3.6 Software Advancement Projects and Workshop Support

Implementation of Finite-Temperature Calculation in TeNeS

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In quantum many-body problems, such as quantum spin systems and strongly correlated electron systems, the dimension of the Hilbert space increases exponentially with the number of spins or particles, making precise analysis of large systems difficult. The tensor network method, which is one technique to overcome such difficulties, represents quantum states as a network constructed by the contraction of small tensors, thereby reducing the effective degrees of freedom and enabling the computation of large systems. The infinite projected entangled pair state/infinite tensor product states (iPEPS/iTPS) is a tensor network that can directly represent the ground state of an infinitely large system. We are developing a tensor network library TeNeS based on iPEPS/iTPS [1, 2]. TeNeS supports MPI and OpenMP hybrid parallelization, and enables us to calculate the ground states of various two-dimensional lattice models.

This year, through the support of Project for Advancement of Software Usability in Materials Science (PASUMS), we have implemented the finite-temperature calculation in TeNeS. The finite-temperature calculation is essential for the analysis of the physical properties of quantum many-body systems, such as the specific heat, and magnetization. The finite-temperature calculation is performed by the imaginary time evolution of the density matrix represented by the infinite projected entangled pair operator/infinite tensor product operator (iPEPO/iTPO) [3] (See Fig. 1). Such imaginary time evolution for iPEPO/iTPO is algorithmically similar to the ground state calculation based on iPEPS/iTPS, and we can easily implement the finite-temperature calculation in TeNeS.

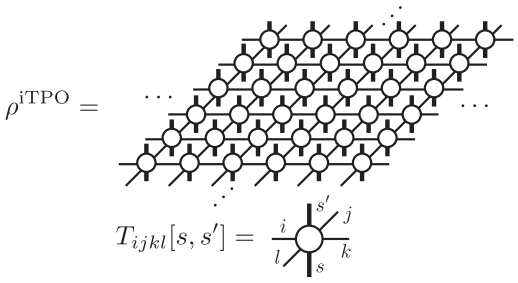

Figure 1: Tensor network diagram of a density matrix ρ represented as an iPEPO/iTPO. Vertical open legs stand for indices of local Hilbert space.

In addition to the finite-temperature calculation, we also implemented the real-time evolution of a pure state using TeNeS. The algorithm of the real-time evolution is essentially the same as the imaginary time evolution. However, usually approximation based on iPEPS/iTPS becomes less accurate for longer time evolution due to the increase of quantum entanglement. Thus, real-time evolution approximated by iPEPS/iTPS is limited to short time evolution.

The finite-temperature calculation and the real-time evolution implemented in TeNeS are useful for the analysis of the physical properties of quantum many-body systems. We hope

that TeNeS can enhance research in the field of quantum many-body systems.

TeNeS was developed with Yuichi Motoyama, Kazuyoshi Yoshimi, Satoshi Morita, Tatsumi Aoyama, Takeo Kato, and Naoki Kawashima.

References

[1] Y. Motoyama, T. Okubo, K. Yoshimi, S. Morita, T. Kato and N. Kawashima, Comput. Phys. Commun. **279**, (2022) 108437.

[2] https://github.com/issp-center-dev/TeNeS

[3] A. Kshetrimayum, M. Rizzi, J. Eisert, and R. Orús, Phys. Rev. Lett. **122**, (2019) 070502.

Development of a tool to create a database of first-principles calculations using high-throughput calculations

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In recent years, approaches to predicting physical properties and designing materials using machine learning (materials informatics) have become popular, in which the generation of a large amount of supervised data is essential for highly accurate prediction and design. From this perspective, databases such as MaterialsProject [1], which store crystal structures, experimental measurement results and first-principles calculations, have been developed and are actively used. On the other hand, machine learning requires the preparation of materials and physical quantities as teacher data, but in many cases the desired materials and physical quantities do not exist in existing databases. If tools and environment can be created to quickly prepare these teacher data, it will provide a research stage for the field of materials informatics and is expected to make a significant contribution to its progress.

We developed HTP tools [2] for exhaustive data generation from crystal structures using first-principles calculations under the support of "Project for advancement of software usability in materials science". Specifically, we developed a script cif2x [3] to generate input files from crystal structures for the first-principles calculation software VASP [4], Quantum ESPRESSO [5], OpenMX [6], and AkaiKKR [7]. Samples and tutorials are provided for each software to explain how to use cif2x with each software.

We also developed a tool to generate batch job scripts, moller [8], which can easily realize exhaustive calculations by bulk execution of jobs on the ISSP supercomputer. Since moller is independent of cif2x in nature, it can be used for general exhaustive calculations with various

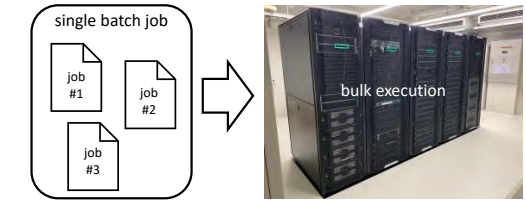

Figure 1: a series of small jobs are executed within a job of large batch classes as a bulk job execution.

solvers. Samples and tutorials are provided that apply HΦ [9] and DSQSS [10] to illustrate the implementation in bulk jobs when multiple calculation scenarios are prepared.

These two software packages, cif2x and moller, are developed as Open Source software and distributed under GPL v.3.0. They have already been pre-installed on the ISSP supercomputer systems. For future plans, we would like to create a computational materials science database using cif2x and moller. It would be interesting to make moller compatible with supercomputing systems other than ISSP supercomputer, to become a standard for exhaustive computations at HPCI. With these tools, we hope that users will make use of them to generate various databases.

References

[1] https://next-gen.materialsproject.org

[2] https://www.pasums.issp.u-tokyo.ac.jp/htp-tools/en/

[3] https://github.com/issp-center-dev/cif2x

[4] https://www.vasp.at

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[8] https://github.com/issp-center-dev/moller

[9] https://github.com/issp-center-dev/HPhi

[10] https://github.com/issp-center-dev/dsqss

Report of CCMS hands-on sessions in the 2023 fiscal year

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In the 2023 fiscal year, Center for Computational Materials Science (CCMS) in the Institute for Solid State Physics (ISSP) held 4 hands-on sessions where the ISSP supercomputer was used [1-4]. In this report, we briefly summarize them.

Table 1 shows the list of the hands-on sessions in the 2023 fiscal year. There are 4 software used in the hands-on sessions: TeNeS, RESPACK, SALMON and 2DMAT. Development of the software except for SALMON was supported by "Project for advancement of software usability in materials science" (PASUMS) [5].

Table 1: List of CCMS hands-on sessions where the ISSP supercomputer was used in the 2023 fiscal year.

Date	Lecturer	Software
Nov. 20	T. Okubo et al.	TeNeS[6]
Jan. 11	K. Yoshimi et al.	RESPACK[7]
Fen. 22	S. Yamada et al.	SALMON[8]
Mar. 28	T. Hoshi et al.	2DMAT[9]

Features of each software are as follows. TeNeS is open-source software for performing simulations for quantum many-body systems by using tensor network methods [6]. RESPACK is a software package for *ab initio* downfolding methods [7]. SALMON is open-source software for performing *ab initio* calculations of electron dynamics in materials [8]. 2DMAT is a Python package to search an optimal result of a given optimization problem by using search algorithms combined with direct-problem solvers [9].

In all of the hands-on sessions, lecturers explained the basics of each software and gave its tutorial. Materials of some hands-on sessions are available on each official page.

References

[1] https://ccms.issp.u-tokyo.ac.jp/event/6260

[2] https://ccms.issp.u-tokyo.ac.jp/event/6293

[3] https://ccms.issp.u-tokyo.ac.jp/event/6310

[4] https://ccms.issp.u-tokyo.ac.jp/event/6432

[5] https://www.pasums.issp.u-tokyo.ac.jp

[6] https://www.pasums.issp.u-tokyo.ac.jp/tenes/en

[7] https://sites.google.com/view/kazuma7k6r

[8] https://salmon-tddft.jp

[9] https://www.pasums.issp.u-tokyo.ac.jp/2dmat/en/

Supercomputer course of Computational Materials Design (CMD®) workshop

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The 41st Computational Materials Design (CMD®) workshop (CMD41) has been held from September 5th to September 9th and the 42nd CMD® workshop (CMD42) has been done from February 20th to February 24th. Both were held online. In this workshop we have the supercomputer course to train up human resources to advance research by using system B supercomputer of ISSP, the University of Tokyo.

In CMD41, nine participants took the supercomputer course and followed a tutorial on STATE-Senri developed by Y. Morikawa. After an introductory lecture on large-scale computing and an explanation of how to use the supercomputer of ISSP by M. Geshi, the participants started constructing computational models for their own research subjects with the help of the lecturers. Then they carried out calculations using supercomputers. Specific themes included molecular adsorption on solid surfaces, chemical reactions of molecules in solutions, chemical reactions of molecules on catalytic surfaces, reactions at solid-solid interfaces, and so on. The participants performed calculations and examined their results.

In CMD42 three participants took the supercomputer course and used the supercomputer of ISSP. They got a tutorial on RSPACE developed by T. Ono. After giving the introductory lecture of large-scale computing by M. Geshi and introducing the calculation method of electronic structures and electron conduction property using RSPACE, exercises instructed in the textbook were carried out. Then, electronic structure calculations were carried out for various molecules, and the electronic density distribution was visualized. The attendees also performed massively parallel calculations to confirm the efficiency for parallel computing. Finally, the electron conduction properties of two-dimensional materials and dialectic materials sandwiched between metallic electrodes were investigated.