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 is to explore the use of high-performance computers for simulations using our open-source software package QuTiP.

The specific 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

We used the Hokusai facilities to simulate complex models of noise and their influence on thermodynamic heat engines via the quantum-jump unravelling of our pseudomode method. We also used it to model correlated transport and Kondo physics.

3. Result

We published a work on using pseudomodes to model electron transport and Kondo physics in Physical Review Research.

A paper on the use of pseudomode unravelings for modelling heat engines is now largely complete, and will be submitted for review.

4. Conclusion

We very much appreciate the Hokusai facilities. It has been extremely useful for the kind of numerical problems we have to tackle.

5. Schedule and prospect for the future

We are still exploring how to optimally use MPI for the kind of problems we have in QuTiP. We plan to continue using Hokusai next year, and explore new problems that can be accelerated by the combination of QuTiP and Hokusai

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

Fiscal Year 2023 List of Publications Resulting from the Use of the supercomputer
 [Paper accepted by a journal]

Mauro Cirio, Neill Lambert, Pengfei Liang, Po-Chen Kuo, Yueh-Nan Chen, Paul Menczel, Ken Funo, and Franco Nori, "Pseudofermion method for the exact description of fermionic environments: From single-molecule electronics to the Kondo resonance"
Phys. Rev. Research 5, 033011 (2023)