Usage Report for Fiscal Year 2022

Project Title:

Parallelization of open quantum systems with QuTiP

Name:
○Neill Lambert (1), Paul Menczel (1), Simon Cross (1)

Laboratory at RIKEN:
Theoretical quantum physics lab
(1) Theoretical Quantum Physics Lab, CPR, RIKEN

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

This project is about the use of QuTiP, our open-source software package, on high-performance computing platforms. Our goal is to explore how well our package works in simulating large quantum systems on a high-performance computer, and apply it to specific problems.

For the latter, we wish to use the Hokusai supercomputer to simulate complex system bath problems using the pseudomode method and the hierarchical equations of motion (HEOM) method, taking advantage of the massive parallelization available.

2. Specific usage status of the system and calculation method

This fiscal year we have continued using Hokusai to explore how well our generalized pseudomode quantum-jump approach works, enabling us to tackle large problems in quantum control and quantum thermodynamics. We also used the facilities to test our HEOM package (see list of publications).

3. Result

We explored in more detail the convergence properties of the pseudomode method and found that it behaves differently from standard quantum jump approaches at long time scales. We are now exploring how to determine when convergence is possible. We also used the Hokusai HPC in testing our HEOM open-source package, which was just accepted for publication in Physical Review Research.

4. Conclusion

The Hokusai HPC has been a valuable resource and enabled us to explore new ideas in how to parallelize the large open quantum system problems we regularly deal with. For example, we plan to explore using it next year for a new method based on stochastic noise, see prospects below.

5. Schedule and prospect for the future

We have developed a stochastic approach based on classical noise averaging and are planning to explore its power using Hokusai next fiscal year.

In addition, we are still exploring how to optimally use MPI features with QuTiP and will use Hokusai as a test bed for this activity.

6. If no job was executed, specify the reason.

Fiscal Year 2022 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Neill Lambert, Tarun Raheja, Simon Cross, Paul Menczel, Shahnawaz Ahmed, Alexander Pitchford, Daniel Burgarth, Franco Nori, “QuTiP-BoFiN: A bosonic and fermionic numerical hierarchical-equations-of-motion library with applications in light-harvesting, quantum control, and single-molecule electronics”, In press, Physical Review Research (2023), arXiv:2010.10806