Development of an integrated dynamical mean-field theory package for correlated electrons

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In condensed matter physics, dynamical mean-field theory (DMFT) [1] is a widely used tool for the study of strongly correlated electron systems. In a DMFT calculation, a correlated lattice model is mapped to an impurity problem whose bath degrees of freedom are self-consistently determined. DMFT can be combined with density functional theory based *ab-initio* calculations as the DFT+DMFT method, to describe strongly correlated materials such as transition metal oxides [2]. The DFT+DMFT method is useful particularly for investigating one-particle excitation of the systems. The DFT+DMFT allows us to compute one-particle spectral functions, which can be compared directly with angle-resolved photoemission spectroscopy (ARPES). Although there are several open-source computational libraries for DMFT calculations, the use of these libraries requires some expertise. This prevents wider use of the DFT+DMFT method in studies of condensed matter physics.

To make this method available to non-experts(including students) in the community in condensed matter physics, we have developed an open-source software `DCore` ver.1 [3] in Project for advancement of software usability in materials science [3] at the fiscal year of 2017. `DCore` is an abbreviation of "integrated DMFT software for CORrelated Electrons". `DCore` is built on the top of elaborate softwares `TRIQS` [5] and `ALPSCore` libraries [6] and related softwares. `DCore` performs calculations based on DMFT with the help of these libraries. As an impurity solver, one can select continuous-time quantum Monte Carlo method or the Hubbard-I approximation. Because `DCore` provides a well-organized text-file-based interface, users can perform the DFT+DMFT calculation with less effort. In a typical DFT+DMFT calculation, the non-interacting Hamiltonian $\mathcal{H}(k)$ is extracted from the results of DFT calculations by projecting the band structure to maximally localized Wannier functions. In `DCore`, we can import $\mathcal{H}(k)$ from outputs of the DFT codes which support `Wannier90` such as `VASP`, `Wien2k`, `Quantum ESPRESSO`, and `OpenMX`.

`DCore` consists of multiple programs, each of which performs a different step of DMFT calculations. To be more specific, `DCore` consists of three layers: interface layer, DMFT loop, and post-processing. Those are performed by the executables `dcore_pre`, `dcore`, `dcore_post`, respectively. Input parameters are provided by a single text file, which is read by all the three programs.

For the interface layer, there are two types of interfaces: standard interface for tight-binding models and `Wannier90` interface for materials. For the standard interface, one can choose one of predefined tight-binding models. On the other hand, for the `Wannier90` interface, one is able to import a tight-binding model constructed by DFT calculations. The data describing the system generated by `dcore_pre` is

```
[model]
seedname = square
lattice = square
norb = 1
nelec = 1.0
t = -1.0
kanamori = [(2.0, 0.0, 0.0)]

[system]
beta = 40.0
nk = 8
n_iw = 1000
prec_mu = 0.001

[impurity_solver]
name = TRIQS/hubbard-I

[control]
max_step = 7

[tool]
broadening = 0.4
nnode = 4
knode = [(G,0.0,0.0,0.0),(X,0.5,0.0,0.0),(M,0.5,0.5,0.0),(G,0.0,0.0,0.0)]
nk_line = 100
omega_max =6.0
omega_min =-5.0
Nomega = 400
```

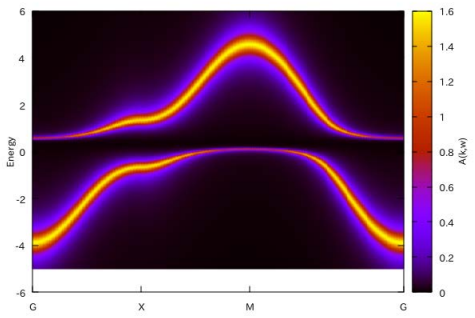

Figure 1: The upper panel shows an example of input file for single-orbital Hubbard model on a square lattice. The lower panel shows the computed momentum-resolved spectrum $A(k, \omega)$.

stored in a file in the HDF5 format, which is read in the later processes. Self-consistent calculations are performed by `dcore` and the results are stored in a separated HDF5 file. One can analyze the result and plot the data by using `dcore_post`.

We show an example for a single-orbital Hubbard model on a square lattice in Fig. 1 using the standard interface. In the input file, one can choose the lattice model, the type of local interactions, and their strengths. Here, the impurity solver is the Hubbard-I approximation using an implementation in `TRIQS`. The computed results are processed by `dcore_post` and are converted into human-readable formats. One can plot the data by using standard tools such as gnuplot (see Fig. 1.) With the `Wannier90` interface, one can perform DFT+DMFT calculations by using a single similar text input file for `DCore`. We refer the interested reader to the website [3] for more examples for real materials.

Finally, we introduce some of available features in `DCore` ver 1 and a future development plan of `DCore`. The feature of `DCore` is to treat many kinds of interactions such as multi-orbital models with non-density-density interactions and spin-orbit coupling. Thus, we can perform collinear magnetic calculations. A future version will support the computation of (free) energy, two-particle quantities such as local magnetic susceptibilities, and the calculations of non-collinear magnetic structures. The software will be preinstalled on the supercomputer (Sekirei) at ISSP in 2018. We hope that DCore promotes wide use of the DFT-DMFT calculations, which is one of excellent methods for understanding strongly-correlated electron systems.

References

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

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

[5] O. Parcollet *et al.*, Comput. Phys. Comm. **196**, 398 (2015).

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