Usage Report for Fiscal Year 2020

Project Title:

Simulating open quantum many-body systems with neural network-approximated quantum trajectories

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1. Background and purpose of the project, relationship of the project with other projects

The analysis of dissipative (interacting) many-body systems, comprising, for instance, steady-state behavior, dissipative phase transitions, and the interplay between interaction and dissipation, lies at the forefront of modern condensed matter research. While their analytical treatment is severely limited, numerical evaluations are extremely costly, due to the exponential growth of the Hilbert space dimension.

One of the hopeful candidates to overcome this problematic situation is to apply machine-learning based technology. Specifically, we aim to circumvent the “curse of dimensionality” by exploiting the expressive power of neural networks, which have been shown to be extremely powerful in the context of classical data processing. The target in our research is among the most challenging simulations in many-body phenomena: the non-equilibrium dynamics of open quantum systems. To be specific, we have been implementing a quantum trajectory-based algorithm, where the full mixed-state dynamics is simulated by stochastic evolution of pure states, such that the full mixed state is recovered by ensemble averaging over the individual trajectories. To reach sufficiently large system sizes, and also to simulate the system dynamics for sufficiently long times, it is necessary to use computing resources that go far beyond the capabilities of private computers, or even smaller clusters/servers; a full-fledged supercomputer appears indispensable.

2. Specific usage status of the system and calculation method

We have installed multiple software packages including *QuTip* and *OpenFermion* for small-size simulations, mainly intended for debugging. Moreover, we have installed *NetKet*, which has been developed to perform large-scale simulations by multi-thread variational Monte Carlo simulation. Using private computers, we have developed the target algorithm that performs the neural network-based quantum trajectory simulation.

3. Result

With the help of the computing power of HOKUSAI, we have been able to confirm that the scaling of the computation time required to run

individual quantum trajectories is significantly reduced in neural-network simulations. While we have not yet established a smoking-gun demonstration that would unambiguously highlight the superiority of our method, we are currently exploring promising candidates such as one- and two-dimensional quantum spin models under local dissipation. In this respect, a key element towards quality assessment of the neural-network approximation is an accurate error accumulation, which is indispensable in variational simulations.

4 . Schedule and prospect for the future

Besides continuing to investigate the applicability of our method, we plan to develop a practical indicator for the simulation accuracy, which can be evaluated during the real time evolution. Such an online accuracy indicator will not only be relevant for the simulation of dissipative quantum systems, but also for other applications, such as the simulation of the non-equilibrium dynamics of closed systems, finite-temperature simulations, etc.