2021年度　利用報告書

プロジェクト名（タイトル）：**Parallelization of open quantum systems with QuTiP**

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1.　本プロジェクトの研究の背景、目的、関係するプロジェクトとの関係

This project has two goals. First, we wish to explore and expand the capability of our open-source software package QuTiP (the QUantum Toolbox in Python) to take advantage of high performance computing. Second, we wish to use these capabilities on a specific problem for simulating the strongly interacting quantum thermal machines using our new pseudo-mode method.

QuTiP is a widely used package for simulating open quantum systems. The data layer backend of QuTiP was recently generalized, and allows for the use of libraries like tensorflow, cupy, and Jax, to make leveraging HPC capabilities easier. We want to use Hokusai to explore these capabilities, and benchmark how our solvers scale.

Secondly, we wish to use QuTiP for a specific physics problem: modelling a quantum machine strongly interacting with multiple thermal environments. We want to demonstrate that our new pseudo-mode method can capture the correct thermodynamics and heat flow even in the strong coupling regime, a parameter regime relevant for experimental realization with superconducting circuits.

2.　具体的な利用内容、計算方法

We began by testing general QuTiP usage on Hokusai and checking that the existing methods supporting parallel operations included in QuTiP work for creating multiple processes on a single node. We are now exploring how generalize these using MPI, so that the same tasks can be performed on multiple nodes.

We also began our pseudo-mode calculations. We developed a generalized quantum-jump approach to efficiently model multiple environments. This quantum-jump approach has two advantages: it uses less memory than a full master equation simulation and can be easily operated in parallel.

3.　結果

For the pseudomode project, we used all cores on a single node, and found convergence in the results with around 100,000 trajectories. We are currently writing a paper incorporating these results.

4.　まとめ

Access to Hokusai Big Wave has been extremely useful for both assessing the capabilities of QuTiP, and for enabling us to simulate a quantum thermal machine strongly interacting with several environments. For the latter, it enabled us to generate the large number of trajectories we needed to numerically simulate this type of large complex system in a reasonable amount of time.

5.　今後の計画・展望

We plan to continue adding features to QuTiP to support HPC use and will use our access to Hokusai to enable this. In addition, after adding MPI support, we will explore how multiple nodes can be used to enable the simulation of more complex systems with our pseudomode approach. As well as continuing our efforts on quantum thermal machines, we wish to use our pseudomode method to simulate Kondo resonance in the scaling limit, which requires a large amount of memory. If we can spread the ODE solving across multiple nodes we can overcome this barrier and demonstrate that our methodology can access this challenging regime.