Project Title:

Parallelization of open quantum systems with QuTiP

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

The purpose of this project was to explore the use of high-performance computers for simulations using our open-source software package QuTiP, and enable new features in QuTiP, like support for MPI.

The specific physics problems we are interested in are complex simulations of quantum noise, based on our recently developed pseudomode method and the hierarchical equations of motion method.

2. Specific usage status of the system and calculation method

The hokusai supercomputer has been important in checking and benchmarking support for MPI we added to QuTiP, our open source package in Python. This focuses on problems relying on unraveling of master equations, where each possible trajectory of evolution can be put on different cores, and batches sent to multiple nodes.

3. Result

We added support for a new parallel-map function in QuTiP that uses MPI4PY to distribute tasks across multiple nodes, allowing users to use QuTiP on their own supercomputer. In addition, the simulations we performed last year, on the unravelling of pseudomode master equations, were published in a APS Physics Review Research paper.

4. Conclusion

The Hokusai supercomputer has been instrumental in both improving QuTiP, and enabling us to perform large scale simulations.

5. Schedule and prospect for the future

We have finished this project for the time being. We plan to explore more uses of supercomputer resources in QuTiP in the future, as the need arises, under a new project.

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

We extended the project through 2024 in case we needed to perform further benchmarking on the MPI support we added to QuTiP, or check results incorporated in our pseudomode article. This turned out not to be necessary, so we did not execute any jobs.

Fiscal Year 2024 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Non-Hermitian pseudomodes for strongly coupled open quantum systems: Unravelings, correlations, and thermodynamics

Paul Menczel, Ken Funo, Mauro Cirio, Neill Lambert and Franco Nori