3.6 Software Advancement Projects and Workshop Support

Advancement of Bayesian Optimization Package PHYSBO

Ryo TAMURA
Center for Basic Research on Materials, National Institute for Materials Science
1-1 Namiki, Tsukuba, Ibaraki 305-0044

Bayesian optimization is an experimental design method that leverages machine-learning-based predictions to identify better conditions with as few trials as possible. In FY2020, under the project for advancement of software usability in materials science(PASUMS) at the Institute for Solid State Physics, the University of Tokyo, we developed PHYSBO, a Bayesian optimization package targeted at physics and materials science [1,2]. In FY2025, we carried out a major update aimed at improving ease of installation and portability across diverse computational environments [3]. The core of this update lies not in changes to the optimization algorithms themselves, but in reducing the burden of practical deployment and operation. In PHYSBO version 2, we changed the license from GPL to MPL in order to enhance compatibility with a wider range of research and software ecosystems. This change provides greater flexibility in how code is handled when the PHYSBO module is imported. In the subsequent version 3, we carried out a fundamental redesign of the implementation, achieving the following functional enhancements and improvements:

- Strengthened support for multi-objective optimization
- Introduction of a range-based policy for continuous-variable optimization
- Elimination of environment dependencies through a Cython-free implementation
- Support for the latest libraries, including NumPy 2

These improvements lower both technical and organizational barriers to adoption and facilitate integration into a wide variety of computational environments and research workflows.

As a result, practical applications using PHYSBO are also accelerating, and the original PHYSBO paper [1] has been cited in numerous influential research articles. Furthermore, PHYSBO has been implemented as the standard engine of NIMO [4], a software package for autonomous materials exploration, and its use is expanding not only within Japan but also internationally.

References

[1] Y. Motoyama, R. Tamura, K. Yoshimi, K. Terayama, T. Ueno, and K. Tsuda, Comput. Phys. Commun. **278**, 108405 (2022).

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

[3] Y. Motoyama, K. Yoshimi, T. Aoyama, K. Terayama, K. Tsuda, R. Tamura, arXiv:2603.01349.

[4] https://www.nims.go.jp/nimo/

Development and Maintenance of Tutorials and Documentation for the First-Principles Quantum Monte Carlo Package TurboRVB

Kosuke NAKANO
Center for Basic Research on Materials (CBRM), National Institute for Materials Science (NIMS)
1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

The goal of this project is to improve the usability and accessibility of the first-principles quantum Monte Carlo (QMC) package TurboRVB [1, 2] and its associated Python tools, TurboGenius [3, 4] and TurboWorkflows [5], within the framework of the FY2025 Project for advancement of software usability in materials science(PASUMS) [6], by developing comprehensive tutorials, manuals, and documentation.

During FY2025, we established a unified documentation portal (Fig. 1) that consolidates the manuals for TurboRVB, TurboGenius, and TurboWorkflows into a single, user-friendly website [7]. The portal guides users to the appropriate manual depending on whether they want to run QMC calculations directly via the core TurboRVB executables, use the higher-level Python interface provided by TurboGenius, or automate multi-step workflows with TurboWorkflows. This development addressed the problem that the relevant information had previously been scattered across separate resources, making it difficult for users to identify the appropriate starting point and understand how these tools should be used in combination.

For TurboRVB, we carried out a comprehensive survey of input variable names for each program in the package. Previously, no systematic list of input parameters existed, making it difficult for new users to set up calculations. The newly compiled input-variable reference covers all major executables and is now included in the TurboRVB manual, thereby resolving this bottleneck significantly lowering the barrier to entry.

For TurboGenius, we prepared tutorials that demonstrate the higher-level Python and command-line interface for common TurboRVB workflows, including geometry optimization, energy calculations, and high-throughput screening setups. These tutorials were developed in response to the problem that, despite the availability of a higher-level interface, practical guidance for standard research use cases had been insufficient. For TurboWorkflows, we documented the remote-execution capabilities, dependency handling, and multi-step workflow orchestration features, thereby addressing the difficulty of routinely using these functions without adequate documentation, enabling users to automate chained QMC jobs across computing resources.

All documentation is publicly available at the TurboTutorials website [7] and is maintained alongside the source code repositories to ensure long-term consistency and updates. Thus, through PASUMS, we improved not only the availability of documentation itself but also the research software support environment by identifying concrete usability issues and providing corresponding solutions.

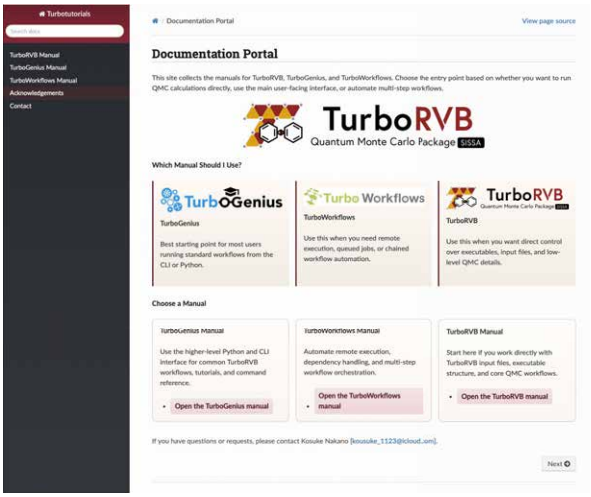

Figure 1: Top page of the TurboTutorials documentation portal, providing unified access to the manuals for TurboRVB, TurboGenius, and TurboWorkflows.

References

[1] TurboRVB, `https://github.com/sissaschool/turborvb`.

[2] K. Nakano, C. Attaccalite, M. Barborini, L. Capriotti, M. Casula, E. Coccia, M. Dagrada, Y. Luo, G. Mazzola, A. Zen, and S. Sorella, J. Chem. Phys. **152**, 204121 (2020).

[3] TurboGenius, `https://github.com/kousuke-nakano/turbogenius`.

[4] K. Nakano, A. Raghav, and S. Sorella, J. Chem. Phys. **159**, 224801 (2023).

[5] TurboWorkflows, `https://github.com/kousuke-nakano/turboworkflows`.

[6] K. Yoshimi, Y. Motoyama, T. Aoyama, T. Kawamura amd N. Kawashima, Science and Technology of Advanced Materials: Methods, **5**,1 (2025).

[7] TurboTutorials, `https://kousuke-nakano.github.io/turbotutorials/`.

Report of CCMS hands-on sessions in the 2025 fiscal year

Masahiro FUKUDA

Institute for Solid State Physics,

The University of Tokyo, Kashiwa-no-ha, Kashiwa, Chiba 277-8581

In the 2025 fiscal year, Center for Computational Materials Science (CCMS) in the Institute for Solid State Physics (ISSP) held 3 hands-on sessions where the ISSP supercomputer was used [1-3]. In this report, we briefly summarize them.

Table 1 shows the list of the hands-on sessions in the 2025 fiscal year. There are 3 hands-on sessions were held. Development of the software except for CrySPY was supported by “Project for advancement of software usability in materials science” (PASUMS) [4].

Features of each software are as follows. DCore [5] is open-source software for performing dynamical mean-field theory (DMFT) calculations for strongly correlated electron systems. ChiQ [6] is a tool for calculating susceptibilities and related response functions based on electronic structure data. CrySPY [7] is open-source software for crystal structure prediction using evolutionary algorithms and other global optimization techniques. ODAT-SE [8] is a framework for managing and automating high-throughput simulations and data analysis workflows in computational materials science.

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/7137

[2] https://ccms.issp.u-tokyo.ac.jp/event/7527

[3] https://mdcl.issp.u-tokyo.ac.jp/scc/news/7779

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

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

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

[7] https://tomoki-yamashita.github.io/CrySPY_doc/

[8] https://www.pasums.issp.u-tokyo.ac.jp/odat-se/en/

Table 1: List of CCMS hands-on sessions where the ISSP supercomputer was used in the 2025 fiscal year.

Date	Lecturer	Software	# of applicants
May. 13	J. Otsuki *et al.*	DCore, ChiQ	20
Oct. 15	T. Yamashita *et al.*	CrySPY	40
May. 27	T. Hoshi *et al.*	ODAT-SE	16

Supercomputer course of Computational Materials Design (CMD®) workshop

Masaaki GESHI[1], Yoshitada MORIKAWA[2], Tomoya ONO[3]

[1]*R^3 Institute for Newly-Emerging Science Design,*
The University of Osaka, Machikaneyama, Toyonaka, Osaka 560-0043

[2] *Department of Precision Engineering, Graduate School of Engineering,*
The University of Osaka, Yamada-oka, Suita, Osaka 565-0871

[3]*Graduate School of Engineering,*
Kobe University, Rokkodai-cho, Nada, Kobe 657-8501

The 47th Computational Materials Design (CMD®) workshop (CMD47) was held from September 1st to September 5th, and the 48th CMD® workshop (CMD48) took place from February 23rd to February 27th. Both were held online. In this workshop, we offer the supercomputer course to train human resources for advancing research using the System B supercomputer at the Institute for Solid State Physics (ISSP), the University of Tokyo.

In CMD47, four 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 including molecular adsorption and reactions on solid surfaces, atom doping in bulk Si, and formation of amorphous SiO2 were investigated. The participants performed calculations and examined their results.

In CMD48, two 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-transport property using RSPACE by T. Ono, Y. Egami, and M. Uemoto, the exercises instructed in the textbook were carried out. Then, electronic structure calculations were carried out for various molecules, and the optimized atomic structures and electronic density distributions were visualized. The attendees also performed massively parallel calculations to confirm the efficiency for parallel computing. Finally, the electronic structures of SiC bulk and/or electronic transport property of molecular junctions were investigated using large scale models.