3.6 Software Advancement Projects, GPGPU Implementation, and Workshop Support

Development of ab-initio configuration sampling toolkit (abICS) for combining first-principles calculations with extended ensemble methods

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In functional materials, varying types of configurational disorder are often employed to obtain favorable properties for a given application. The ability to simulate such disorder as a function of temperature should be immensely helpful for comparing with experiment. It would also enable prediction and design of properties in materials with realistic levels of disorder. To achieve this, a natural way may be to combine first-principles calculations with the Metropolis Monte Carlo algorithm. However, this is quite costly in terms of computational power, so many workers have opted to first derive lightweight models from first-principles calculations, then use that model for Monte Carlo sampling. The problem is that deriving lightweight *and* reliable models becomes increasingly difficult with increasing complexity of the system (various dopants, charged defects, interfaces, etc.).

In last year's ISSP joint-use project, SK proposed to bypass such fitting and instead rely on efficient parallel algorithms for thermodynamic sampling. Figure 1 shows our computational scheme. There are N_{rep} Metropolis samplers running in parallel at different temperatures. Each of the samplers spawns parallel DFT processes (we used VASP [1]) to perform local structural relaxation and energy calculation at every Metropolis step. The temperatures are swapped according to the replica exchange algorithm [2] to speed up the sampling. We successfully demonstrated that sufficient sampling can be performed on meaningfully large supercells by calculating the degree of disorder in $MgAl_2O_4$ [3].

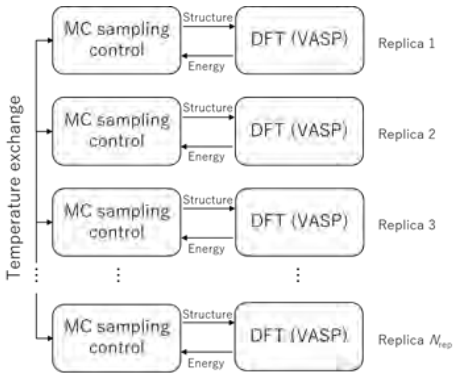

Figure 1 Our scheme for parallel configuration sampling. Reproduced from Ref. [3].

As this year's Software Advancement Project, we proposed to develop an easy-to-use interface for this computational scheme. The result has been released as ab-Initio Configuration Sampling toolkit, or *abICS* for short. It is written in Python 3 and is registered at PyPI (Python Package Index; pypi.org). It can thus be installed in most environments rather easily through the command "`pip install --user abics`". Now, abICS can sample using the replica exchange Monte Carlo algorithm, and we are planning to add support for other extended ensemble methods soon. The parameters for the sampling are controlled by an input file in TOML format, which is a minimal and easy-to-read configuration format that is being used in many software projects [4]. The parameters for the DFT calculations such as k-point sampling, basis set specification, convergence parameters, etc. are controlled by input formats of the specified solver. As the solver, abICS supports the use of DFT codes VASP, Quantum Espresso [5], and OpenMX [6] as of May 2020. It also has experimental support for aenet [7], which uses neural network potentials. Preprocessing scripts are provided for converting structure files to abICS input.

We believe that abICS will be immensely useful for making efficient use of next-generation supercomputers due to its multi-layered parallelism. We are also aiming to bring together information science, materials simulation, and statistical physics using abICS as a hub. Because of modular coding practices employed in our project, it should be relatively easy to implement interfaces for other solvers, or to implement new sampling schemes. Please have a look at our homepage [8] and do not refrain from contacting us if you are interested in using or extending this software.

References

[1] https://vasp.at/

[2] K. Hukushima and K. Nemoto: J. Phys. Soc. Jpn. **65** (1996) 1604.

[3] S. Kasamatsu and O. Sugino: J. Phys.: Condens. Matter **31** (2019) 085901.

[4] https://github.com/toml-lang/toml

[5] https://www.quantum-espresso.org/

[6] http://www.openmx-square.org/

[7] http://ann.atomistic.net/

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

GPU acceleration for solving Bethe-Salpeter equation

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The Bethe-Salpeter equation (BSE) provides two-particle responses in interacting many-body systems. In the context of dynamical mean-field theory (DMFT), for example, the momentum-dependent dynamical susceptibility $\boldsymbol{\chi}(\boldsymbol{q}, i\nu_n)$ is obtained by solving the BSE.

The BSE is symbolically written as

$$\widetilde{\boldsymbol{\chi}}(\boldsymbol{q}, i\nu_n) = [\widetilde{\boldsymbol{\chi}}_0^{-1}(\boldsymbol{q}, i\nu_n) - \boldsymbol{\Gamma}(i\nu_n)]^{-1}, \quad (1)$$

where the bold symbols indicate matrices of size $M = N_{\rm sp}^2 N_{\rm orb}^2 N_\omega$. Here, $N_{\rm sp}$ is the number of spin components, $N_{\rm orb}$ is the number of orbitals, and N_ω is the number of the fermionic Matsubara frequencies. Solving Eq. (1) requires computations of matrix multiplications and the inverse of a matrix. Therefore, the computational cost is $\mathcal{O}(M^3)$.

The matrix size M for typical models is shown in Table 1. Here, the value of N_ω is fixed at 20, but a larger value is necessary to address low-temperature properties. Namely, M in Table 1 should be regarded as a minimum estimation. We see that d-orbital systems require $M = 500$ without spin-orbit coupling (SOC) and $M = 2{,}000$ with SOC. For the f-orbital, we need $M \approx 4{,}000$.

Table 1: The matrix size M for typical models.

Model	$N_{\rm sp}$	$N_{\rm orb}$	N_ω	M
1 orbital	1	1	20	20
2 orbital	1	2	20	80
3 orbital	1	3	20	180
5 orbital	1	5	20	500
5 orbital (SOC)	2	5	20	2,000
7 orbital (SOC)	2	7	20	3,920

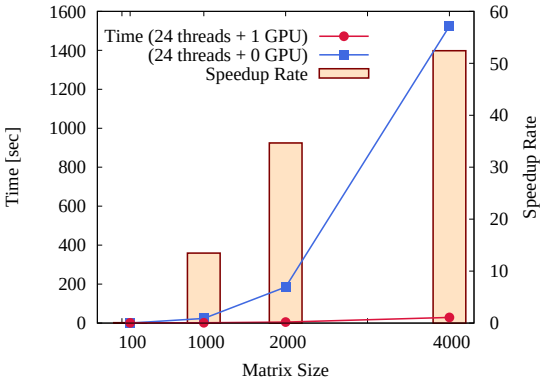

Figure 1: Computation time for solving the BSE (left axis) and the speedup rate achieved by the use of GPU (right axis).

Figure 1 shows a benchmark. We used 1 node (24 thread) of System B in ISSP supercomputer center. Without GPU, the computational time grows in proportion to M^3 as expected (filled squares). Use of GPU suppresses the growth of the time (filled circles). A significant speedup is achieved for $M \gtrsim 100$: The speedup rate (the time without GPU divided by the time with GPU) is 13 and 52 for $M = 1{,}000$ and 4,000, respectively. This benchmark indicates that the GPU acceleration is highly beneficial for d and f orbitals especially on the existence of SOC.

As a future work, our BSE code will be integrated into the open-source DMFT software `DCore` developed under the support of ISSP [1].

Acknowledgment: This work was supported by support service of program portability to GPGPU.

Reference:

[1] `https://github.com/issp-center-dev/DCore`

Report of CCMS hands-on sessions in the 2019 fiscal year

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In the 2019 fiscal year, center for computational materials science (CCMS) in institute for solid state physics (ISSP) held two hands-on sessions by using supercomputer (sekirei) of ISSP. A list of the hands-on sessions is shown in Table 1. In this report, we briefly summarize the hands-on sessions in the order of date.

DSQSS [1] is an open-source software package for solving quantum many-body problems using the quantum Monte Carlo method that sample the Feynman path integral using the worm update. Development of DSQSS was supported by "Project for advancement of software usability in materials science"(PASUMS) [2] in the 2018 fiscal year. In the hands-on session, Naoki Kawashima and co-developers explained the basics of the quantum Monte Carlo method and gave a tutorial of DSQSS [3].

DCore [4] is a tool for performing quantum many-body simulations based on the dynamical mean-filed theory (DMFT). Development of DCore was also supported by PASUMUS in the 2017 fiscal year. In the hands-on session, Hiroshi Shinaoka and co-developers explained the basics of the DMFT and gave a tutorial of DCore [5].

Date	Software	Main lecturer
Jun. 6	DSQSS	N. Kawashima
Dec. 26	DCore	H. Shinaoka

Table 1: List of software packages used in CCMS hands-on sessions.

References

[1] https://ma.issp.u-tokyo.ac.jp/en/app/180

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

[3] https://ccms.issp.u-tokyo.ac.jp/event/1942

[4] https://ma.issp.u-tokyo.ac.jp/en/app/1004

[5] https://ccms.issp.u-tokyo.ac.jp/event/2486

Supercomputer course of Computational Materials Design (CMD®) workshop

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The 35rd Computational Materials Design (CMD®) workshop (CMD35) has been held from September 2nd to September 6th and the 36th CMD® workshop (CMD36) has been done from February 17th to February 21st at Graduate School of Engineering Science, Osaka University. In this workshop we have the supercomputer course to train up human resources to advance researches by using system B supercomputer of ISSP, the University of Tokyo.

In CMD35 eight participants took the supercomputer course and got a tutorial on STATE-Senri developed by Y. Morikawa. After giving the introductory lecture of large-scale computing by M. Geshi and explaining how to use the supercomputer of ISSP and explaining how to use STATE-Senri, calculation models on each research subject of the participants were built and their calculations were carried out. Specific subjects include oxidation of solid surfaces, chemical reactions on two-dimensional materials, atomic diffusion on solid surfaces, dry reforming of methane, chemical reactions in solid oxide fuel cell, and so on. The participants performed the calculations and examined the results.

In CMD36 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 describing the calculation method of electronic states and electron conduction property using RSPACE, exercises published in the manual were carried out by Y. Egami. Then, electronic state calculations were carried out for several molecules, and the electronic density distribution was visualized. Finally, the atomic structure optimization of the defects in GaAs bulks was carried out, and the calculation of carrier scattering property by the defects was investigated.