MISTIQS: An open-source software for performing quantum dynamics simulations on quantum computers

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Abstract.
We present MISTIQS, a Multiplatform Software for Time-dependent Quantum Simulations. MISTIQS delivers end-to-end functionality for simulating the quantum many-body dynamics of systems governed by time-dependent Heisenberg Hamiltonians across multiple quantum computing platforms. It provides high-level programming functionality for generating intermediate representations of quantum circuits which can be translated into a variety of industry-standard representations. Furthermore, it offers a selection of circuit compilation and optimization methods and facilitates execution of the quantum circuits on currently available cloud-based quantum computing backends. MISTIQS serves as an accessible and highly flexible research and education platform, allowing a broader community of scientists and students to perform quantum many-body dynamics simulations on current quantum computers.

Keywords:
quantum dynamics simulation; quantum computing
1. Motivation and Significance

With Google’s recent experimental realization of quantum supremacy for a proof-of-concept problem [1] and IBM’s announced roadmap for scaling quantum computers up to over a thousand qubits as early as 2023, there is a growing demand for the use of quantum computers for nontrivial scientific applications. A highly anticipated application is as a universal simulator of quantum many-body systems, an idea originally conceived of by Richard Feynman in the 1980s [2] and later elaborated by Seth Lloyd [3]. The last decade has witnessed the growing success of quantum computing for simulating static properties of quantum systems, i.e., the ground state energy of small molecules [4-9]. However, it remains a challenge to simulate quantum many-body dynamics on current-to-near-future noisy intermediate-scale quantum (NISQ) computers [10].

To facilitate the adoption of quantum computing for studying quantum dynamics, we have developed open-source software to perform non-trivial many-body quantum dynamics on the publicly available IBM-Q and Rigetti quantum computers. While there are general open source platforms such as Cirq [11] for developing general quantum circuits to be run on quantum computers, a host of emergent quantum programming languages [20], and other problem-specific platforms such as OpenFermion [12] for solving static electronic structure problems on quantum computers, no such platform is widely available for studying time-dependent quantum many-body dynamics. Here, we present MISTIQS (Multiplatform Software for Time-dependent Quantum Simulation), an open-source software package dedicated to enabling the dynamic simulation of quantum many-body systems that can be represented by the Heisenberg model, a ubiquitous model that captures the behavior of a variety of quantum materials and systems. An early prototype of this software was successfully used to simulate ultrafast control of emergent magnetism by terahertz radiation in atomically thin Re-doped MoSe$_2$ monolayers [13], and has since been expanded to simulate the dynamics of broader material systems that are described by the Heisenberg model.

In addition, MISTIQS also includes a domain-specific quantum circuit compiler for simulating a subgroup of the Heisenberg model known as the transverse field Ising model (TFIM) [22]. By lowering the gate count of the circuits for simulating the many-body dynamics, this special-purpose compiler allows for more accurate, longer-time simulations by reducing the compounding gate error [14], while also significantly reducing the wall-clock compilation time over backend-native general-purpose compilers. In total, MISTIQS employs a user-friendly, object-orientated framework for formulating, optimizing, and executing quantum circuits for dynamic many-body simulations on quantum computers with the goal of expanding education and spurring the development of research in this field.

2. Software Description

MISTIQS is written in Python, with backend-specific libraries only imported as needed per each use case. MISTIQS provides a full-stack solution for the direct quantum simulation of spin systems governed by the Heisenberg model Hamiltonian, taking the following form for $N$ spins:

$$H(t) = -\sum_{i=1}^{N-1} [J_x \sigma_i^x \sigma_{i+1}^x + J_y \sigma_i^y \sigma_{i+1}^y + J_z \sigma_i^z \sigma_{i+1}^z] - h(t) \sum_{i=1}^{N} \sigma_i^k \quad k \in \{x, y, z\}$$

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Here, $J_x$, $J_y$, and $J_z$ give the exchange interaction strengths between nearest neighbor spins in the $x$-, $y$-, and $z$-directions respectively, $h(t)$ gives the time-dependent external magnetic field to which the spins are exposed, and $\sigma_i^k$ is the $k$-th Pauli matrix acting on qubit $i$. The dynamics of systems modeled by this class of Hamiltonians can be simulated on digital quantum computers by mapping the states of the spins to those of the qubits, and translating the Hamiltonian-dependent time-evolution operator into a quantum circuit. Execution of the resultant quantum circuits on a quantum computer produces results that can be post-processed to show the dynamic evolution of the system.

The workflow for MISTIQS is described by Fig. 1. First, the user must define the coefficients of the Hamiltonian specific to the material system of interest, along with other simulation parameters such as number of time-steps, step-size, and quantum backend. MISTIQS then generates quantum circuits that simulate the time-evolution of the system. These circuits can then be executed on the chosen NISQ backend. Finally, the results can be post-processed to reveal the evolution of the spins over the course of the simulation. It is worth emphasizing that MISTIQS accepts a user-specified function for the time dependence of the external magnetic field, defined as $h(t)$ in Equation 1, allowing researchers to more accurately model the specific conditions of their experiments. The specifics of this full-stack functionality are shown in more detail in Fig. 2a.

The user can also choose to only use portions of MISTIQS’s functionality. For example, if the user just wants to output a list of quantum circuits compatible on IBM quantum devices, they can choose to skip circuit execution and post-processing. There is also the option to use the domain-specific compilers on externally generated circuits to output compiled circuits for IBM’s or Rigetti’s platforms.
2.1. Software Architecture

Upon downloading the software from https://github.com/USCCACS/MISTIQS, the following directories will be present:

- **src/:** Directory containing *MISTIQS* source code.
- **docs/:** Directory containing user’s manual for *MISTIQS*.
- **examples/:** Directory containing demonstrative examples covering some different use cases of *MISTIQS*.

Upon running any portion of the software, the following subdirectory will be created:

- **data/:** Directory containing simulation results, graphics (if applicable), and the logfile generated by executing the software.

*MISTIQS* is comprised of three core modules, described below with additional information about their key member functions:

- **quantum_circuits:** Code defining quantum logic gate and quantum circuit objects native to *MISTIQS* that allow it to operate above the syntax of any one quantum computing platform.
  - **Gate:** Takes as input a quantum gate name, rotation angles (if applicable), and the set of qubits it acts on to create an intermediate quantum gate representation.
  - **Program:** Builds an intermediate quantum circuit representation from a list of *Gate* objects.
- **Heisenberg:** Code that generates, compiles, and executes quantum circuits using user-defined Hamiltonian and simulation as input.
  - **generate_circuits:** From the input file, this method uses the user-specified Hamiltonian parameters, as well as user choices regarding backend and compilation. First, it generates intermediate quantum circuits needed to simulate the time-evolution of the system, then it compiles these circuits into the native gate sets and syntax of the user-specified quantum computing backend.
  - **connect_ibm:** For IBM use cases, this method connects to the IBMQ backend (needed for quantum circuit compilation and execution). Takes in IBMQ API key and account overwrite boolean as needed.
  - **run_circuits:** From the input file, this method uses the backend and quantum device choice, as well as user choices regarding post-processing of results. Its functionality is to execute the quantum circuits on the user-specified quantum device and post-process the results to the user’s specifications.
- **ds_compiler:** Code for domain-specific compilation of circuits for the TFIM (which is a special case of the general Hamiltonian in Equation 1) into the native gate sets employed by IBM and Rigetti.
  - **ds_compile_ibm:** Domain-specific quantum compiler for circuits simulating time-evolution of the TFIM. Takes in a high-level quantum circuit and returns a compiled quantum circuit executable on IBM quantum computers.
• **ds_compile_rigetti**: Domain-specific quantum compiler for circuits simulating time-evolution of the TFIM. Takes in a high-level quantum circuit and returns a compiled quantum circuit executable on Rigetti quantum computers.

The described roles and key member functions of these modules are illustrated in Fig. 2b. In this figure, information inlets and outlet paths are also highlighted, and the optional compiler-only use case is included in the context of the nominal workflow.

![Diagram](image)

**Fig. 2.** a) Full-stack representation of MISTIQS workflow. b) Key roles and member functions of MISTIQS modules.

This multi-output architecture allows MISTIQS to serve a variety of education-facing and research-facing applications; utilizing the full feature stack allows for streamlined visualizations of key observable evolutions under the Hamiltonian of interest, while the ability to output the generated simulation circuits allows for researchers to utilize their own compilers or transform circuits into the syntax appropriate for alternate quantum hardware backends.

### 2.2. Prerequisites

The MISTIQS codebase was intentionally written to minimize the number of required external libraries; it only requires the *numpy* library to be installed. If the user would like to generate plots of the simulation results, then the *matplotlib* library must be installed as well. Otherwise, any additional required libraries are solely dependent on the quantum-computing platform the user would like to produce quantum circuits for; *qiskit* [17] is required to generate circuits for IBM devices, *pyquil* [18, 19] is required for Rigetti use cases, and *cirq* [11] is likewise required for Google use cases.

### 2.3. Generalized Workflow

To use MISTIQS, the user must first define any parameters that need to be changed from their default values in a simple text-based input file. The customizable parameters are described in the appendix. A *Heisenberg* object is then created, which stores all of the input system parameters. Note that while attributes of the object are initially set from the input file, they can be changed
later in the code as any time. Next, the software transforms the input Hamiltonian and simulation parameters into a series of quantum programs (an intermediate representation of quantum circuits) that will simulate the dynamics of the system of interest via Trotter approximation. This intermediate circuit representation (native to MISTIQS) facilitates the transformation of the quantum circuits into the equivalent native circuits for various quantum computing platforms. This is crucial because quantum computing platforms can vary widely in not only in circuit object syntax, but also the native quantum gate set allowed on their hardware.

MISTIQS then compiles the circuits, if desired, using either the compilers native to the specified quantum computing platform or the built-in domain-specific quantum compilers. If execution of the quantum simulation is desired, MISTIQS will run the circuits on the specified quantum device. Once successfully run, the software can post-process the results and save the average magnetization data for each qubit over the duration of the simulation in individual output files. It can also generate and save plots of this data. A logfile is kept during each use, and this, along with all generated qubit data and plots, will be saved in a data folder.

2.4. Software Functionalities

MISTIQS can perform quantum dynamics simulations for any variant of the time-dependent Heisenberg model, including the important XX chain model, XXZ chain model, and TFIM [21]. The time-dependent external magnetic field, set to a sinusoidal function of a tunable frequency by default, can also be customized by the user, allowing for greater flexibility in the pulse shapes that can be simulated by this software. Another key functionality of the software is quantum circuit compilation, as its built-in domain-specific compilers are optimized for TFIM simulations on IBM and Rigetti backends.

3. Illustrative Examples

3.1. XX Chain Model Domain Wall Quench Simulation

In this example, we use a 16-qubit noiseless quantum simulator to explore the dynamics of a 6-spin XX chain forming a domain wall. We are interested in measuring and plotting the average magnetization of each spin over time. An XX spin chain is a subcase of Equation 1 where \( J_x = J_y \neq 0 \) and \( J_z = h(t) = 0 \), with \( J_z \) set by the material being simulated. While it is one of the simplest subsets of the Heisenberg model, it has shown relevance in entanglement teleportation and low-energy quantum chromodynamics (QCD) [15,16].

For this example, we configure the initial spins of the spin chain by setting the initial_spins parameter so that half of the spins start in a spin-down configuration in order to form a domain wall. To run the simulation, we first initialize the Heisenberg object with the relevant input file, then generate the circuits with the generate_circuits() method, then run the simulation with the run_simulation() method. Fig. 3a illustrates the spin states of each spin in this domain wall example over the course of a 50 fs simulation, with the evolution of the second spin highlighted in green, and the corresponding plot of the evolution of the second spin produced by MISTIQS is shown in Fig. 3b. The results align with those presented in Fig 2 of ref [21].

3.2. Quantum Ising model Simulation of Emergent Magnetism in MoSe2:
In this example, we will explore the emergent magnetism of a Re-doped MoSe$_2$ monolayer, which we model with the TFIM, by performing a 5-qubit quantum simulation on IBM’s 5-qubit “Ourense” quantum computer. TFIM spin chains are governed by Equation 1 where $J_x = J_y = 0$, $J_z \neq 0$, and $k = x$. Physically, this describes a system with inter-spin coupling only in the $z$-direction in the presence of an external magnetic field aligned with the $x$-direction. To run a quantum simulation of such a system with MISTIQS, set the $J_z$ parameter to the value matching the system of interest, set the ext_dir parameter to ‘$X$’, then set the $h_{ext}$ to a nonzero value. Then, the num_qubits parameter is set accordingly, and the initial_spins parameter is set to reflect standard spin-up configuration. Other general simulation parameters, such as simulation length and backend, are also set. A complete example input file, TFIM_input_file.txt, is found in the examples directory.

To run the simulation, a Heisenberg object is created with the relevant input file, then the user is connected to the IBM Q backend by running the connect_IBM() method. Next, the quantum circuits are generated by running the generate_circuits() method, and the simulation is executed and post-processed by running the run_circuits() method. The resulting plot of average magnetization should resemble Fig. 3c, although differences will inevitably arise due to device noise.

3.3. Standalone Compiler for the Quantum Ising Problem:

In this example, we will use the domain-specific (DS) compilers built into MISTIQS to optimize the quantum circuits of a TFIM simulation. The user need only import the ds_compiler module, and call the ds_compile method on the circuits, providing the desired backend to compile to as an argument. If running the sample circuits described above, this backend argument would be “ibm”. The optimized circuits will be returned as a new list. Input circuits may be generated by initializing a Heisenberg object with the TFIM example input file (see Section 3.2), and using the output of the return_circuits() method of the Heisenberg object. Alternatively, the user may input externally created circuits.

The examples directory contains an example use case that directly implements these steps, then runs the same circuits through IBM’s native compiler to directly compare the performances of the two compilers. This will produce a comparison of quantum gate counts between the identical circuits compiled by the domain-specific compiler built into MISTIQS and the native IBM compiler resembling Fig. 3d.
Fig. 3. (a) Average magnetization of the domain wall example spin chain over time. (b) Average magnetization of the second spin over time as output by MISTIQS. (c) Example average magnetization evolution of a TFIM chain spin executed by MISTIQS on both a noiseless quantum simulator and an IBM quantum computer. (d) Comparison of quantum gate counts in a sample TFIM circuit when compiled with the IBM native compiler and the domain-specific compiler integrated into MISTIQS.

4. Impact

The three major impacts of MISTIQS are: (1) to provide an open-source platform enabling accessible, end-to-end quantum dynamics simulations across the major quantum computing platforms open to public use; (2) to accelerate quantum dynamics simulation research by wrapping quantum circuit formation, compilation, execution, and basic post-processing into a user-friendly package; and (3) to facilitate quantum computing education, where the accompanying examples and tutorials can be used as self-contained course modules in classroom and workshop settings.

MISTIQS aims to bridge the gap between quantum computation and fields such as chemistry, materials science, and condensed matter physics by making quantum dynamics simulations on NISQ-era devices accessible to a wider range of researchers. It is our hope that this high-level programming library can spur new acceleration in exploring the power of current quantum devices across a wide range of applications. Already, beta versions of this software have been successfully used to perform quantum simulations of ultrathin materials under the TFIM exploring emergent magnetism phenomena [13].

5. Conclusions

In summary, MISTIQS is an end-to-end software solution for performing quantum simulations of systems governed by any subset of the time-dependent Heisenberg model Hamiltonians on current quantum computers. By simplifying and streamlining the workflow from the material’s Hamiltonian to the post-processed quantum computer data, as well as providing effortless cross-
platform functionality between IBM, Google, and Rigetti quantum computing platforms, researchers outside of the field of quantum computation can easily leverage the power of quantum computers in their work. MISTIQS has already proven its utility in the simulation of quantum materials, and is expected to accelerate quantum simulation research in a wide variety of applications including quantum chemistry, materials science, and condensed matter physics.

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Appendix

List and Descriptions of Customizable Parameters

| Parameter Name | Description |
|----------------|-------------|
Jx Controls inter-spin coupling in the X direction
Jy Controls inter-spin coupling in the Y direction
Jz Controls inter-spin coupling in the Z direction
h_ext Controls amplitude of the Hamiltonian’s external magnetic field term
ext_dir Sets the direction of the external magnetic field
num_qubits Specifies the number of qubits of the quantum simulation
initial_spins Sets the initial spins of each qubit
delta_t Sets the timestep of the quantum simulation
steps Specifies the number of timesteps in the quantum simulation
QCQS Specifies whether the circuits will be run on a quantum computer or a quantum simulator
shots Sets the number of shots to execute on the quantum device
noise_choice If using a quantum simulator, this sets whether a noisy simulator is desired.
device_choice Specify the quantum device to generate the circuits for and/or run the circuits on
plot_flag Sets whether post-processed results from running the quantum simulation should be plotted and saved.
time_dep_flag Specifies whether time dependence is desired in the Hamiltonian external field term
freq Specifies the frequency of the optional time dependent function in the Hamiltonian external field term
custom_time_dep Sets whether the software should look for a user-defined time dependence function for the Hamiltonian external field term
backend Sets the choice of quantum computing platform (IBM, Rigetti, Google)
compile Sets whether the software should compile the generated quantum circuits
auto_smart_compile Sets whether the integrated domain-specific compilers should automatically be applied to detected TFIM circuits (IBM and Rigetti backends only)
default_compiler Sets whether the software defaults to compilers native to the backend of choice or the integrated domain-specific compilers (IBM and Rigetti backends only)

B- Required Metadata

B1 Current executable software version

Table 1 – Software metadata

| Nr | (executable) Software metadata description | Please fill in this column |
|----|--------------------------------------------|---------------------------|

| S1        | Current software version | v1.0       |
|-----------|--------------------------|------------|
| S2        | Permanent link to        | https://github.com/USCCACS/MISTIQS |
|           | executables of this     |            |
|           | version                  |            |
| S3        | Legal Software License  | MIT License|
| S4        | Computing platform /     | Linux      |
|           | Operating System         |            |
| S5        | Installation requirements & | Python 3.8, numpy, matplotlib*, qiskit*, pyquil*, cirq* |
|           | dependencies             | *optional depending on use case |
| S6        | If available Link to user | https://github.com/USCCACS/MISTIQS/tree/master/docs |
|           | manual - if formally     |            |
|           | published include a      |            |
|           | reference to the         |            |
|           | publication in the       |            |
|           | reference list           |            |
| S6        | Support email for        | cdpowers@usc.edu |
|           | questions                |            |

**Table 2** – **Code metadata**

| Nr | Code metadata description | Please fill in this column |
|----|---------------------------|----------------------------|
| C 1| Current Code version      | v1.0                       |
| C 2| Permanent link to code / | https://github.com/USCCACS/MISTIQS |
|    | repository used of this   |                            |
|    | code version              |                            |
| C 3| Legal Code License        | MIT License                |
| C 4| Code Versioning system    | git                        |
|    | used                      |                            |
| C 5| Software Code Language    | python                     |
|    | used                      |                            |
| C 6| Compilation requirements, | Python 3.8, numpy, glob*, |
|    | Operating environments & | matplotlib*, qiskit*,     |
|    | dependencies              | pyquil*, cirq*             |
|    | *optional depending on use| case                      |
| C 7| If available Link to      | https://github.com/USCCACS/MISTIQS/tree/master/docs |
|    | developer documentation /|                            |
|    | manual                    |                            |
| C 8| Support email for questions | cdpowers@usc.edu          |