3.6 Software Advancement Projects, GPGPU Implementation, and Workshop Support

Development of first principles electronic-structure calculation software by combining effective-model derivation code RESPACK and model-analysis codes $\mathcal{H}\Phi$ and mVMC

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As Project for advancement of software usability in materials science at the fiscal year of 2018, we have released a new version of the software RESPACK [1] for many-body perturbation calculation and effective low-energy model derivation. RESPACK is possible to derive parameters for the effective low-energy model from first principles. The new version includes *ab initio* GW calculation and utility tool such as transfer analysis and interfaces to model-analysis solvers mVMC [2] and $\mathcal{H}\Phi$ [3]. Users can now automatically obtain the model-analysis-software inputs via RESPACK.

RESPACK consists of five programs:

- Wannier function calculation (`wannier`)

- Dielectric function calculation (`chiqw`)

- Electronic interaction calculation for direct and exchange integrals (`calc_w3d`, `calc_j3d`),

- *Ab initio* GW calculation (`calc_gw`),

- Utility code for transfer analysis (`transfer_analysis`)

These programs are run under the following inputs:

- Input file for RESPACK calculation (`input.in`)

- Band-calculation outputs contained in a directory `dir-wfn`

RESPACK supports *ab initio* band calculation codes using norm conserving pseudopotentials plus plane wave basis set, and officially supports xTAPP [4] and Quantum ESPRESSO [5] packages. Automatic generation scripts which convert results of the band calculation to inputs for RESPACK is prepared for xTAPP and Quantum ESPRESSO codes. An input file for specifying RESPACK calculation conditions is designed pursuing simplicity and is given in a namelist format. It supports OpenMP/MPI and can be used in both laboratory-computer environment and System B at ISSP, the University of Tokyo. RESPACK has a wide application including simple metals, semiconductors, $3d/4d$ transition-metal compounds, organic and aromatic compounds, etc. In this report, we present an *ab initio* calculation of the excitation spectrum of an impurity system using three software: xTAPP, RESPACK, and $\mathcal{H}\Phi$.

Figure 1(a) is the atomic geometry of the impurity system of ruby (Al_2O_3:Cr), and the panel (b) is our calculated band structure, where we see two impurity bands near the Fermi level due to the Cr impurity. Blue dotted curves are the Wannier interpolated band

obtained from `wannier` program. We also performed `chiqw`, `calc_w3d`, and `calc_j3d` and calculated effective interactions.
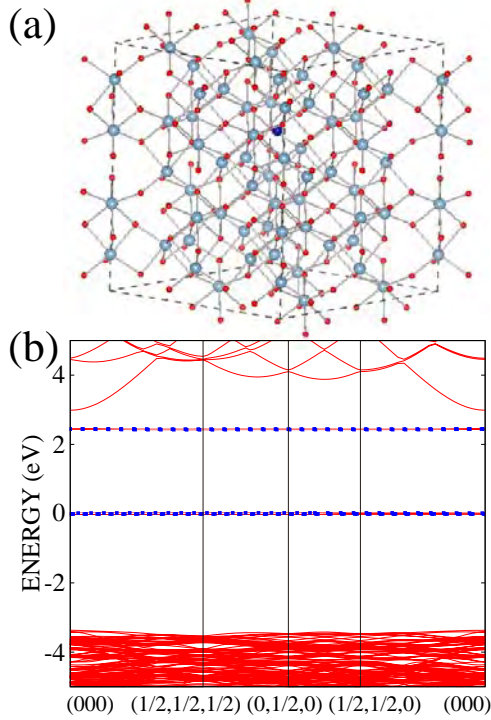

Figure 1: (a) Atomic geometry for impurity sistem: $Al_{47}CrO_{72}$ ($2\times2\times1$ supercell). (b) Calculated xTAPP band structure with $5\times5\times5$ k-point sampling and 100-Ry cutoff.

When the RESPACK job (`wannier`, `chiqw`, `calc_w3d`, `calc_j3d`) is executed, a directory `dir-mvmc` is generated under the calculation directory, and the files necessary for model-analysis softwares mVMC and $\mathcal{H}\Phi$ are output. Using these data and a standard-mode input for mVMC and $\mathcal{H}\Phi$, all inputs of the model calculations are automatically generated under the following command:

`HPhi -s stan.in (or vmc.out -s stan.in)`

Here, `HPhi` and `vmc.out` are execution files of $\mathcal{H}\Phi$ and mVMC, respectively, and `stan.in` is an input file for standard mode. This interface code has the lattice conversion function; when the user moves from *ab initio* calculation to model one, the lattice adopted at the *ab initio* calculation can be flexibly changed. Also, the code has an option for avoiding the Hartree-term double count; user can adjust one-body correction $\Delta_{i\mathbf{0}}$ by optional parameter α,

$$
\begin{aligned}
\Delta_{i\mathbf{0}} =\ & \alpha U_{i\mathbf{0},i\mathbf{0}} D^{\mathrm{KS}}_{i\mathbf{0},i\mathbf{0}} \\
& + \sum_{\mathbf{R}\neq\mathbf{0}} \sum_k D^{\mathrm{KS}}_{k\mathbf{0},k\mathbf{0}} \Big(U_{i\mathbf{0},k\mathbf{R}} - (1-\alpha) J_{i\mathbf{0},k\mathbf{R}} \Big),
\end{aligned}
\tag{1}
$$

where U, J, and D are the direct integral, exchange integrals, and density matrix with the Kohn-Sham orbital, respectively.

Table 1 shows our calculated excitation energy diagram of the impurity model. The excitation energy depends on α in Eq. (1), and the results correcting of the Hartree-term double counting reasonably reproduce the experimental result.

Table 1: Calculated energy diagram of impurity model from RESPACK. The unit is eV. Values of the ground state (GS) are the total energy.

Expt	Theory		
-	$\Delta_{i\mathbf{0}} = 0$	$\alpha = 0.5$	$\alpha = 1$
GS(^4A)	47.9(^4A)	5.60(^4A)	−3.04(^4A)
1.79(^2E)	1.67(^2E)	1.61(^2E)	1.62(^2E)
1.87(^2T)	1.78(^2T)	1.73(^2T)	1.84(^2T)
2.23(^4T)	2.29(^4T)	1.79(^4E)	2.32(^2A)
2.62(^2T)	2.46(^4T)	2.23(^4T)	2.56(^4T)
3.10(^4T)	2.69(^2T)	2.60(^4A)	2.78(^4T)

For code developments of RESPACK, we thank to Yoshihide Yoshimoto, Yoshiro Nohara, Yusuke Nomura, Terumasa Tadano, and Maxime Charlebois.

References

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

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

[3] http://issp-center-dev.github.io/HPhi/index.html

[4] http://xtapp.cp.is.s.u-tokyo.ac.jp/

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

DSQSS - A PIMC-based quantum lattice model solver [1]

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Among many numerical solutions to the quantum many-body problems on lattices, the path-integral Monte Carlo method (PIMC) has probably the most broad range of applicability [1]. By using PIMC, we can calculate the thermal expectation values of observables of interest with no systematic error for larger systems than can be handled by exact methods. The method works in arbitrary dimension at finite temperature as long as the system is free from the sign problem. The Monte Carlo method generally suffers from the slow convergence near the critical point ('critical slowing down'). For discrete space problems, several update methods, e.g., the loop algorithm and the directed-loop algorithm (DLA), have been developed to overcome the critical slowing down. These methods have been extended for massive parallelization for modern supercomputers.

While the loop-type update algorithms are quite powerful in selected problems, the worm-type update algorithm, the DLA included, are more frexible in various applications. Representative examples are boson systems and, equivalently, antiferromagnets with uniform magnetic field. In spite of these broad range of applicability, very few DLA-based open-source software has been available for parallel computation. Therefore, we proposed to develop one in the ISSP software-development/improvement project, to make it easier for non-experts to run DLA simulation on pararell machines without much effort.

Specifically, We are developing a PIMC program package for quantum lattice problems, which we call DSQSS (Discrete Space Quantum Systems Solver). Since DSQSS adopts the DLA for update scheme, it can update configurations effectively even under a symmetry-breaking field, DSQSS supports arbitrary Hamiltonians and lattices while it comes with additional tools to make it easier to define standard Hamiltonians and lattices. For example, models such as XXZ model defined on hypercubic lattice are pre-defined in DSQSS. As a result, in many cases of interest, users can perform QMC calculation by providing only a small amount of information (typically a few ten lines of text file) to define the condition of the simulation precisely. DSQSS also offers the parallelized multi worm algorithm for massively parallel calculation.

[1] This report is based on collaboration of Y. Motoyama (ISSP), K. Yoshimi (ISSP), A. Masaki-Kato (Hitachi Ltd.), N. K., and T. Kato (ISSP).

[2] The software website is https://github.com/issp-center-dev/dsqss

GPGPU implementation of divide-and-conquer density-functional tight-binding molecular dynamics

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Many biochemical systems, including rhodopsin in vertebrate eyes and photoactive yellow protein in purple bacteria, exhibit photo activity. After photon absorption, a photoactive protein converts the light energy into chemical energy or a signal with conformational changes such as proton and electron transfers. Although hydrogen atoms and/or protons play important roles in protein function, it is difficult to identify their position experimentally due to spatial resolution restrictions. Quantum mechanical molecular dynamics (QM-MD) simulations is a powerful tool for the analysis of geometric and electronic structures. One of the challenges in QM-MD simulations is the applicability to large systems on account of high computational demands with respect to the system size. In our group, divide-and-conquer density-functional tight-binding (DC-DFTB) [1] has been developed to reduce the computational cost and shown to perform reasonably well for many large systems.

In this study, the Graphical processing units (GPU) code for DC-based DFTB methods is implemented to enable long-time QM-MD simulation for support service of GPGPU implementation. The GPU code is heterogynous algorithm on CPU and GPU architectures. The construction of Hamiltonian and evaluation of the derivative terms is accelerated on GPU. The diagonalization of Hamiltonian is performed on CPU. Table 1 shows the wall-clock times for DC-DFTB calculations of water cluster $500H_2O$. The heterogynous algorithm achieves 2.46-fold and 3.43-fold speedups for construction of Hamiltonian and evaluation of derivative term, respectively.

Table 1. Wall-clock times for DC-DFTB calculations of water cluster $500H_2O$.

	CPU	GPU
Construction of Hamiltonian	11.3	4.6
Evaluation of derivative term	16.7	4.9

References

[1] H. Nishizawa, Y. Nishimura, M. Kobayshi, S. Irle, H. Nakai, J. Comput. Chem. **37** (2016) 1983.

Report of CCMS hands-on sessions in the 2018 fiscal year

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In the 2018 fiscal year, center for computational materials science (CCMS) in institute for solid state physics (ISSP) held five 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.

DCore is a tool for performing quantum many-body simulations based on the dynamical mean-filed theory (DMFT). Development of DCore was supported by "Project for advancement of software usability in materials science"(PASMS) [1] in the 2017 fiscal year. Hiroshi Shinaoka and co-developers explained the basics of the DMFT and gave a tutorial on DCore [2, 3].

MateriApps LIVE! is a Debian Live Linux system that contains OS, editors, several materials science application software packages. Synge Todo explained how to install and used MateriApps LIVE! [4, 5] and explained how to use several software packages included in MateriApps LIVE!.

xTAPP is a first-principles plane-wave pseudo-potential code. In the hands-on session in xTAPP [6, 7], Yoshihide Yoshimoto and Kanako Yoshizawa explained the basic usages of xTAPP and how to use it in sekirei.

$\mathcal{H}\Phi$ is an exact diagonalization package and its development was supported by PASMS in the 2015 and 2017 fiscal years. Youhei Yamaji and co-developers explained the how to use HΦ [8, 9] and recently implemented functions such as the real-time evolution.

RESPACK is a first-principles calculation software package for evaluating the interaction

Date	Software	Main lecturer
Jul. 30	DCore	H. Shinaoka
Aug. 28	MateriApps LIVE!	S. Todo
Oct. 19	xTAPP	Y. Yoshimoto
Dec. 12	$\mathcal{H}\Phi$	Y. Yamaji
Mar. 1	RESPACK	K. Nakamura

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

parameters of materials and its development was partially supported by PASMS in the 2018 fiscal year. Kazuma Nakamura explained the details of RESPACK [10, 11] and how to use it.

References

[1] http://www.issp.u-tokyo.ac.jp/supercom/softwaredev

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

[3] https://ccms.issp.u-tokyo.ac.jp/event/570

[4] https://ma.issp.u-tokyo.ac.jp/en/app/275

[5] https://ccms.issp.u-tokyo.ac.jp/event/653

[6] https://ma.issp.u-tokyo.ac.jp/en/app/741

[7] https://ccms.issp.u-tokyo.ac.jp/event/697

[8] https://ma.issp.u-tokyo.ac.jp/en/app/367

[9] https://ccms.issp.u-tokyo.ac.jp/event/1101

[10] https://ma.issp.u-tokyo.ac.jp/en/app/772

[11] https://ccms.issp.u-tokyo.ac.jp/event/1331

Supercomputer course of Computational Materials Design (CMD®) workshop

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The 33rd Computational Materials Design (CMD®) workshop (CMD33) has been held from September 3 to September 7 and the 34th CMD® workshop (CMD34) has been done from February 18 to February 22 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 CMD33 nine participants took the supercomputer course and got a tutorial on STATE-Senri developed by Y. Morikawa. After 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. Concrete themes were molecular adsorption on solid surfaces, chemical reactions at electrode interfaces, adsorption and diffusion of atoms on graphene, electronic structures of oxides for ion batteries and so on. The participants performed the calculations and examined the results.

In CMD34 thirteen participants took the supercomputer course and four participants used the supercomputer of ISSP. They got a tutorial on RSPACE developed by T. Ono. After describing the calculation method of electronic states and electron conduction property using RSPACE, exercises published in the manual were carried out. Then, electronic state calculations were carried out on a plurality of molecular systems, and the electronic density distribution was visualized. Finally, the atomic structure optimization of the system in which molecules are sandwiched between metal electrodes was carried out, and the calculation of electron conduction properties of molecules was analyzed.