プログラム名： 量子人工脳を量子ネットワークでつなぐ高度知識社会基盤の実現
PM 名： 山本喜久
プロジェクト名：量子シミュレーション

委 託 研 究 開 発

実 施 状 況 報 告 書（成果）

平成 28 年度

研究開発課題名：

現代コンピュータに実装できる量子多体系の新計算手法の開発(理論研究)

研究開発機関名：

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Ⅰ　当該年度における計画と成果

１．当該年度の担当研究開発課題の目標と計画

Our goals for 2016 were to refine and expand several features of the Quantum Toolbox in Python software (QuTiP). In particular, we planned to extend and improve the functions we started developing in 2015 for calculating counting statistics and solving exact system-bath problems. Secondary goals were to improve overall performance of QuTiP.

２．当該年度の担当研究開発課題の進捗状況と成果

2-1 進捗状況

We succeeded in refining and improving the counting statistics functions, and the hierarchy equation of motion package for the exact solution of a system coupled to a bosonic environment, which were both officially released in QuTiP v4.1.

With collaborators, we also made substantial changes to low-level parts of QuTiP to improve performance in various areas.

Note that QuTiP has been mentioned in very high-profile and quite visible publications, like Nature Physics and The Economist.　Thus it is having an ImPACT in society.

2-2 成果

1) For the counting statistics methods, we developed easy-to-use functions so that users can model transport of particles through arbitrary nanostructures, and calculate, using counting statistics techniques, quantities like current, shot noise, and frequency-dependant spectra. We also made codes showing various simple examples of how to use these functions.

2) We finalized a user-friendly version of the Hierarchy Equations of Motion. This solver allows users to model non-Markovian and non-perturbative environments for open quantum systems. This powerful method was originally proposed by Tanimura and Kubo, and has applications in various fields, including quantum information, physical chemistry, and quantum biology. Our code allows users to apply it to arbitrary systems, with great efficiency (It is now approximately 20x faster than our preliminary development code).

3) With our collaborators, among other changes we made the following low-level improvements to general QuTiP performance:

- Updated Steady state solvers
  - Direct and inverse-power routines are now 100x+ faster using Intel Pardiso solver
- Batch mode for Propagator construction
  - One can compute the propagator of a system's dynamics by evolving all possible initial basis states simultaneously using a block-concatenated Hamiltonian.　Allows for faster construction of a propagator at the cost of a larger memory overhead.
- Sparse matrix-vector multiplication: We now make use of both SSE3 (Streaming Symmetric Instructions and Multiple Data Extensions), a very highly optimized low level instruction set, and OPENMP (Open Multi-Processing) open source library.　This leads to:

○ SSE3 leads to Fast complex-complex matrix-vector multiplication, with a 40% faster single-thread (single CPU) performance.
○ Enhanced parallel performance with OPENMP.

● Sparse Matrices:　New Fast CSR (Compressed Sparse Row) matrix class
○ Up to 20x improvement in the time needed to create a CSR matrix.
○ Up to 100x+ improvement in CSR adjoint & transpose operations.
○ Up to 100x+ improvement in Hermitian verification.
○ Up to 100x+ improvement in Kronecker tensor product.
○ Up to 100x+ improvement in partial trace (tracing out sub-systems).
○ 100% compatible with standard SciPy CSR matrix class.

These improvements led to substantial speed-up in many solvers, like the Hierarchy Equations of motion mentioned above.

2-3 新たな課題など

We plan to continue developing QuTiP as a powerful tool for the community, by both improving performance and adding new features. Our primary goals for 2017 are:

1) We plan to add support for time-dependant Hamiltonians and loss terms to the functions used to calculate correlations and spectra.

We also plan to improve the underlying Lindblad and Monte-Carlo solvers, by adding more sophisticated support for parallelization on multi-core machines.

2) We also plan to add support for time-dependant Hamiltonians to the Hierarchy equations of Motion solver. This will allow users to treat quantum control problems with an exact method.

In the longer term, beyond 2017, we plan to add new solvers to treat fermonic environments. This will allow users of QuTiP to study sophisticated many-body physics like the Kondo effect.

We also plan to continue integration of various modules in QuTiP, in particular the Quantum Information Processing (QIP) module, and the quantum control module. In the former, we also plan to add increased functionality, including simulated heralded near-deterministic multi-qubit controlled phase gates with integrated error detection.

３．アウトリーチ活動報告

Our software QuTiP (Quantum Toolbox in Python) has been featured (early 2017) in the well-known magazine “The Economist”, in an article on software for quantum computers. The article appeared in the print edition in the Technology Quarterly section, which covered quantum devices.

The software QuTiP is mentioned in an article in Nature. The article writes that: "QuTip, another Python package, enables researchers working on quantum mechanics to define a system and then simulate how it behaves."

The outreach and usefulness of this software is also proved by the 25,473 unique visitors to qutip.org in 2016.