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Qiskit Dynamics: A Python package for simulating the time dynamics of quantum systems

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Summary

Qiskit Dynamics is an open-source Python library for numerically simulating the time dynamics of finite-dimensional quantum systems. The goal of the package is to provide flexible configuration of the numerical methods used for simulation: general tools for transforming models of quantum systems for more efficient simulation (rotating frames and the rotating wave approximation), choice of array representations (dense vs. sparse, and different array libraries), and access to different types of underlying solvers (standard ODE vs. geometric solvers). The package also contains advanced functionality for computing time-dependent perturbation theory expressions used in robust quantum control optimization (Haas et al., 2019; Puzzuoli et al., 2023).

As part of the Qiskit Ecosystem (https://qiskit.org/ecosystem), the package interfaces with other parts of Qiskit (Qiskit contributors, 2023b). Most notably, Qiskit Dynamics provides tools for simulating control sequences specified by Qiskit Pulse (Alexander et al., 2020), which gives a pulse representation of quantum circuit instructions. Higher-level interfaces allow users to build and interact with simulation-based objects that target the same constraints (qubit layout, control sequence sampling rate, etc.) as a specified IBM Quantum computer.

Lastly, to facilitate high-perfomance applications, Qiskit Dynamics is compatible with the JAX array library (Bradbury et al., 2018). As such, all core computations are just-in-time compilable, automatically differentiable, and executable on GPU.

Statement of need

Numerical simulation of time-dependent quantum systems is a useful tool in quantum device characterization, design, and control optimization. As these applications often involve the expensive process of repeatedly simulating a system across different parameters (e.g., in exploratory parameter scans or in optimizations), users need to be able to easily select the numerical methods that are most performant for their specific problem. The ability to automatically differentiate and compile simulations is also critical for control optimization research. To ensure flexibility and broad applicability, it is important that all of these capabilities work for arbitrary user-specified models.

Furthermore, having a simulation-based drop-in replacement for real quantum computing systems is useful for developers building software tools for low-level control of experiments, such as Qiskit Pulse (Alexander et al., 2020) and Qiskit Experiments (Kanazawa et al., 2023).

Related open source packages

Due to its importance, many open-source packages contain time-dependent quantum system simulation tools. In Python, these include QuTiP (Johansson et al., 2013), TorchQuantum (Wang et al., 2022), and C3 (Wittler et al., 2021). C++ packages (also with Python interfaces) include lindbladmpo (Landa & Misguich, 2023) and Quandary (Günther et al., 2021). Packages also exist in other languages, such as the Hamiltonian open quantum system toolkit (HOQST) (Chen & Lidar, 2022) and a Framework for Quantum Optimal Control (Goerz et al., 2023) in Julia, and Spinach (Hogben et al., 2011) in MATLAB. The features in Qiskit Dynamics for simulating Qiskit Pulse control sequences replace those previously offered in Qiskit Aer (Qiskit contributors, 2023a).

Documentation and community

Qiskit Dynamics documentation, including API docs and tutorials, is available at https://qiskit.org/ecosystem/dynamics/. A public Slack channel for community discussion can be found here: https://qiskit.slack.com/archives/C03E7UVCDEV.

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