量子格子模型プログラムパッケージ

DCore (integrated DMFT software for CORrelated Electrons)の概要

品岡寛

埼玉大学

発表概要

1. 背景：強相関電子電子系
2. 第一原理計算・動的平均場近似の概要
3. DCoreの説明

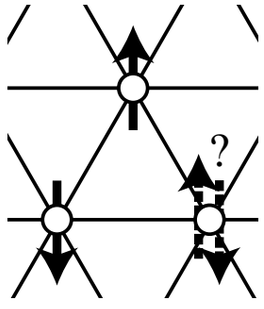
背景: 強相関電子系の広がり

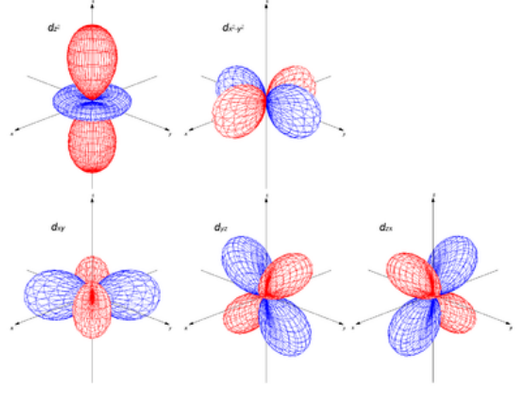
超伝導

鉄系遷移金属酸化物、有機導体等

スピン、軌道、電荷秩序

フラストレート磁性体、マルチフェロイック





トポロジカル相

5*d*遷移金属酸化物、界面・表面

⇨ 定量的な物性予測を強く要請されている

第一原理計算とは？

密度汎関数理論

P. Hohenberg and W. Kohn (1964)
W. Kohn and L. J. Sham (1965)

- 様々な近似: 局所密度近似(LDA)、一般化勾配近似 (GGA)
- 全電子計算 or not
- 基底関数の種類: 平面波＋α、FP-LAPW、数値原子基底

	全電子計算	基底関数
VASP	N	PAW
Quantum ESPRESSO	N	PAW
Wien2k	Y	FP-LAPW
OpenMX	N	数値原子基底

Free

Free

Abinit, Elk, AkaiKKR, QMAS, *etc*.

Quantum ESPRESSO

https://www.quantum-espresso.org

- 擬ポテンシャル法
- Wannier90との連携

  (symmetry-adapted Wannier functions)

OpenMX

http://www.openmx-square.org

Welcome to OpenMX

Open source package for Material eXplorer

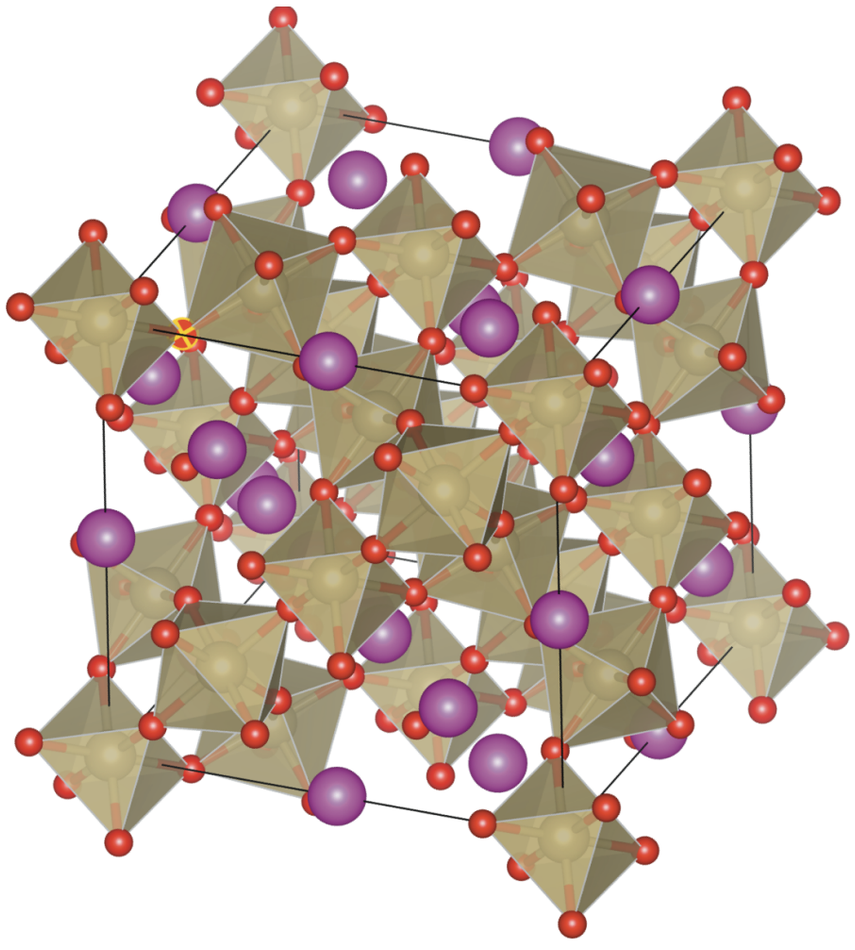
Contents

- **What's new**
  - International Summer Workshop for July 2nd-12th, 2018
  - Patch (Ver. 3.8.5) to OpenMX Ver. 3.8 (June 12, 2018)
- What is OpenMX?
- Download
- Manual of Ver. 3.8
- Manual of Ver. 3.7
- Technical Notes
- Video Lectures
- Publications
- OpenMX Forum
- OpenMX Viewer
- Workshop
- Database of VPS and PAO
  - Ver. 2013
- ADPACK
- Miscellaneous informations
- Contributors
- Acknowledgment
- Opening positions
- Links

- 擬ポテンシャル＋数値原子軌道基底
- 大規模系の計算
- Wannier90との連携
- 対称操作は無し

密度汎関数理論＋動的平均場近似

LDA/DFT+DMFT　　G. Kotliar *et al.*, RMP **78**, 865 (2006)



相関効果が強い原子軌道への射影

三

動的平均場

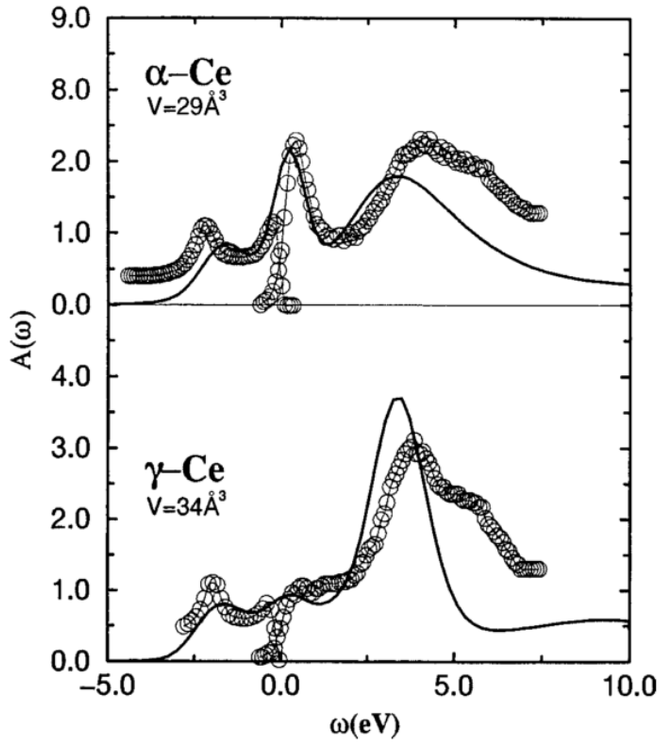
$$\Sigma(k,\omega) \rightarrow \Sigma(\omega)$$

- 格子問題を量子不純物問題へマップ
- 動的物理量の計算: スペクトル関数、動的感受率
- 摂動理論による拡張が可能 (DMFT+GWなど)

計算できる量

- スペクトル関数

$$A(k,\omega) = -\frac{1}{\pi}\mathrm{Im}G(k,\omega + i0^{+})$$



McMahan *et al*., 2003

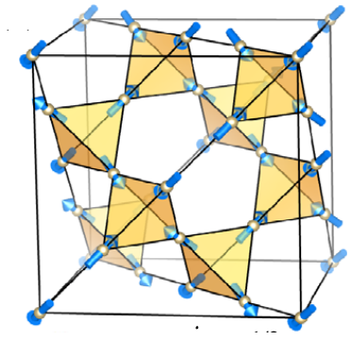
→光学実験との直接比較

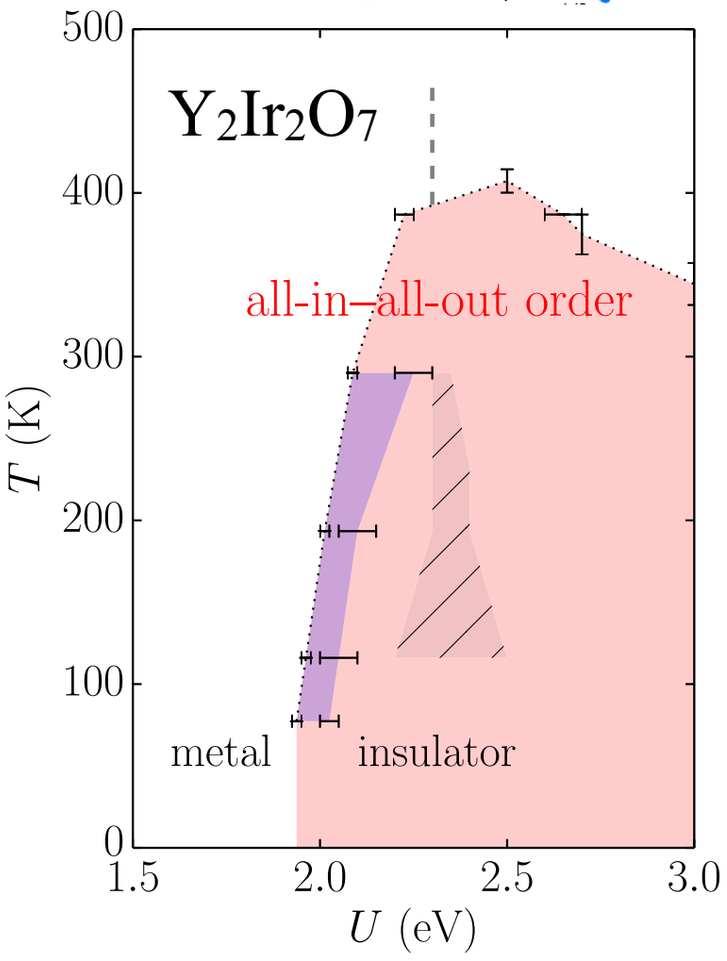
- 静的・動的感受率

M. Jarrell (1992), H. Park *et al*. (2011), L. Boehnke *et al*. (2011), J. Kuneš *et al*. (2017)

- 構造緩和　K. Haule and G. L. Pascut (2016)

- 複雑な磁気構造





HS, S. Hoshino, M. Troyer and P. Werner (2015)

DFT+DMFTの計算スキーム

G. Kotliar *et al*., RMP **78**, 865 (2006)

バンド計算プログラム

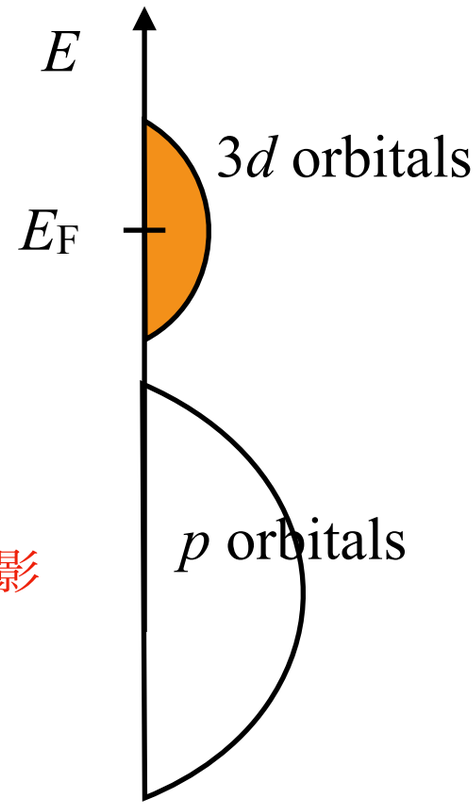
電子密度

構造緩和には必須

バンド構造

局在軌道への射影

最局在ワニア関数、射影ワニア関数など



$$G_{\rm loc}(i\omega_n) = \left\langle \frac{1}{i\omega_n - \mathcal{H}(k) - \Sigma(i\omega_n)} \right\rangle_k$$

$$\mathcal{G}_0^{-1} = \Sigma + G_{\rm imp}^{-1}$$

(多軌道)量子不純物問題

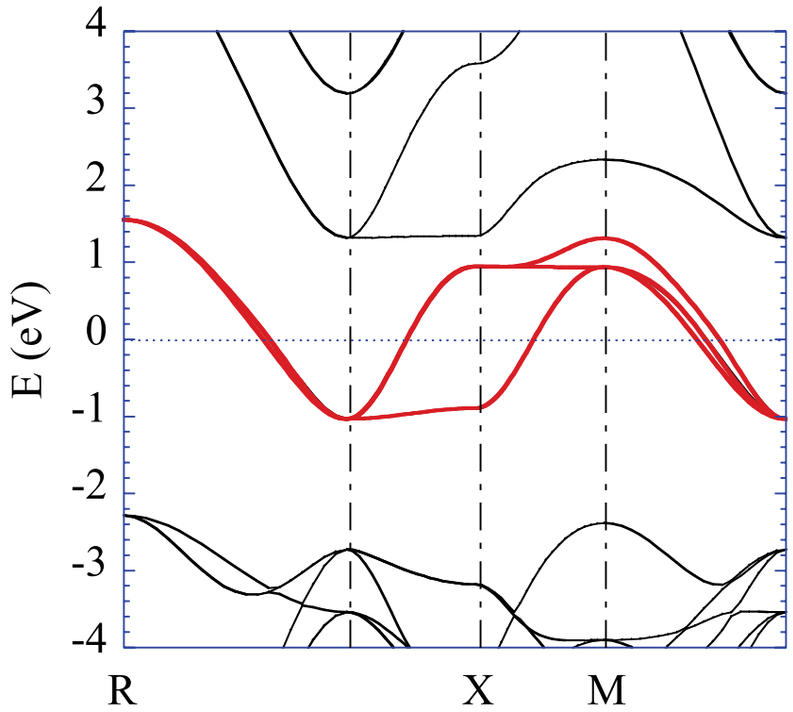
$$S_{\rm imp} = \int d\tau d\tau' c^\dagger(\tau)\mathcal{G}_0^{-1}(\tau,\tau')c(\tau') + S_{\rm int}$$

$$\Sigma = \mathcal{G}_0^{-1} - G_{\rm imp}^{-1}$$

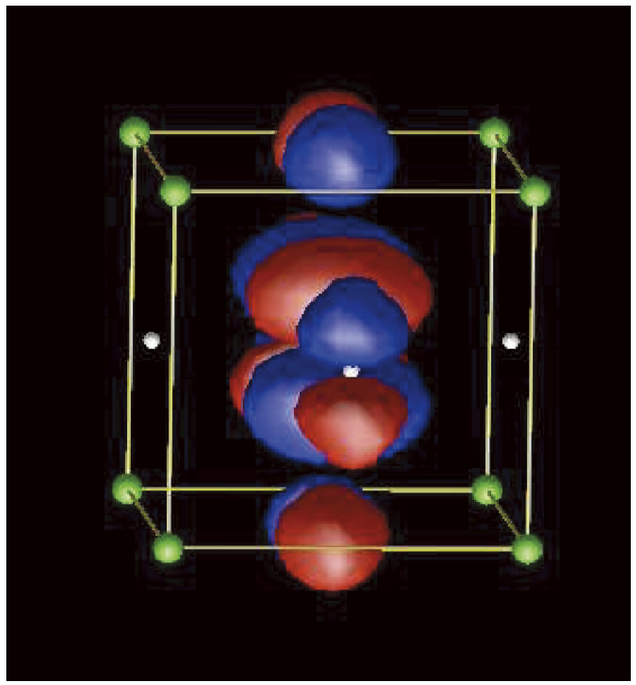
動的平均場

最局在ワニア関数

N. Marzari and D. Vanderbilt (1997), I. Souza *et al*. (2001)



波数、軌道に依存
したゲージ変換



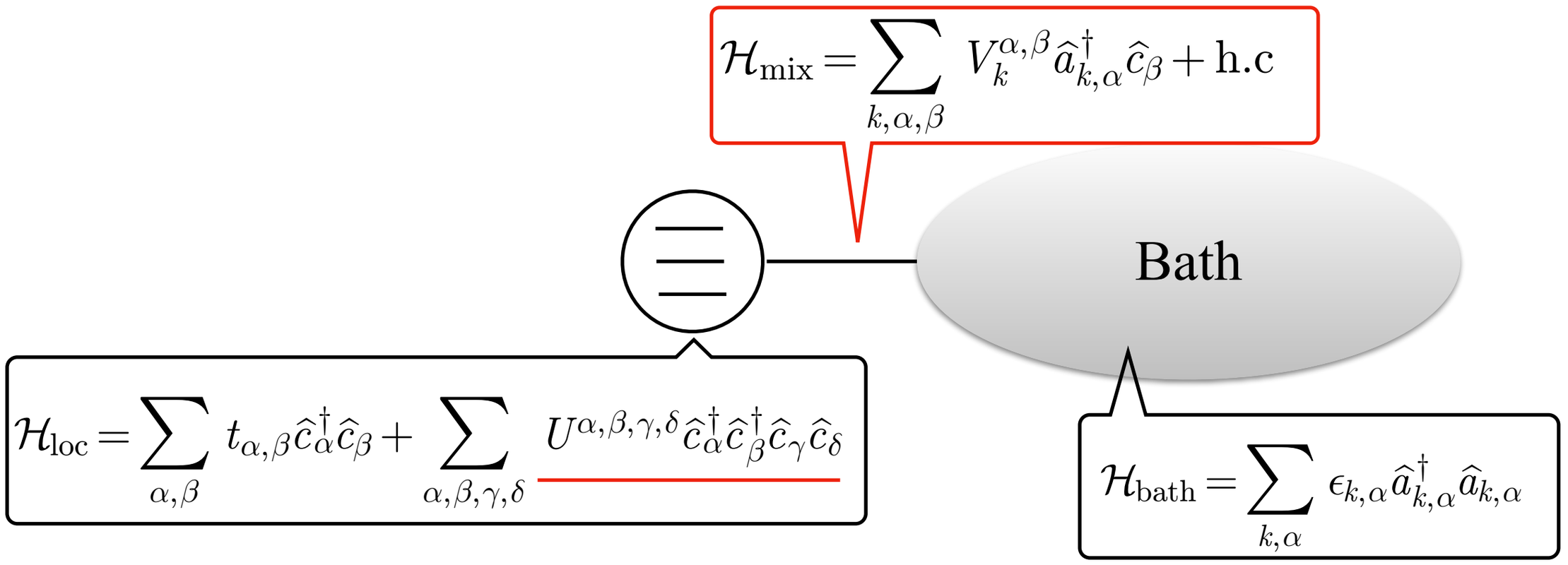
$SrVO_3$: M. Imada and T. Miyake (2010)

- DFTコードが使う基底に依存しない
- ワニア関数の最適化が必要

Projectors

http://hauleweb.rutgers.edu/tutorials/Overview.html
M. Aichorn *et al*., PRB **80**, 085101 (2009)
https://triqs.github.io/dft_tools/master/_downloads/TutorialDmftproj.pdf

Quantum (Anderson) impurity problem



Continuous-time QMC, Hubbard-I approximation, exact diagonalization, *etc*.

Exact but expensive

Continuous-time Monte Carlo method

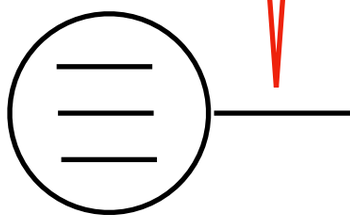
Review: E. Gull *et al*., RMP **83**, 349 (2011)

$$\mathcal{H}_{\mathrm{mix}} = \sum_{k,\alpha,\beta} V_k^{\alpha,\beta} \hat{a}_{k,\alpha}^{\dagger} \hat{c}_{\beta} + \mathrm{h.c}$$

Hybridization expansion (CT-HYB)

P. Werner *et al*., PRL **97** 076405 (2006)

P. Werner *et al*., PRB **74** 155107 (2006)



Bath

$$\mathcal{H}_{\mathrm{loc}} = \sum_{\alpha,\beta} t_{\alpha,\beta} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\beta} + \sum_{\alpha,\beta,\gamma,\delta} U^{\alpha,\beta,\gamma,\delta} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\beta}^{\dagger} \hat{c}_{\gamma} \hat{c}_{\delta}$$

$$\mathcal{H}_{\mathrm{bath}} = \sum_{k,\alpha} \epsilon_{k,\alpha} \hat{a}_{k,\alpha}^{\dagger} \hat{a}_{k,\alpha}$$

Interaction expansion (CT-INT)

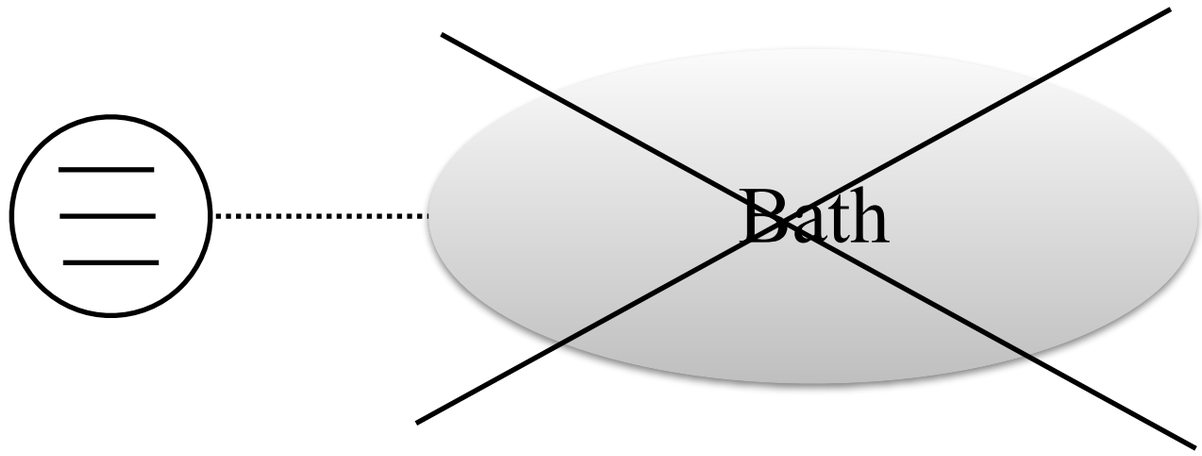
A. N. Rubtsov *et al*., PRB **72**, 035122 (2005)

- Exact: A serious expansion of partition function
- Sign problem in solving multi-orbital model
- Parallel computing is necessary!

Hubbard I approximation

J. Hubbard, Proc. Roy. Soc. London A**276**, 238 (1963)

- Insulating solution at integer fillings
- Multi-orbital systems
- Real-frequency data
- Can be ran on a laptop



既存のソフトウェア

- TRIQS: A Toolbox for Research on Interacting Quantum Systems

  https://triqs.ipht.cnrs.fr/

  - Green's function libraries
  - Quantum impurity solvers
  - Interface with *ab-initio* codes

- ALPSCore project

  https://alpscore.org

  - Continuous-time quantum impurity solvers
    - Hybridization-expasion algorithm

      HS, E. Gull, P. Werner (2017)
    - Interaction-expansion algorithm

      HS, Y. Nomura, E. Gull (2018)

Pythonでライブラリを組み合わせて、物質、模型ごとにプログラムを作る必要あり

- DFT + Embedded DMFT Functional

  http://hauleweb.rutgers.edu/tutorials/

  Rutger's university

  - Quantum impurity solvers
  - Charge self consistency with Wien2k
  - *License issues*

- iQIST (Interacting Quantum Impurity Solver Toolkit)

  https://github.com/iqist/iqist

  - Quantum impurity solvers

- w2dynamics

  M. Wallerberger *et al*., arXiv:1801.10209v1

  - Quantum impurity solver

誰もが簡単に使えるようなソフトウェアが必要　（理論家にも実験家にも）　→　DCore

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3. DCoreの説明
   - 概要
   - 入力パラメータの概要

Development of DCore ver. 1.0

DCore

Development of DCore was
proposed by H. Shinaoka in 2017.

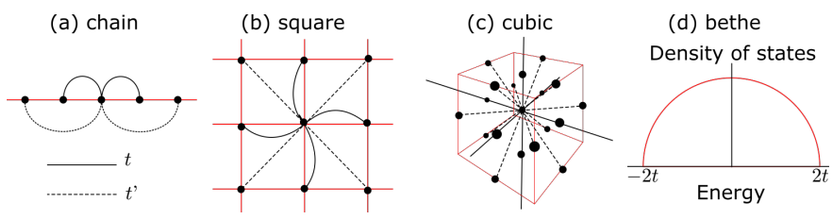
Released in April 2018

Openness:3 ★★★ Document quality:3 ★★★

A tool for performing quantum many-body simulations based on dynamical mean-field theory. In addition to predefined models, one can construct and solve an ab-initio tight-binding model by using wannier 90 or RESPACK. We provide a post-processing tool for computing physical quantities such as the density of state and the momentum resolved spectral function. DCore depends on external libraries such as TRIQS and ALPSCore.

ref.) https://ma.issp.u-tokyo.ac.jp/en/app/1004

Predefined models



Wannier90 format

QUANTUMESPRESSO

OPEN

RESPACK
第一原理多体摂動計算

DCore

DMFT calculations
using TRIQS and ALPS

Pure Python implementation
GPLv3

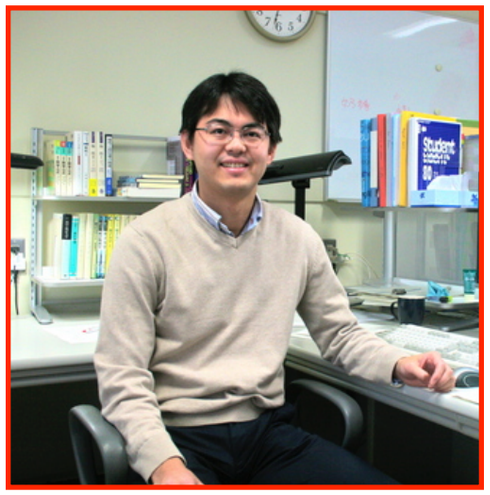
DCore v2：基本情報

- **DCore 開発者 (自分は除く)**

Released in May 2019

Okayama univ.

J. Otsuki



N. Takemori

ISSP

K. Yoshimi

M. Kawamura

Acknowledgments to T. Kato and Y. Motoyama

- **必要環境**
  - Python2.7
  - **TRIQS 1.4 or 2.1+**
    C++14 (1.4) or C++17 (2.1+), gccもしくはclangが楽

- **ライセンス**

オープンソースソフトウェアなので、誰でも利用&貢献可能！

- **動作環境**
  - Linux , OS Xでの動作確認済

DCore v2 機能一覧

- **モデル**
  - 格子形状
    - 標準的な格子：Bethe, chain, square, cubic lattice
    - Wannier90形式： DFT calculations with/without spin-orbit coupling
  - 相互作用
    - Slater-Kanamori interaction, *etc*.
- **自己無撞着計算** New
  - 非磁性計算、非共線磁気構造
- **物理量**
  - 自己エネルギー　$\Sigma(i\omega_n)$
  - スペクトル関数　$A(\omega)$, $A(k, \omega)$
- **MPI並列**
- **対応量子不純物ソルバーの追加**

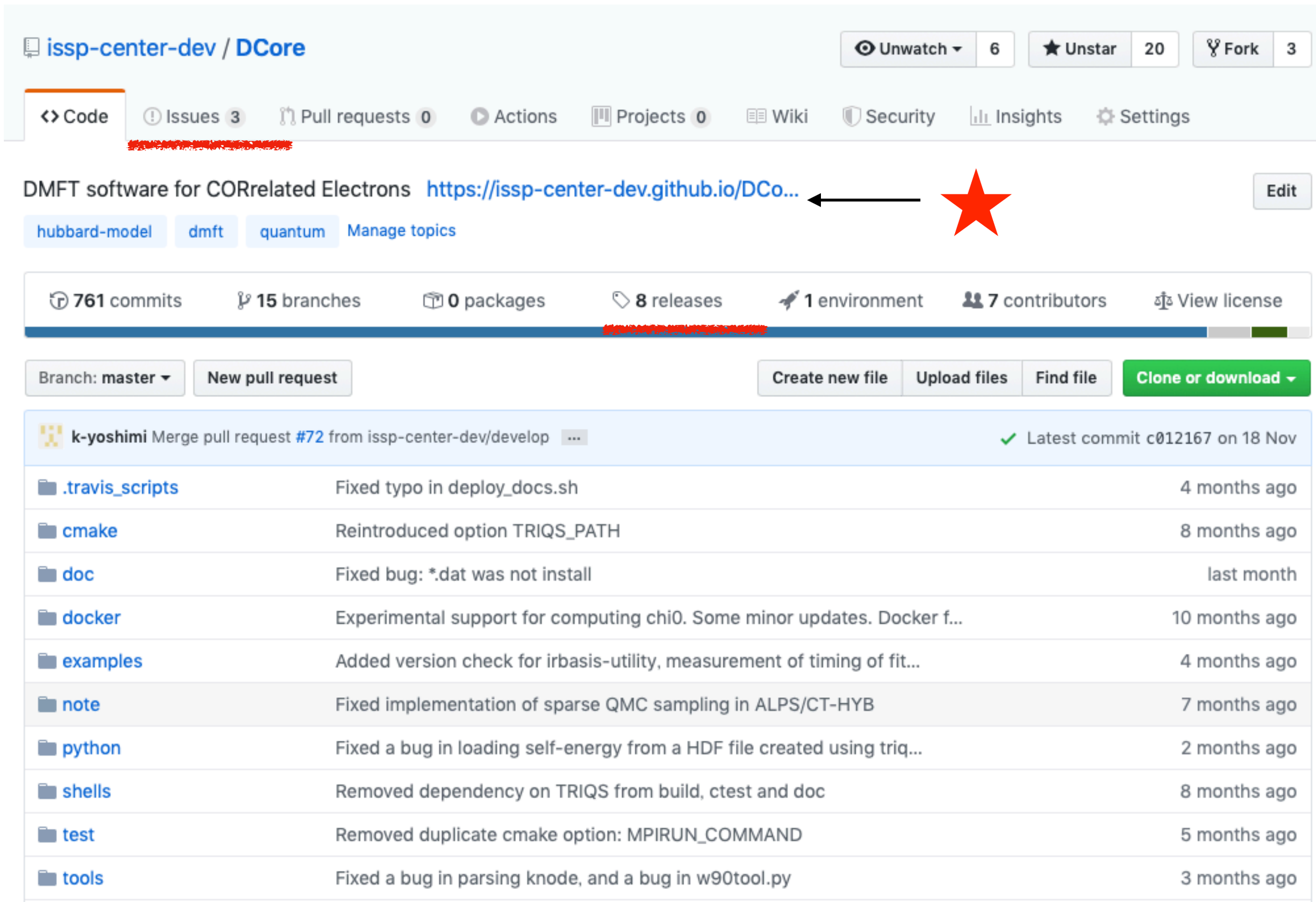
  ALPS/CT-HYB, TRIQS/cthyb, TRIQS/Hubbard-Iに加えて、ALPS/CT-HYB-SEGMENT, pomerolを追加 New

物理量は今後追加予定
開発者としての参加を歓迎！

ソルバーの追加が簡単に

公式開発サイト

https://github.com/issp-center-dev/DCore



公式マニュアル

https://issp-center-dev.github.io/DCore/master/index.html

- インストール手順、入力・出力ファイル解説、パラメータ一覧、サンプル、謝辞など

Quick search

Go

DCore

integrated **D**MFT software for **Cor**related **e**lectrons

What is DCore?

DCore is aimed at model calculations and ab-initio calculations by the dynamical mean-field theory (DMFT). This package consists of programs with text-based and hdf5-based interface. These programs enable users to perform DMFT calculations and analyze results without writing computer code.

License

The DCore package is published under the GNU General Public License, version 3.

The following files are from the TRIQS (Toolbox for Research on Interacting Quantum Systems).

- https://github.com/issp-center-dev/DCore/blob/develop/python/impurity_solvers/triqs_hubbard_I_impl.py
- https://github.com/issp-center-dev/DCore/tree/develop/python/converters

We would like to express our sincere gratitude to TRIQS's developers.

This package of ver.1.0 was developed under the support of "Project for advancement of software usability in materials science" by The Institute for Solid State Physics, The University of Tokyo. The copyright of DCore ver.1.0 belongs to The University of Tokyo.

Authors & Quotation

Developers:

謝辞

https://issp-center-dev.github.io/DCore/master/index.html#authors-quotation

Authors & Quotation

Developers:

- ver. 2.0
  H. Shinaoka, J. Otsuki, K. Yoshimi, M. Kawamura, N. Takemori, Y. Motoyama
- ver. 1.1 (released on 2019/1/25)
- ver. 1.0 (released on 2018/3/24)
  H. Shinaoka, J. Otsuki, K. Yoshimi, M. Kawamura, T. Kato

Related papers: This package depends on TRIQS libraries and applications. Please cite relevant papers for these original libraries.

- TRIQS libraries
- TRIQS/DFTTools

In addition to the above two libraries, you may use impurity solvers listed below.

- TRIQS/cthyb
- TRIQS/hubbardI
- ALPS/CT-HYB
- ALPS/CT-HYB-SEGMENT

For some of them, they provide a BibTeX entry for each paper in the above cites.

DCore v2の解説論文も準備中！

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計算の流れ

入力テキストファイルの作成

第一原理計算から導出したパラメータを使用する場合、
Wannier90形式のファイルも用意
(hopping, Interaction)

モデル生成：dcore_pre
(出力: HDF5)

ハミルトニアン [$H(k)$, 相互作用行列]データの生成

DMFT計算 ：dcore
(出力: HDF5)

DMFT自己無撞着計算
自己エネルギー等の出力

収束チェック ：dcore_check
(出力：標準出力、画像)

計算後処理： dcore_post
(出力: テキスト、画像)

$A(k, \omega)$ 等の計算や表示

入力ファイル

全6つのblockから構成される

[model]：模型に関する設定
格子
軌道の数・種類
電子数
相互作用の種類
相互作用の大きさ

[system]：系に関する設定
虚時間の分点の数
松原振動数の分点の数
逆温度
化学ポテンシャル
etc…

[mpi]：MPI並列計算の設定
mpirunコマンド名など

[impurity_solver]：不純物ソルバーの設定
TRIQS/hubbard-I, TRIQS/cthyb,
ALPS/CT-HYBなど

[control]：DMFT計算条件の設定
次のステップに進む際のmixingパラメータ
DMFT-loopの最大ループ数
再計算フラグ

[tool]：ポスト処理時の設定
最大・最小実振動数
k点の始点・終点と分点数
振動数の虚部のシフト量
etc.

レファレンスマニュアル

https://issp-center-dev.github.io/DCore/master/reference.html

Reference Manual

各プログラムの入力・出力ファイル

入力パラメータ一覧

出力ファイル

不純物ソルバー

[model] block

	`dcore_pre`	`dcore`	`dcore_check`	`dcore_post`
[model]	Yes	Yes	Yes	Yes
[system]		Yes	Yes	Yes
[impurity_solver]		Yes		Yes
[control]		Yes		
[tool]			Yes	Yes
[mpi]		Yes		Yes

[model] block

This block includes parameters for defining a model to be solved.

Name	Type	Default	Description
seedname	String	dcore	Name of the system. The model HDF5 file will be seedname.h5.
lattice	String	chain	Chosen from “chain”, “square”, “cubic”, “bethe”, “wannier90”, and “external”
t	Float	1.0	Transfer integral (Nearest neighbor)
t’	Float	0.0	Transfer integral (Second nearest)
nelec	Float	1.0	Number of electrons per unit cell.
norb	String	1	Number of orbitals at each correlated shell (*ncor* integers separated by commas or spaces.)
ncor	Integer	1	Number of correlated shells in a unit cell (for lattice = wannier90).
corr_to_inequiv	String	None	Mapping from correlated shells to equivalent shells (for lattice = wannier90)
bvec	String	[(1.0,0.0,0.0),(0.0,1.0,0.0),(0.0,0.0,1.0)]	Reciprocal lattice vectors in arbitrary unit.
nk	Integer	8	Number of *k* along each line
nk0	Integer	0	Number of *k* along b_0 (for lattice = wannier90, external)
nk1	Integer	0	Number of *k* along b_1 (for lattice = wannier90, external)
nk2	Integer	0	Number of *k* along b_2 (for lattice = wannier90, external)
spin_orbit	Bool	False	Whether the spin-orbit case.
interaction	String	kanamori	Chosen from “slater_uj”, “slater_f”, “kanamori”, “respack” (See below)
density_density	Bool	False	If true, only the density-density part of the interaction is used (See below).
kanamori	String	None	U (Diagonal Coulomb pot.), U’ (Off-diagonal Coulomb pot.) and J (Hund coupling) (See below).
slater_f	String	None	Angular momentum, Slater integrals F (See below).
slater_uj	String	None	Angular momentum, Slater integrals in U and J (See below).
local_potential_matrix	String	None	dict of {ish: ‘filename’} to specify local potential matrix of ish-th shell
local_potential_factor	String	1.0	Prefactors to the local potential matrix (float or list with len=ncor)

格子

相互作用

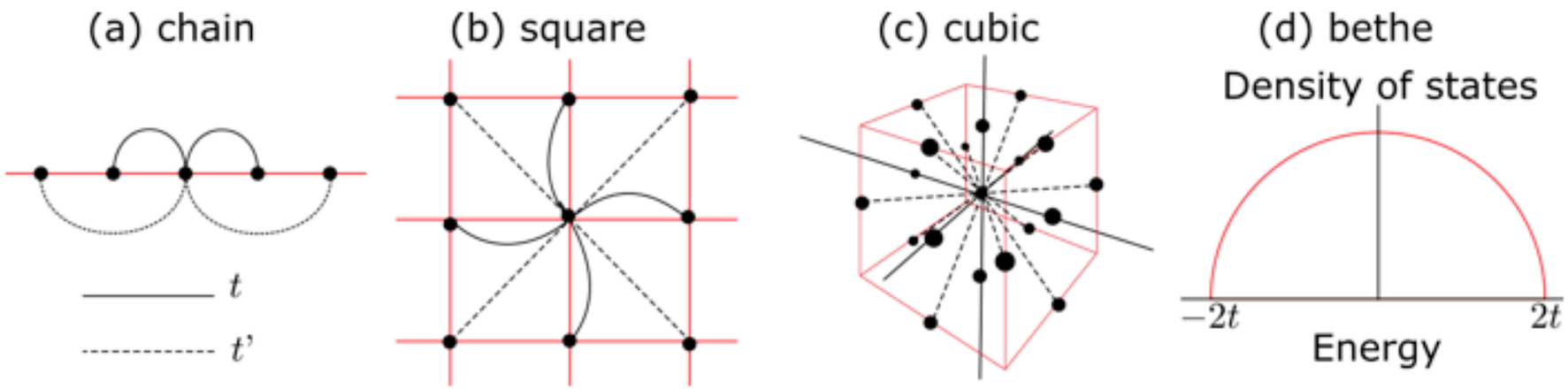
配位子場

格子の種類

lattice

For model calculations, the following preset models are defined:

- **chain**
- **square**
- **cubic**
- **bethe** (semicircular DOS with energy ranges [-2t:2t])



For DFT+DMFT calculations, hopping parameters in the Wannier90 format can be imported by

- **wannier90**

  Place the Wannier90 file in the current directory with the name *seedname*_hr.dat.

For experts, the lattice data may be prepared by your own. In this case, use

- **external**

  In this mode, you should make all necessary data in `dft_input` group of *seedname*.h5. The data structure follows **DFTTools**. For details, see the reference manual of DFTTools.

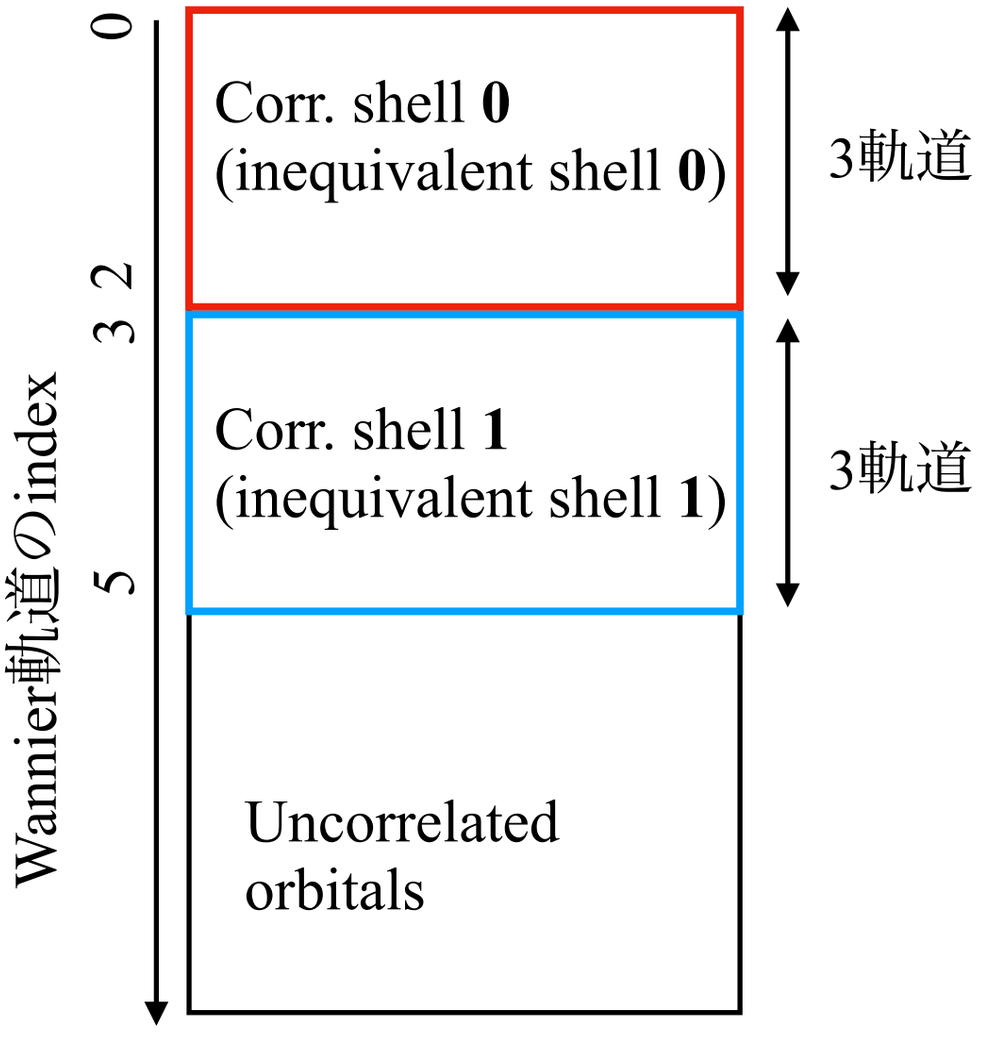
  The pre-process `dcore_pre` does not touch the data in `dft_input` group, and write only additional data such as interactions into `DCore` group.

Correlated shellとinequivalent shell

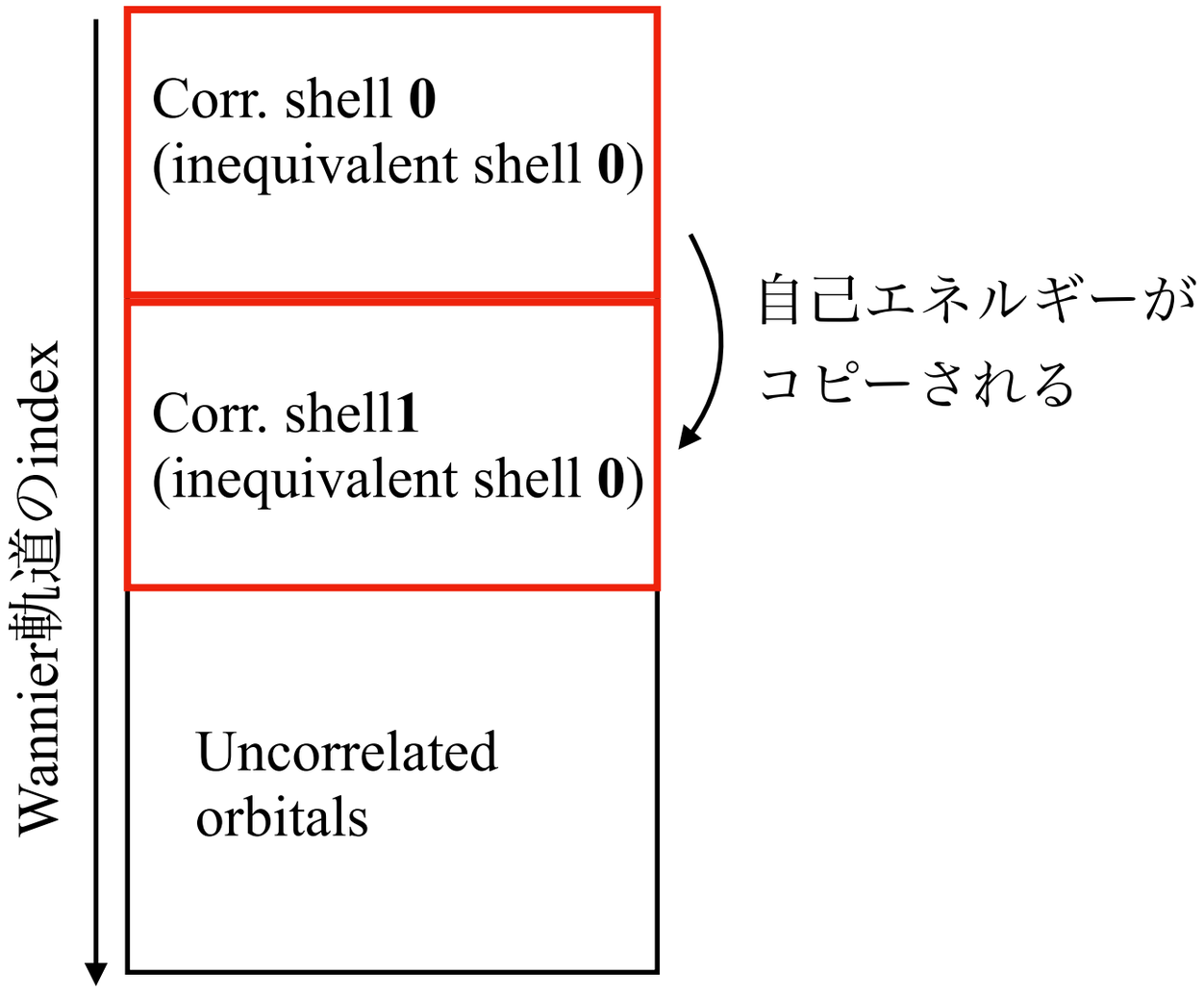
3軌道・2原子系 (spin_orbit=False)

デフォルト

[model]
ncor = 2
norb = 3, 3
spin_orbit = False



[model]
ncor = 2
norb = 3
corr_to_inequiv = 0, 0
spin_orbit = False



グリーン関数

	↑	↓
↑	≠0	0
↓	0	≠0

Correlated shellとinequivalent shell

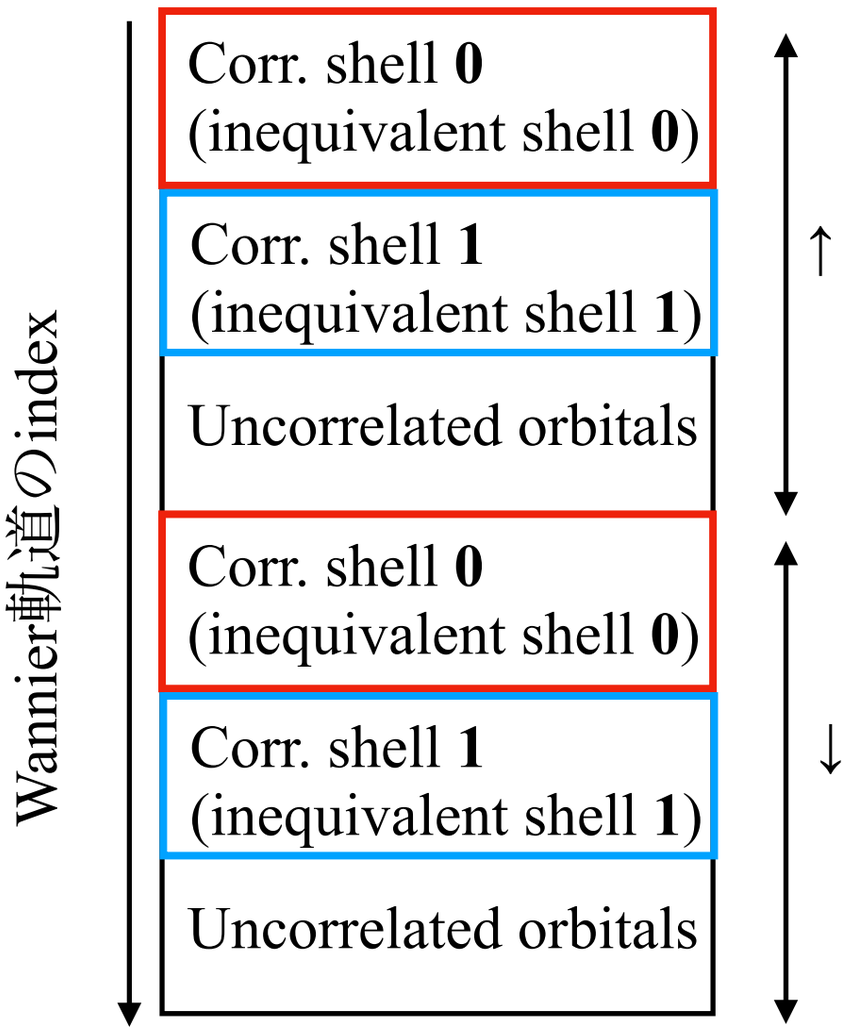
3軌道・2原子系 (spin_orbit=True)

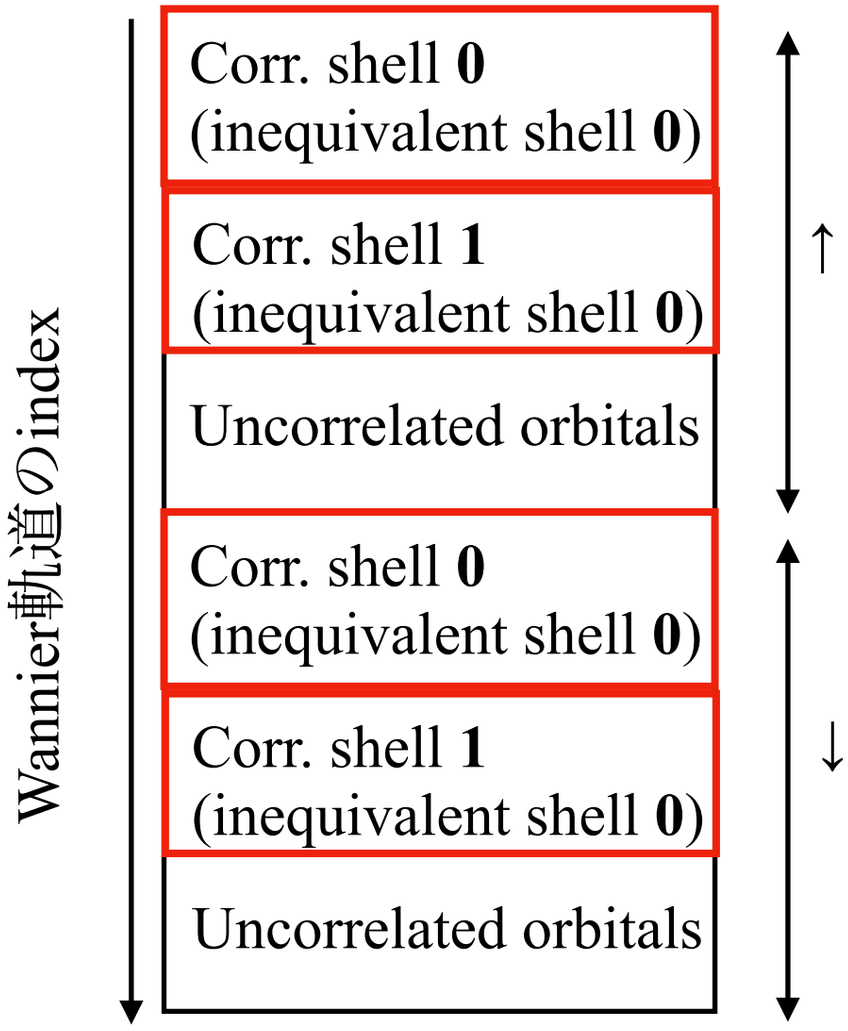
[model]
ncor = 2
norb = 3, 3

[model]
ncor = 2
norb = 3
corr_to_inequiv = 0, 0

グリーン関数

	↑	↓
↑	≠0	≠0
↓	≠0	≠0





相互作用の種類

Inequivalent shell毎に設定可能

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{i,\alpha\beta\gamma\delta,\sigma\sigma'} U^{i}_{\alpha\beta\gamma\delta} c^{\dagger}_{i\alpha\sigma} c^{\dagger}_{i\beta\sigma'} c_{i\delta\sigma'} c_{i\gamma\sigma}.$$

Slater-Kanamori相互作用

$$\begin{aligned}
U_{\alpha\alpha\alpha\alpha} &= U, \\
U_{\alpha\beta\alpha\beta} &= U' \qquad (\alpha \neq \beta), \\
U_{\alpha\beta\beta\alpha} &= J \qquad (\alpha \neq \beta), \\
U_{\alpha\alpha\beta\beta} &= J \qquad (\alpha \neq \beta),
\end{aligned}$$

where U, U', J at each correlated shell are specified by the parameter kanamori as

```
interaction = kanamori
kanamori = [(U_1, U'_1, J_1), (U_2, U'_2, J_2), ... ]
```

Slater型などの他のパラメータ化、ファイル入力もサポート

[system] block

	`dcore_pre`	`dcore`	`dcore_check`	`dcore_post`
[model]	Yes	Yes	Yes	Yes
[system]		Yes	Yes	Yes
[impurity_solver]		Yes		Yes
[control]		Yes		
[tool]			Yes	Yes
[mpi]		Yes		Yes

[system] block

This block includes thermodynamic parameters and some technical parameters such as the number of Matsubara frequencies.

Name	Type	Default	Description
beta	Float	1.0	Inverse temperature. This parameter is overridden, if T is given.
T	Float	-1.0	Temperature. If this parameter is given, beta is overridden by 1/T.
n_iw	Integer	2048	Number of Matsubara frequencies
fix_mu	Bool	False	Whether or not to fix chemical potential to a given value.
mu	Float	0.0	Initial chemical potential.
prec_mu	Float	0.0001	Threshold for calculating chemical potential with the bisection method.
with_dc	Bool	False	Whether or not use double counting correction (See below)

If the parameter `with_dc` is specified to `True`, the following part of the self-energy is subtracted to avoid the double-counting error of the self-energy.

$$\Sigma^{\mathrm{dc-imp}}_{i,\alpha\sigma\beta\sigma'} = \delta_{\sigma\sigma'} \sum_{\gamma\delta\sigma_1} U_{\alpha\gamma\beta\delta} \langle c^\dagger_{\gamma\sigma_1} c_{\delta\sigma_1} \rangle_0 - \sum_{\gamma\delta} U_{\alpha\gamma\delta\beta} \langle c^\dagger_{\gamma\sigma'} c_{\delta\sigma} \rangle_0,$$

where $\langle \cdots \rangle_0$ indicates the expectation value at the initial (Kohn-Sham) state.

[impurity_solver] block

	`dcore_pre`	`dcore`	`dcore_check`	`dcore_post`
[model]	Yes	Yes	Yes	Yes
[system]		Yes	Yes	Yes
[impurity_solver]		Yes		Yes
[control]		Yes		
[tool]			Yes	Yes
[mpi]		Yes		Yes

対応不純物ソルバー

	General interaction (non density-density)	Spin-orbit coupling	備考
ALPS/CT-HYB	○	○	品岡等が開発
ALPS/CT-HYB-SEGMENT	-	-	比較的高速
TRIQS/cthyb	○	△	
TRIQS/hubbard-I	○	○	Hubbard-I近似 (TRIQS 1.4のみ)
pomerol	○	○	Hubbard-I近似 (Bathの離散化を次期バージョンで追加)

ソルバー毎の解説

https://issp-center-dev.github.io/DCore/master/impuritysolvers.html

不純物ソルバーの指定法

https://issp-center-dev.github.io/DCore/master/impuritysolvers.html

[impurity_solver] block

This block specifies an impurity solver to be used and necessary parameters for running the solver program.

Name	Type	Default	Description
name	String	null	Name of impurity solver. Available options are null, TRIQS/cthyb, TRIQS/hubbard-I, ALPS/cthyb, ALPS/cthyb-seg, pomerol.
basis_rotation	String	None	You can specify either 'Hloc', 'None', or the location of a file..

- TRIQS/hubbard-I

```
[impurity_solver]
name = TRIQS/hubbard-I
```

- ALPS/CT-HYB

```
[impurity_solver]
name = ALPS/cthyb
timelimit{int} = 300
exec_path{str} = $HOME/opt/CT-HYB/bin/hybmat
```

不純物ソルバー固有のパラメータを指定可能 (型指定が必要)

[control] block

	`dcore_pre`	`dcore`	`dcore_check`	`dcore_post`
[model]	Yes	Yes	Yes	Yes
[system]		Yes	Yes	Yes
[impurity_solver]		Yes		Yes
[control]		Yes		
[tool]			Yes	Yes
[mpi]		Yes		Yes

[control] block

This block includes parameters that control the self-consistency loop of DMFT.

Name	Type	Default	Description
max_step	Integer	100	Maximum steps of DMFT loops
sigma_mix	Float	0.5	Mixing parameter for self-energy
restart	Bool	False	Whether or not restart from a previous calculation stored in a HDF file.
initial_static_self_energy	String	None	dict of {ish: 'filename'} to specify initial value of the self-energy of ish-th shell. The file format is the same as local_potential_matrix.
initial_self_energy	String	None	Filename containing initial self-energy in the same format as sigma.dat generated by dcore_check.
time_reversal	Bool	False	If true, an average over spin components are taken.
symmetry_generators	String	None	Generators for symmetrization of self-energy.

[tool] block

	`dcore_pre`	`dcore`	`dcore_check`	`dcore_post`
[model]	Yes	Yes	Yes	Yes
[system]		Yes	Yes	Yes
[impurity_solver]		Yes		Yes
[control]		Yes		
[tool]			Yes	Yes
[mpi]		Yes		Yes

[tool] block

This block includes parameters that are solely used by `dcore_post`.

Name	Type	Default	Description
nnode	Integer	0	[NOT USED] Number of node for the *k* path
nk_line	Integer	8	Number of *k* along each line
knode	String	[(G,0.0,0.0,0.0), (X,1.0,0.0,0.0)]	The name and the fractional coordinate of each k-node.
omega_min	Float	-1.0	Minimum value of real frequency
omega_max	Float	1.0	Max value of real frequency
Nomega	Integer	100	Number of real frequencies
broadening	Float	0.1	An additional Lorentzian broadening
eta	Float	0.0	Imaginary frequency shift for the Pade approximation
omega_pade	Float	5.0	Cutoff frequencies for the Pade approximation. Data in [-i omega_pade, i omega_pade] is used.
omega_check	Float	0.0	Maximum frequency for dcore_check. If not specified, a fixed number of Matsubara points are taken.

[mpi] block

	dcore_pre	dcore	dcore_check	dcore_post
[model]	Yes	Yes	Yes	Yes
[system]		Yes	Yes	Yes
[impurity_solver]		Yes		Yes
[control]		Yes		
[tool]			Yes	Yes
[mpi]		Yes		Yes

[mpi] block

This block includes parameters which are read by `dcore` and `dcore_post`.

Name	Type	Default	Description
command	String	mpirun -np #	Command for executing a MPI job. # will be relaced by the number of processes.

dcore, dcore_post内部でMPIを起動するときに使われる