chemically well-defined?, Journal of Chemical Theory and Computation (2019).

[63] A. F. Izmaylov, M. Díaz-Tinoco, and R. A. Lang, On the order problem in construction of unitary operators for the variational quantum eigensolver, Phys. Chem. Chem. Phys. 22, 12980 (2020).

[64] O. Higgott, D. Wang, and S. Brierley, Variational quantum computation of excited states, Quantum 3, 156 (2019).

[65] A. Pérez-Salinas, A. Cervera-Lierta, E. Gil-Fuster, and J. I. Latorre, Data re-uploading for a universal quantum classifier, Quantum 4, 226 (2020).

[66] M. Ponce, R. van Zon, S. Northrup, D. Gruner, J. Chen, F. Etinaz, A. Fedoseev, L. Groer, F. Mao, B. C. Mundim, et al., Deploying a top-100 supercomputer for large parallel workloads: The niagara supercomputer, in Proceedings of the Practice and Experience in Advanced Research Computing on Rise of the Machines (learning) (2019) pp. 1–8.

[67] C. Loken, D. Gruner, L. Groer, R. Peltier, N. Bunn, M. Craig, T. Henriques, J. Dempsey, C.-H. Yu, J. Chen, et al., Scinet: lessons learned from building a power-efficient top-20 system and data centre, in Journal of Physics-Conference Series, Vol. 256 (2010) p. 012026.