TRIQS

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Ab initio DMFT: introduction to DFTTools, solid_dmft, and related tools

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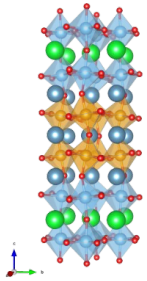
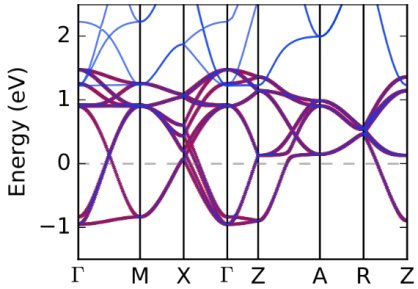
[1]Center for Computational Quantum Physics, Flatiron Institute, Simons Foundation

05/27/2024

Ab initio DMFT / Quantum Embedding

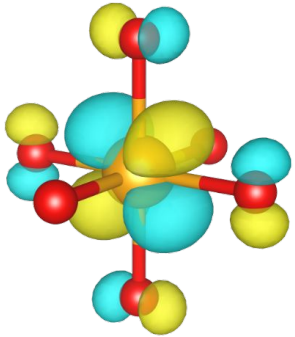


Density Functional Theory



$$P_{m\nu}(\mathbf{k}) = \langle w_{m\mathbf{k}} | \Phi_{\nu\mathbf{k}} \rangle$$

Downfolded Hamiltonian

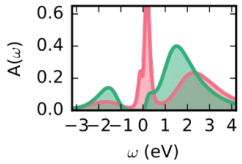


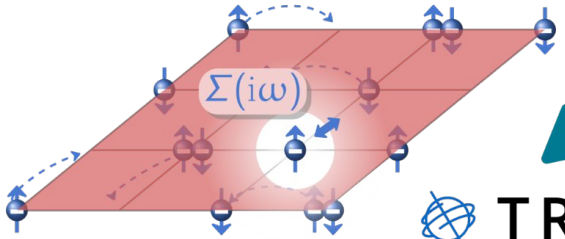
$$\hat{G}(\mathbf{k}, i\omega_n) = \sum_{\nu\nu'} \left[i\omega_n + \mu - \hat{\epsilon}(\mathbf{k}) - \Delta\hat{\Sigma}(\mathbf{k}, i\omega_n) \right]^{-1}_{\nu\nu'} \Pi_{\nu\nu'}(\mathbf{k})$$

$$G^{\mathrm{loc}}_{mm'}(\mathrm{i}\omega_n) = \sum_{\mathbf{k}\nu\nu'} P_{m\nu}(\mathbf{k}) G_{\nu\nu'}(\mathbf{k}, \mathrm{i}\omega_n) P^*_{\nu' m'}(\mathbf{k})$$

charge self-consistency

$$\Delta\Sigma_{\nu\nu'}(\mathbf{k}) = \sum_{\nu\nu'} P^*_{\nu m}(\mathbf{k}) \Delta\Sigma_{mm'} P_{m'\nu'}(\mathbf{k})$$





$$+ \hat{H}_{int} = \frac{1}{2} \sum_{mm'm''m'''} U_{mm'm'''m''} \hat{c}^\dagger_m \hat{c}^\dagger_{m'} \hat{c}_{m'''} \hat{c}_{m''}$$

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Dynamical Mean-Field Theory

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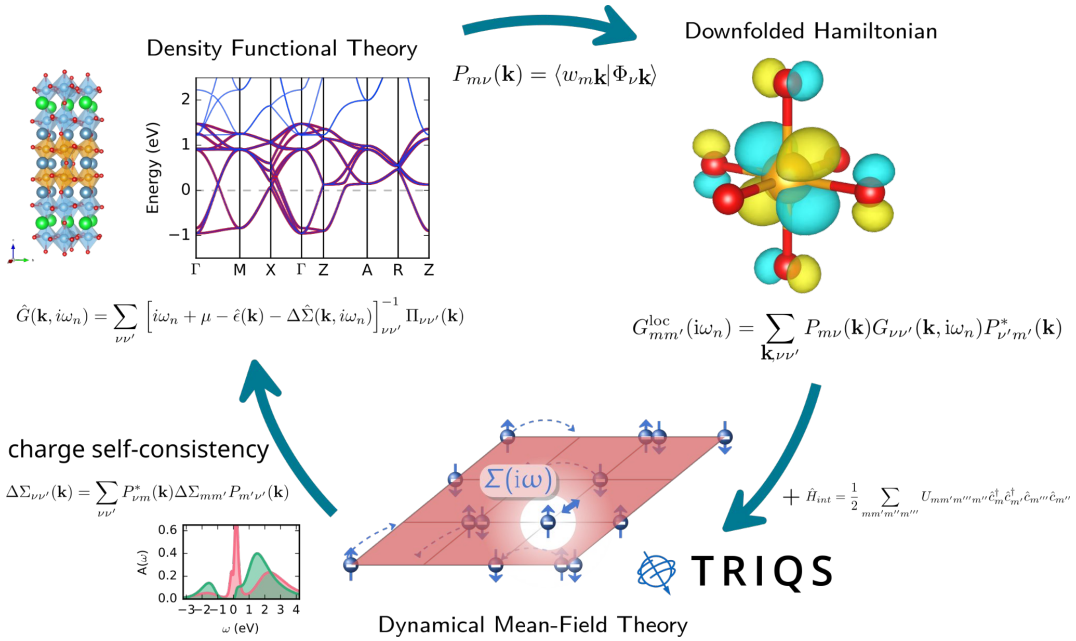
Ab initio DMFT / Quantum Embedding

Model -> DFT+DMFT:

- projector choice: KS basis vs localized orbitals
- interaction Hamiltonian for these orbitals (screening)
- double counting
- charge self-consistency
- post-processing

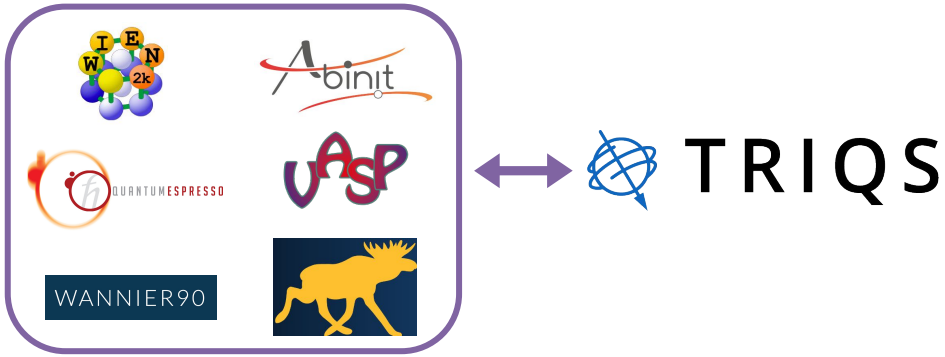


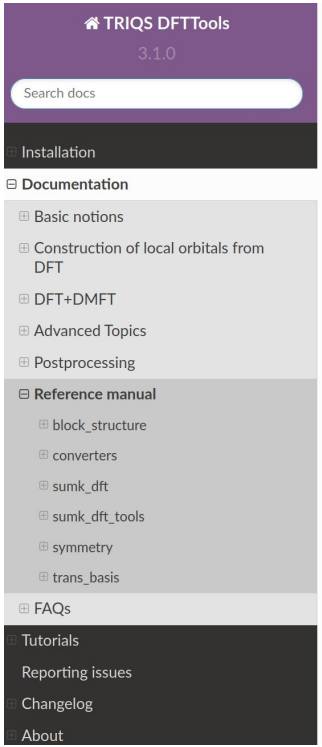
DFT+DMFT within the TRIQS ecosystem

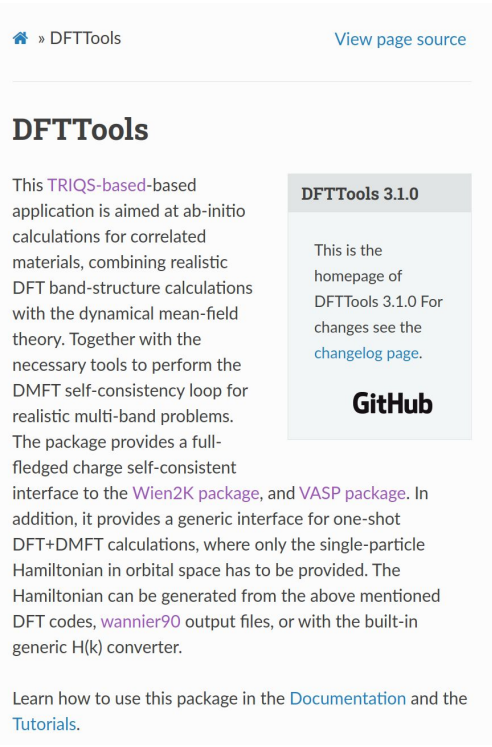
1. TRIQS/DFTTools: connection to ab initio codes
2. TRIQS/solid_dmft: full DFT+DMFT wrapper
3. Impurity solvers in TRIQS
4. Analytic continuation with TRIQS
5. FermiSee: phenomenology & visualization
6. solid_dmft tutorial

1. TRIQS/DFTTools: triqs.github.io/dft_tools

- same structure as TRIQS main project, i.e. automatic reference manual and tutorials
- issues and discussions on github.com/triqs/dft_tools
- M. Aichhorn *et al. CPC* '16 ~ 170 citations







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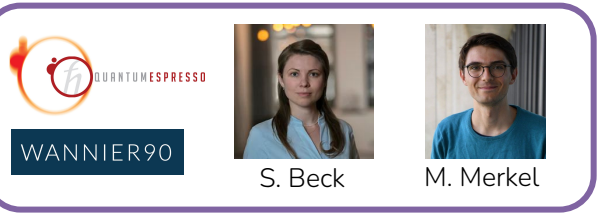

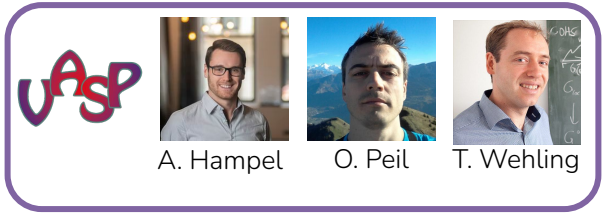

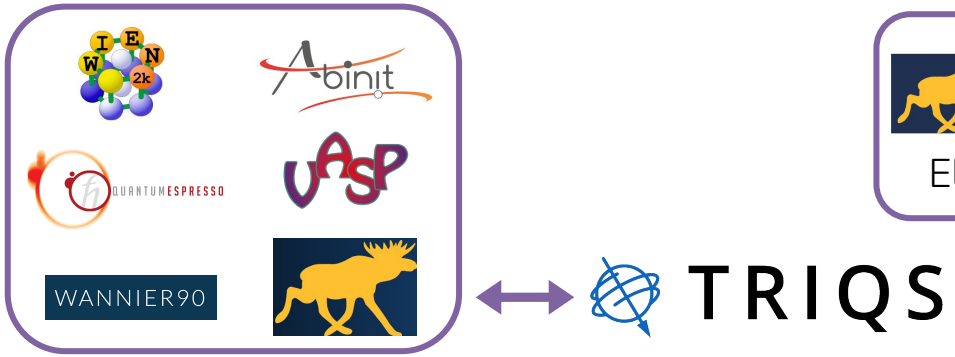

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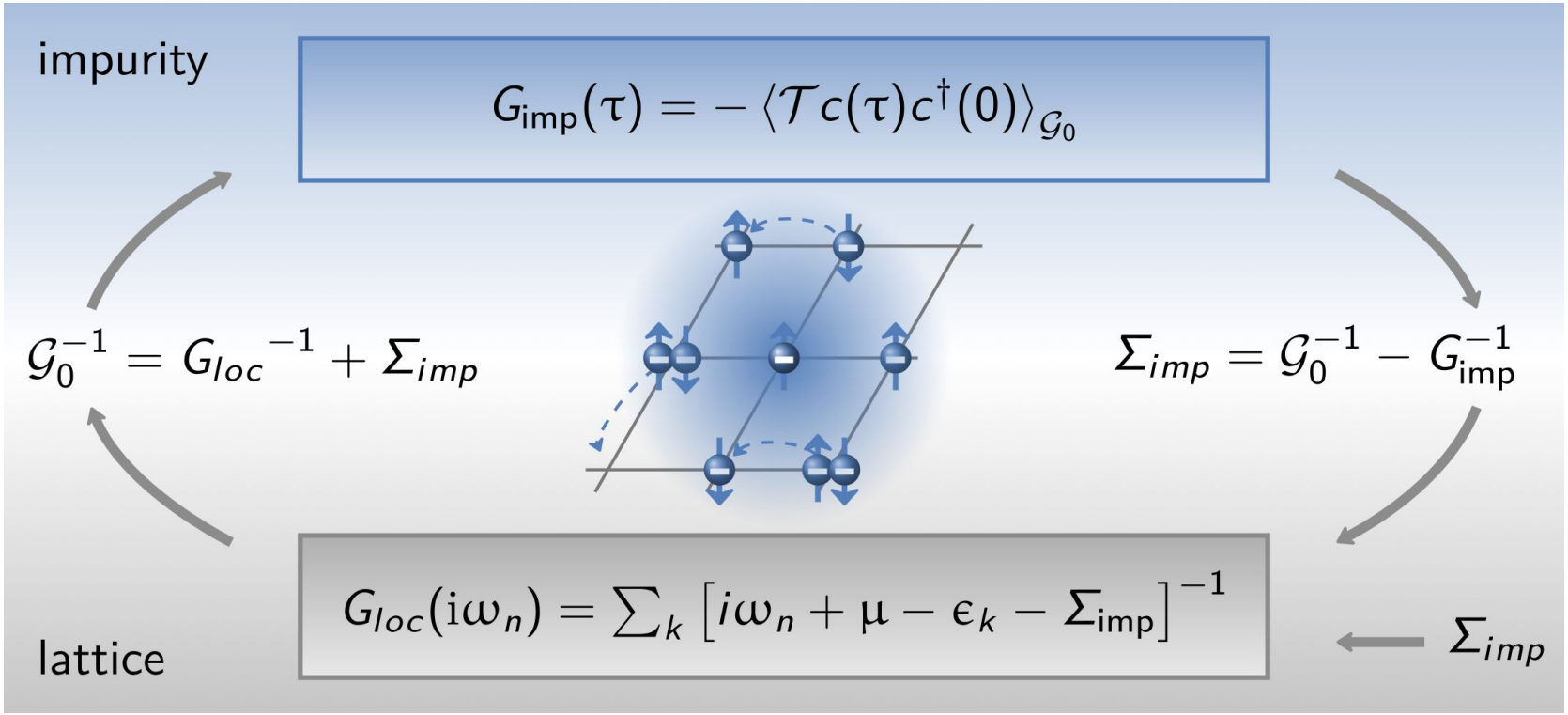
1. TRIQS/DFTTools: electronic structure interface



Adapted from S.Beck

1. TRIQS/DFTTools: core functionality

- `lattice_gf()` $G(\mathbf{k},\omega)$
- `extract_G_loc()` $G(\omega)=\sum_k G(\mathbf{k},\omega)$
- `downfold / upfold` $P_{m\nu R}(\mathbf{k})$
- `calc_mu()` μ
- `calc_dc()` $\mathbf{\Sigma}^{DC}$
- `blockstructure class: analyse_block_structure_from_gf()`

1. DFTTools example: Wannier90 converter + basics

```
from triqs_dft_tools.sumk_dft import SumkDFT
from triqs_dft_tools.converters import Wannier90Converter
from triqs.gf import *

Converter = Wannier90Converter(seedname='svo_t2g')
Converter.convert_dft_input()

mesh = MeshImFreq(beta=40, S='Fermion', n_iw=1025)
sumk = SumkDFT(hdf_file='svo_t2g.h5', mesh=mesh)

sumk.calc_mu()

Gloc_iw = sumk.extract_G_loc()

sumk.analyse_block_structure_from_gf(Gloc_iw)

sumk.set_Sigma(Sigma)
```

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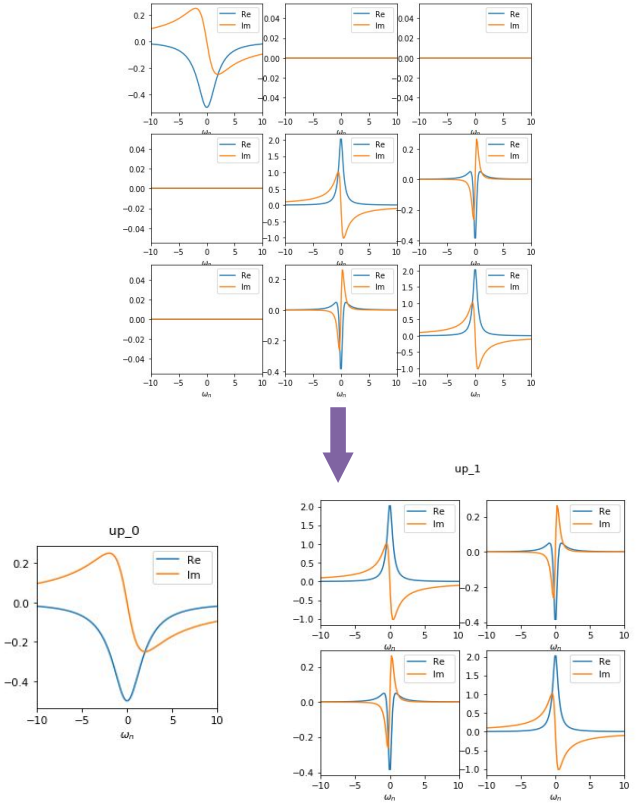
1. DFTTools functionality: SumkDFT

- tutorials for DMFT calculation with Wien2k, Elk, Vasp, and QE / Wannier90
- post-processing:
  - spectral function: `density_of_states()`, `spaghettis()`
  - Fermi surfaces: `spectral_contours()`
  - transport / optical conductivity $\sigma(\Omega)$
- manipulate orbital structure with `blockstructure` class (right)
- charge self-consistency updates of ρ



1. DFTTools functionality: double counting

- Problem: What has been already accounted for in KS-DFT ($\sum^{DC}$) for the localized orbitals?
- ill-posed problem due to the formally incompatible footing: diagrammatic vs. non-perturbative
- different analytic expressions have been proposed: FLL, AMF, ANI, Kunes, nominal … [1]
- more sophisticated numerical evaluation in [2]

$$\hat{H}_{\mathrm{DFT+}} = \hat{H}_{\mathrm{KS}} + \hat{H}_{\mathrm{U}} - \hat{H}_{\mathrm{DC}}$$

$$E^{DFT+U}[\rho^\sigma] = E^{DFT}[\rho^\sigma] + \sum_\alpha E^U[n_\alpha] - E^{DC}[n_\alpha]$$

$$E_{\mathrm{H}}[\rho(\mathbf{r})] + E_{\mathrm{XC}}[\rho(\mathbf{r})]$$

DFT+DMFT

$$\Delta\Sigma^{\mathcal{R}}_{\alpha\beta} = \Sigma^{\mathrm{imp}}_{\alpha\beta} - \Sigma^{\mathrm{DC}}_{\alpha\beta}$$

$$\Sigma^{\mathrm{DC}}[n_R] = U_{\mathrm{avg}}\left(n_R - \frac{1}{2}\right) - J_{\mathrm{avg}}\left(n^\sigma_R - \frac{1}{2}\right)$$

[1] good overview over DC: Karolak, M. : Electronic Correlation Effects in Transition Metal Systems: From Bulk Crystals to Nanostructures, PhD thesis, (2013), link: ediss.sub.uni-hamburg.de/volltexte/2013/6526/
[2] K. Haule, PRL 115, 196403 (2015)

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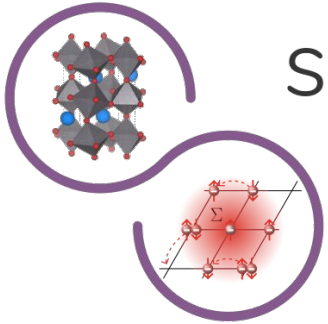
1. TRIQS: interaction Hamiltonian

- `triqs.operators.util.U_matrix` provides functions to create full Uijkl tensors with:
  - spherical symmetry (Slater like)
  - cubic symmetry (Kanamori)
- provides also functions to manipulate 4 index tensors
- `triqs.operators.util.U_matrix` provides functions to create triqs many-body operators from Uijkl tensors:
  - `h_int_density`: density-density only
  - `h_int_kanamori`: only Kanamori relevant 2 index
  - `h_int_slater`: full Uijkl used

2. solid_dmft: DFT+DMFT calculations

- 🚢 TRIQS flagship implementation of DFT+DMFT
- 📈 Scalability with scriptable config file
- 🔗 interface to Vasp and Quantum Espresso for CSC calculations [2]
- 🔬 Reproducibility: versioning, h5 storage, convergence metrics
- ⚛ Flexible solver choice: cthyb, ctseg, ctint, FTPS, Hubbardl, Hartree, …
- 📋 Online documentation & tutorials: triqs.github.io/solid_dmft



solid_dmft

A versatile python wrapper to perform DFT + DMFT calculations utilizing the TRIQS software library.


S. Beck


M. Merkel (ETH)


A. Carta (ETH)


A. Hampel

[1] M. Merkel, A. Carta, S. Beck, AH, JOSS, doi.org/10.21105/joss.04623 (2022)
[2] S. Beck, AH, O. Parcollet, C. Ederer, and A. Georges, JoP: Condensed Matter, 34 (2022)

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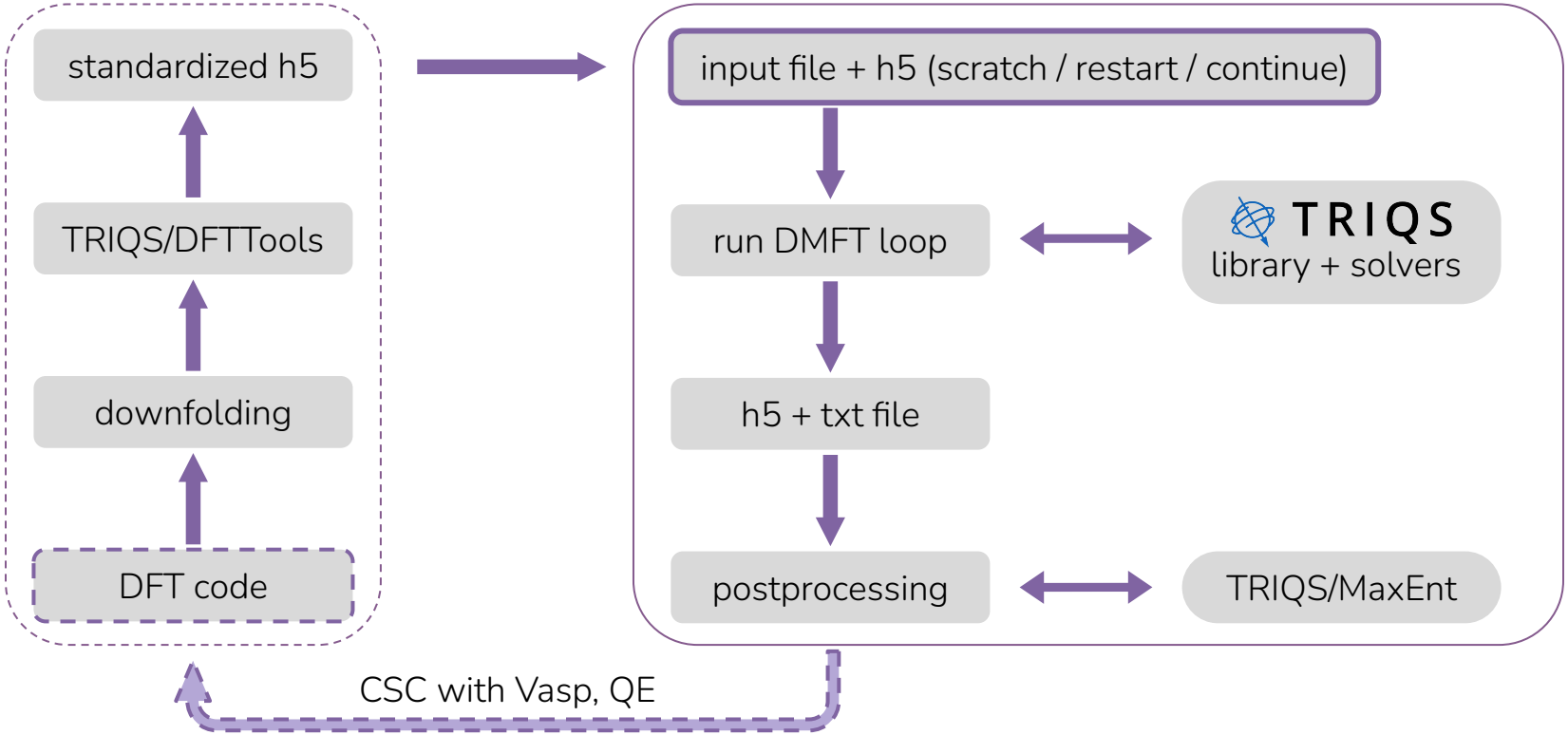
2. solid_dmft: workflow

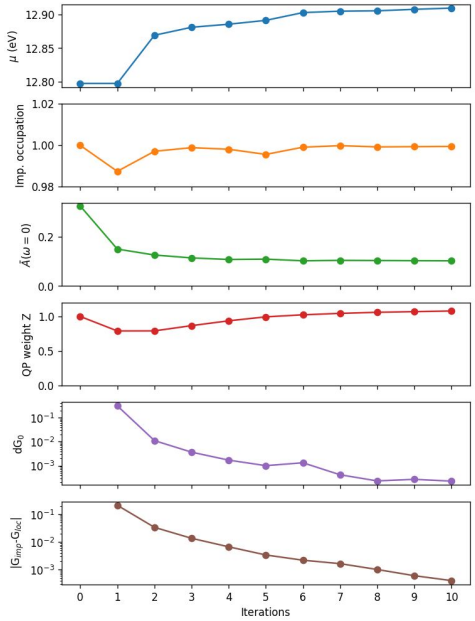


2. solid_dmft: example & tutorials

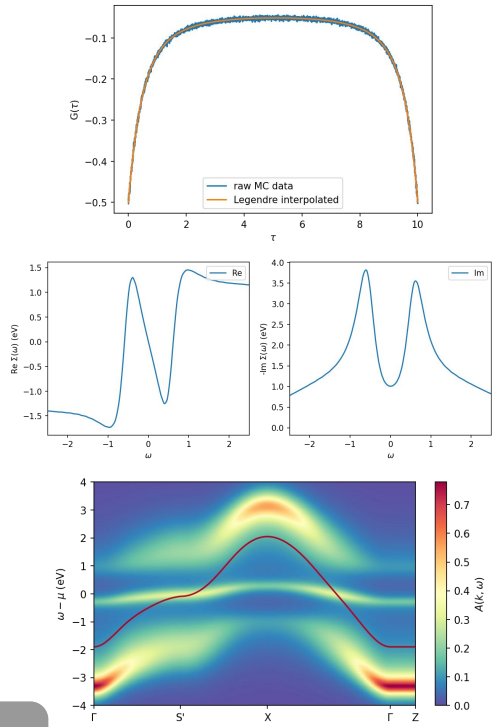
example config file:

```
[general]
seedname = "lco_wannier"
jobname = "b10-U5.0"

beta = 10
n_iw = 251
n_tau = 5001
n_iter_dmft = 6

prec_mu = 1e-4

h_int_type = "kanamori"
U = 3.6
J = 0.0
dc_type = 0

[solver]
type = "cthyb"
length_cycle = 60
n_warmup_cycles = 1e+4
n_cycles_tot = 2e+6
measure_density_matrix = true
```

mpirun solid_dmft



postprocessing



github.com/TRIQS/tutorials/AbinitioDMFT
more tutorials: triqs.github.io/solid_dmft/tutorials

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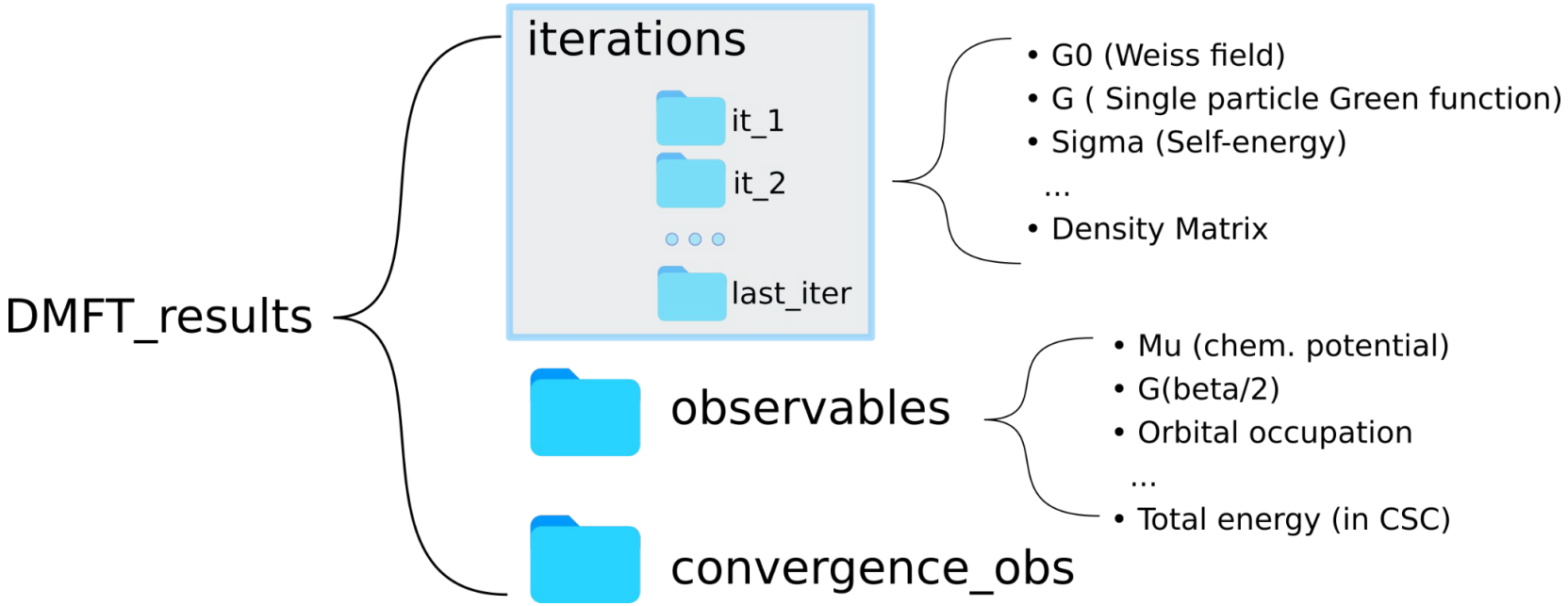
2. solid_dmft: input

- toml bases input parser
- divided into 4 sections:
  - general
  - solver
  - dft
  - advanced
- all defaults in `solid_dmft/io_tools/default.toml`
- `triqs.github.io/solid_dmft/input_output/DMFT_input/input`

```
[general]
seedname = SVO
csc = true
beta = 10
n_iter_dmft_first = 5
n_iter_dmft = 12

h_int_type = "kanamori"
U = 6.5
J = 0.65
dc_type = 1
dc_dmft = true
calc_energies = true

[solver]
type = "cthyb"
length_cycle = 100
n_warmup_cycles = 1e+4
n_cycles_tot = 1e+6
measure_density_matrix = true

[dft]
dft_code = "vasp"
dft_exec = "vasp_std"
n_cores = 1
```

2. solid_dmft: standardized output for reproducibility



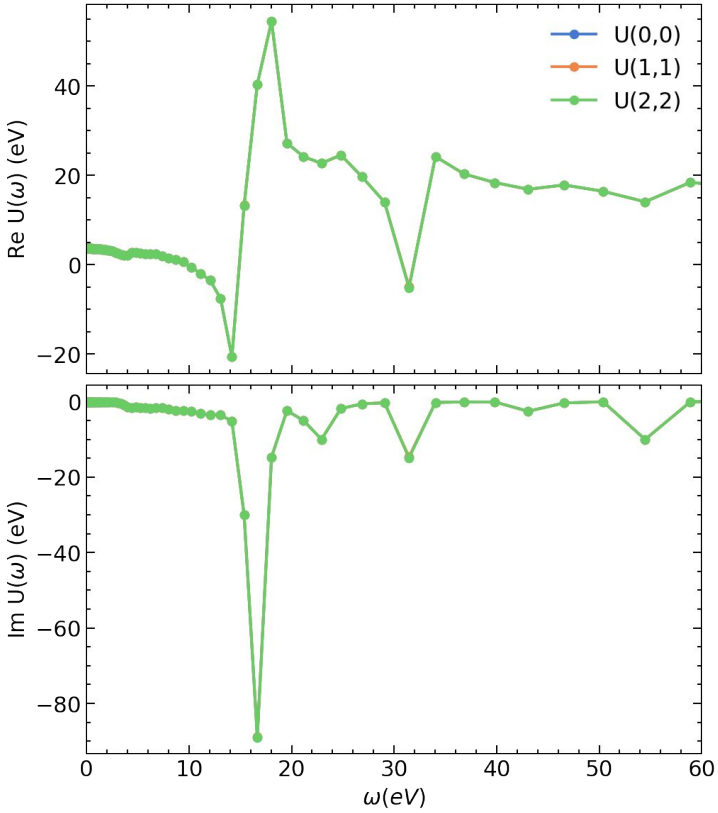
standardized output to continue previous calculations or just load self-energy

2. solid_dmft utils: cRPA

- RESPACK results reader

```
from solid_dmft.postprocessing.eval_U_cRPA_RESPACK
import read_interaction

RP = read_interaction(seed='svo',
                      path='./cRPA')

for key, value in RP.__dict__.items():
    print(key)
```

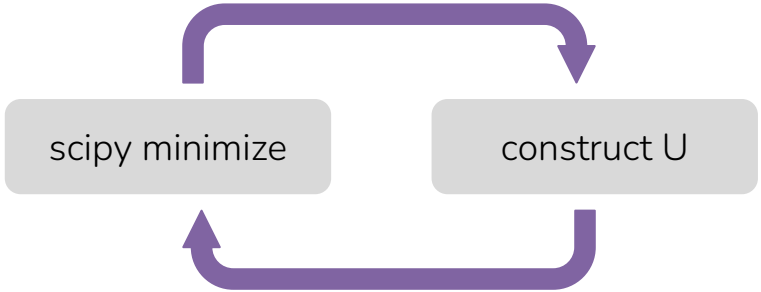
- gives access to numpy arrays of:
  - U_R, V_R, J_R, X_R
  - Uijkl, Vijkl
  - Uij_w, Jij_w
- same for Vasp cRPA
- results can be used in DMFT run*



2. solid_dmft utils: parameterize Coulomb tensor

- module `eval_U_cRPA_Vasp.py`:

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{\sigma\sigma'} \sum_{mm'm''m'''} U_{mm'm''m'''} \; c^{\dagger}_{m\sigma} c^{\dagger}_{m'\sigma'} c_{m'''\sigma'} c_{m''\sigma}$$

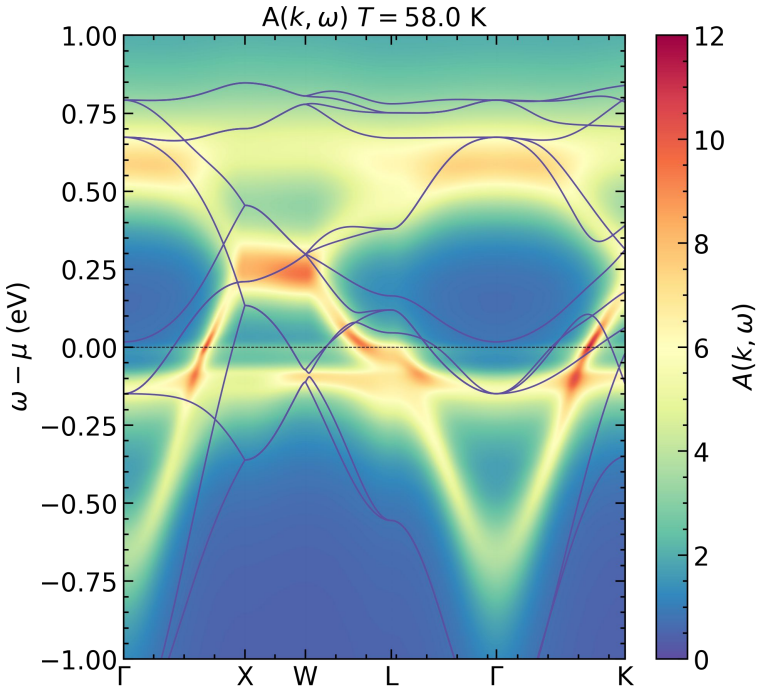


- `fit_kanamori(uijkl, n_orb, fit_2, fit_3, fit_4)`
- `fit_slater_fulld(u_ijij, u_ijji, U_init, J_init, fixed_F4_F2)`

$$\begin{aligned}
\hat{H}_{\text{kan}} = & \frac{1}{2} \sum_{\sigma} \sum_{m} \mathcal{U} \; \hat{n}_{m\sigma} \hat{n}_{m\bar{\sigma}} \\
& + \frac{1}{2} \sum_{\sigma} \sum_{m \neq m'} \left[\mathcal{U}' \; \hat{n}_{m\sigma} \hat{n}_{m'\bar{\sigma}} + (\mathcal{U}' - \mathcal{J}) \hat{n}_{m\sigma} \hat{n}_{m'\sigma} \right] \\
& + \frac{1}{2} \sum_{\sigma} \sum_{m \neq m'} \left[\mathcal{J} \; c^{\dagger}_{m\sigma} c^{\dagger}_{m'\bar{\sigma}} c_{m\bar{\sigma}} c_{m'\sigma} + \mathcal{J}_C \; c^{\dagger}_{m\sigma} c^{\dagger}_{m\bar{\sigma}} c_{m'\bar{\sigma}} c_{m'\sigma} \right]
\end{aligned}$$

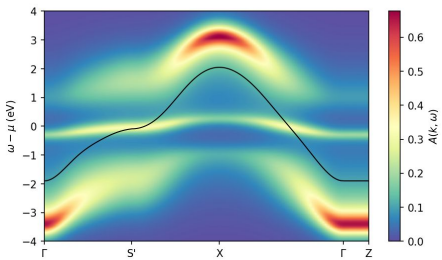
2. solid_dmft post-processing with H(*R*)

- leverage Wannier interpolation to calculate G(k, ω)
- no pre-computing of projectors on k-path necessary
- high precision mesh allows to find contours and QP dispersion
- loads automatically self-energy and other parameters from solid_dmft h5



2. solid_dmft post-processing with H(*R*)

```
from solid_dmft.postprocessing import plot_correlated_bands as pcb

w90_dict = {'w90_path': './data/mlwf/', 'w90_seed': 'lco',
            'n_orb': 1, 'mu_tb': 12.7367}

tb_dict = {'bands_path': [('G', 'S\''), ('S\'', 'X'), ('X', 'G'), ('G', 'Z')],
           'n_k': 50, 'G': [ 0.0,  0.0,  0.0],
           …}

sigma_dict = {'dmft_path': 'b10-U3.6/lco_wannier.h5',
              'it': 'last_iter', 'spin': 'up'}

tb_bands, alatt_kw, freq = pcb.get_dmft_bands(with_sigma='calc',
                                              **w90_dict, **tb_dict, **sigma_dict)

fig, ax = plt.subplots(1)
pcb.plot_bands(fig, ax, alatt_kw, tb_bands, freq, n_orb=w90_dict['n_orb'],
               alatt=True, colorscheme_bands='Greys', colorscheme_alatt='Spectral_r')
```



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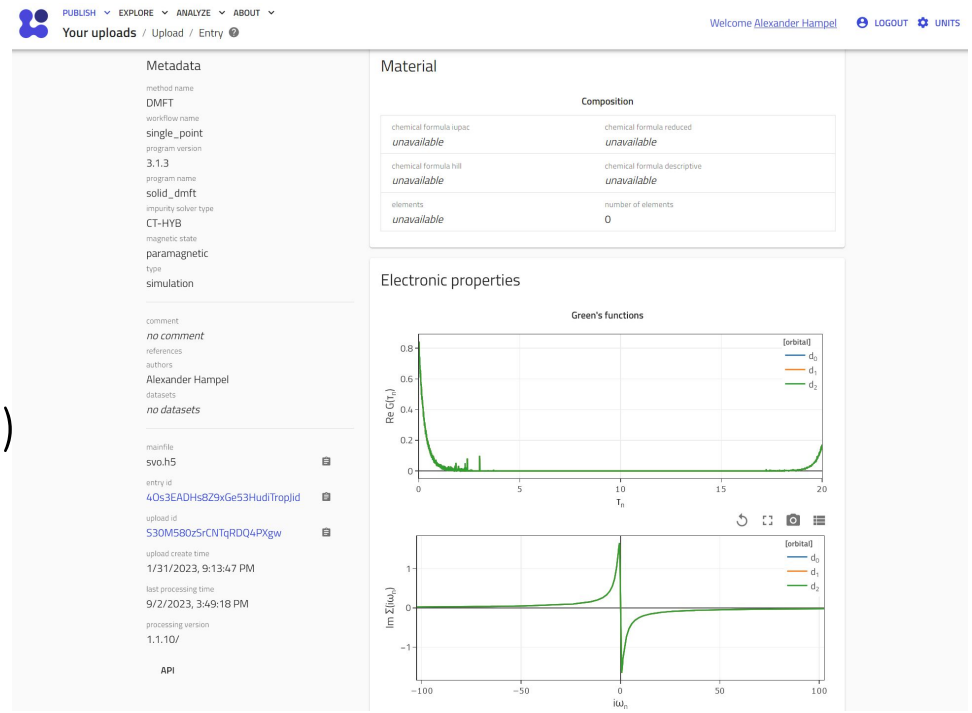
2. solid_dmft: NOMAD parser

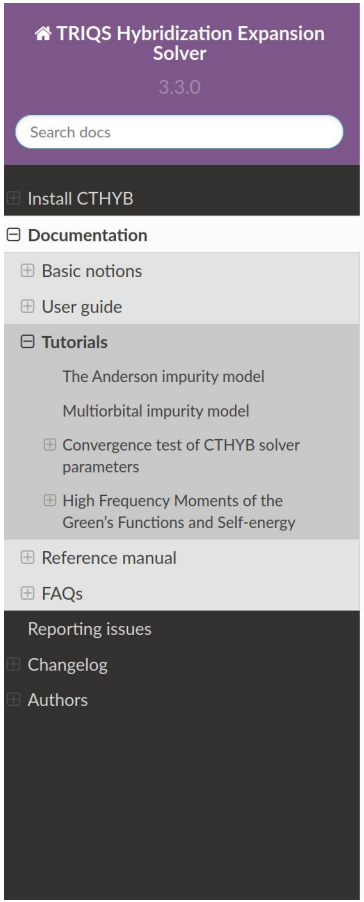
- material science data management and sharing: nomad-lab.eu/nomad-lab/
- automatic processing of h5 archives from DMFT calculations (solid_dmft)
- processing of results with unique identifiers



3. TRIQS impurity solvers

solver name	method	# orb	measure	comments	approximation
cthyb	ct-qmc hyb expansion	~5	$G(\tau)$, $G^{(2)}$, χ_{AB}, ρ_{imp}	small U/Δ, off diag $\Delta \rightarrow$ sign	exact
ctseg	ct-qmc hyb segment picture	~8	$G(\tau)$, $G^{(2)}$, χ_{AB}, ρ_{imp}	small U/Δ, nn int only, $U(\tau)$	exact
ctint	ct-qmc interaction expansion	~80	$G(\tau)$, $G^{(2)}$, χ_{AB}	small Δ/U, nn int only, $U(\tau)$	exact
forkTPS	fork tensor product states	~5	$G(t)$, χ_{AB}	η~1e-2 , Kanamori only	exact
hartree_fock	Hartree / Hartree-Fock	~20	$\sum^{HF}$	no ω, HF only	only HF diagrams
hubbardI	ED of impurity problem	~7	$G(i\omega_n)$, $G(\omega)$, $G^{(2)}$, χ_{AB}		neglect hyb
nrgljubljana_interface	NRG	~3	$G(\omega)$, $A(\omega)$, χ_{AB}	log mesh around ω=0	exact
pomerol2triqs	ED of impurity problem	~3	$G(\omega)$, $G(i\omega_n)$, $G^{(2)}$, χ_{AB}	discretized bath	finite size bath
w2dynamics_interface	ct-qmc hyb / seg exp + worm	~5	$G(\tau)$, $G^{(2)}$ + worm, χ_{AB}, ρ_{imp}	small U/Δ, off diag $\Delta \rightarrow$ sign, $U(\tau)$	exact

2. TRIQS impurity solvers: tutorials



User guide

- Setting the parameters
- Building DMFT calculations
- Random number generators
- Measuring static observables / impurity density matrix
- Multiplet analysis & particle number histograms
- Dynamical spin-spin susceptibility \(\chi_{S_z S_z}(\tau)\)
- Perturbation order histograms

Tutorials

- The Anderson impurity model
- Multiorbital impurity model
- Convergence test of CTHYB solver parameters
- High Frequency Moments of the Green's Functions and Self-energy

Reference manual

`triqs_cthyb.multiplet_tools`	functions for analyzing the multiplet structure in cthyb
`triqs_cthyb.solver`	the triqs_cthyb solver class
`triqs_cthyb.tail_fit`	tail fitting and high frequency moments
`triqs_cthyb.util`	utility functions

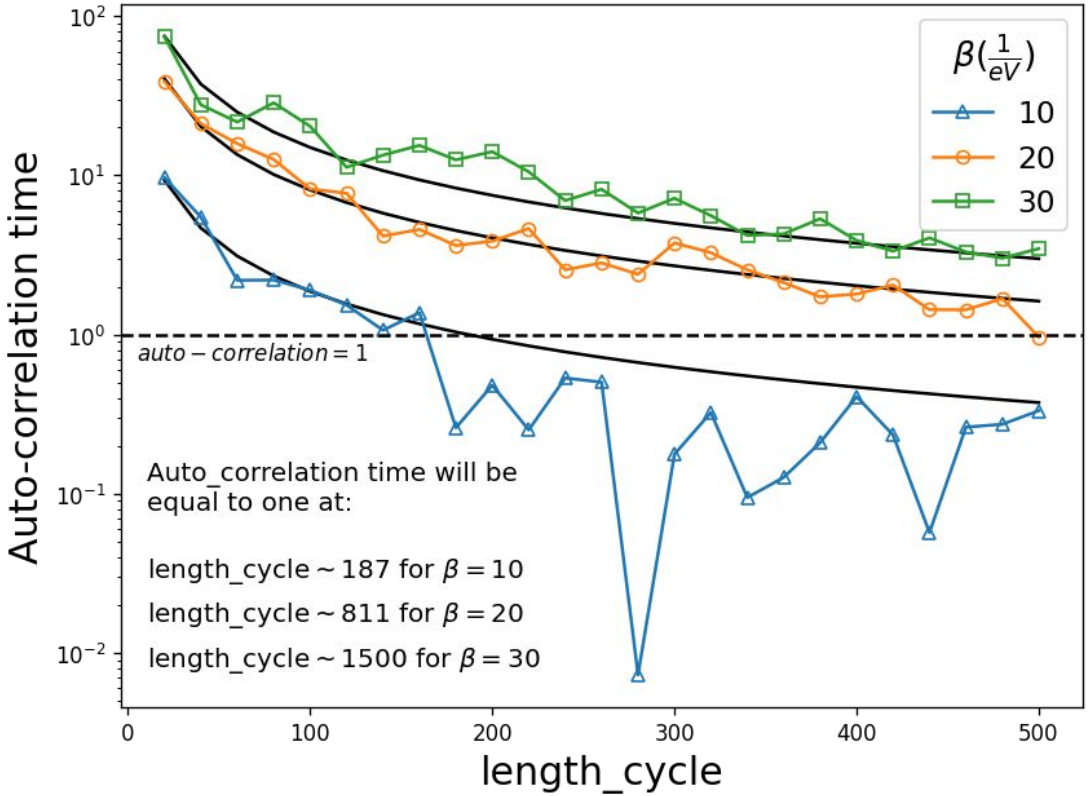
Link to all relevant solver parameters:

- triqs_cthyb.solver.Solver.solve_parameters
- triqs_cthyb.solver.Solver.constr_parameters

2. TRIQS impurity solvers: QMC convergence

- `length_cycle`
- `n_warmup_cycles`
- `n_cycles`
- `n_tau`
- `n_iw`

triqs.github.io/cthyb/latest/guide/cthyb_convergence_tests.html [1]



[1] Tutorial by Azin Kazami-Moridani

4. analytic continuation: TRIQS

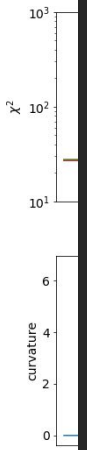
- TRIQS provides several apps to analytically continue Matsubara Green functions:

$$G(i\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{i\omega_n - \omega} A(\omega) \quad \text{or} \quad \mathbf{G} = \mathbf{KA} \text{ (matrix form)}$$

- triqs.github.io/maxent
  - G. J. Kraberger et al. , PRB 96 (2017)
- triqs.github.io/Nevanlinna
  - S. Iskakov et al. , CPC (2023)
- triqs.github.io/omegamaxent_interface
  - ΩMaxEnt code, D. Bergeron and A.-M.S. Tremblay, PRE 94 (2016)
- krivenko.github.io/som
  - Stochastic Optimization Method, I. Krivenko et al. , CPC 239 (2019)

4. analytic continuation: TRIQS/maxent

- triqs.github.io/maxent
- different ways to choose α implemented:
  - line-fit
  - from curvature of log(χ^2) vs log(α)
  - Bryan
- matrix valued continuation
- self-energy continuation (element-wise)




```
G_iw = GfImFreq(beta=10, indices=[0])
G_iw << SemiCircular(1)-0.5*SemiCircular(0.5)
G_tau = GfImTime(beta=10, indices=[0],
n_points=2501)
G_tau.set_from_fourier(G_iw)
G_tau.data[:, 0, 0] += 1.e-5 *
np.random.randn(len(G_tau.data))

from triqs_maxent import *
tm = TauMaxEnt(cost_function='bryan',
probability='normal')
tm.set_G_tau(G_tau)
tm.set_error(1e-4)
# run maxent
result = tm.run()
result.get_A_out('LineFitAnalyzer')
```

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4. analytic continuation: solid_dmft + maxent

- integration between solid_dmft and maxent (block structure, DC, μ)
- MPI parallelized over blocks
- continuation of:
  - G_{imp}: `postprocessing.maxent_gf_imp`
  - G_{latt}: `postprocessing.maxent_gf_latt`
  - $\sum_{imp}$: `postprocessing.maxent_sigma`
  - $\sum_{imp}$: `postprocessing.pade_sigma`
- writes result back to h5
- automatically used by post-processing routines

```
from solid_dmft.postprocessing import maxent_sigma

# use pcb maxent script to continue self energy
Sigma_real_freq =
maxent_sigma.main(external_path=h5_file,
                  omega_min=-10, omega_max=10,
                  maxent_error=0.03,
                  iteration=None,
                  n_points_maxent=101,
                  n_points_alpha=50,
                  analyzer='LineFitAnalyzer',
                  n_points_interp=2001,
                  n_points_final=1001,
                  continuator_type='inversion_dc')
```

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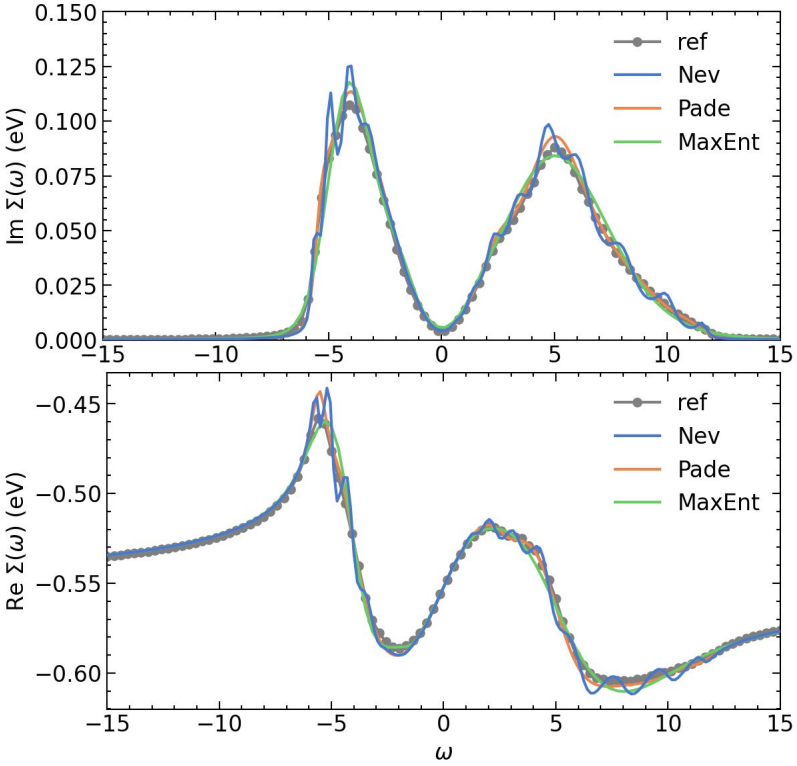
4. analytic continuation: TRIQS/nevanlinna & Pade

- Nevanlinna, matrix valued Caratheodory, and Pade
- Nevanlinna / Caratheodory work best for non-continuous spectra
- further extension necessary for noisy data
- triqs.github.io/Nevanlinna/latest/documentation
- Pade: `triqs.gf.gf_fnt.set_from_pade()`

1 band GW self-energy example:



5. FermiSee: WebApp for data visualization

$$A(\omega, \mathbf{k}) = -\frac{1}{\pi}\mathrm{Im} \sum_{\alpha=\alpha'} [\omega + \mu - \epsilon(\mathbf{k}) - \Sigma(\omega)]^{-1}_{\alpha\alpha'}$$

🔬 fermisee.flatironinstitute.org

🧰 github.com/TRIQS/FermiSee

👷 testers and developers welcome

TRIQS

WANNIER90 PythTB


S. Beck


S. Rahim


A. Hampel

plotly | Dash

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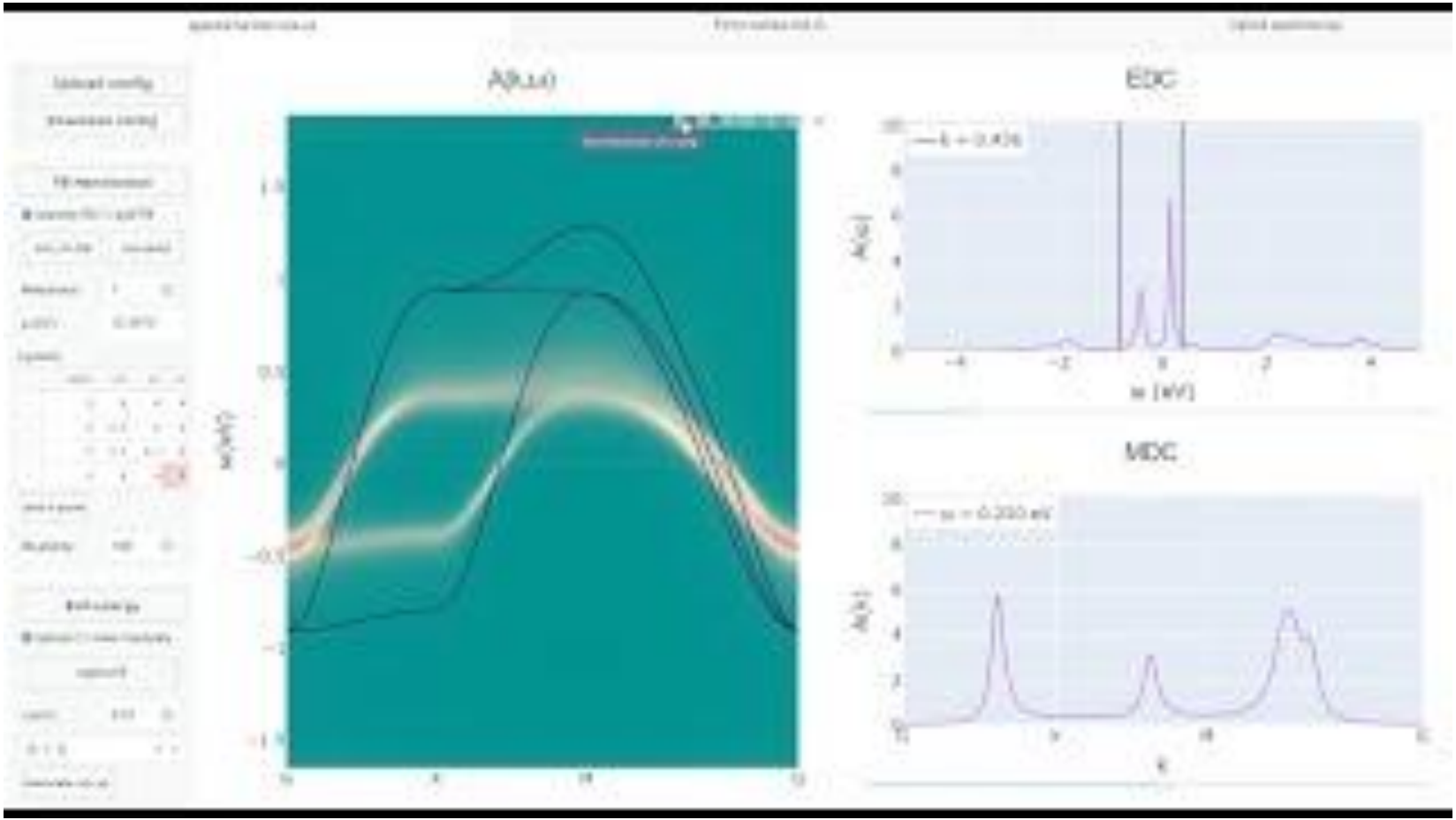
5. FermiSee demo



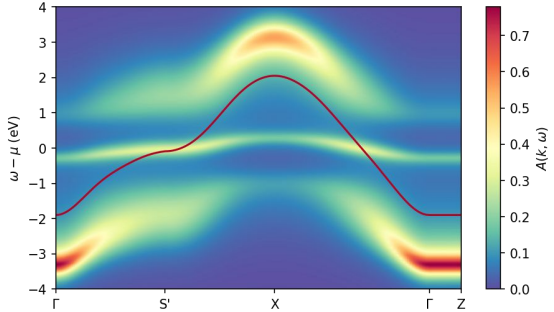
Summary

TRIQS

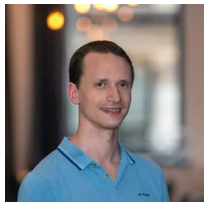
solid_dmft

A versatile python wrapper to perform DFT + DMFT calculations utilizing the TRIQS software library.

- TRIQS ecosystem to perform ab-initio simulations for correlated electron systems
- solid_dmft as flagship implementation for DFT+DMFT and embedding
- impurity solvers
- Analytic continuation packages
- FermiSee: webapp for data visualization



Acknowledgements:


N. Wentzell


S. Beck


O. Parcollet


A. Georges

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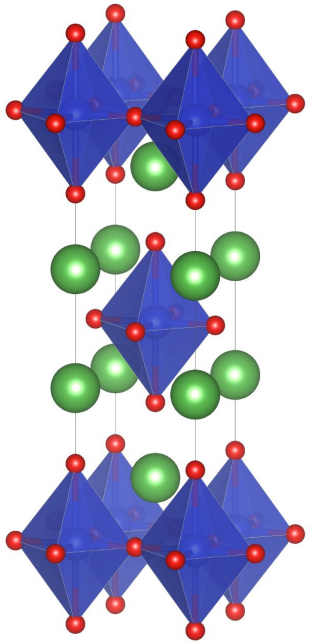
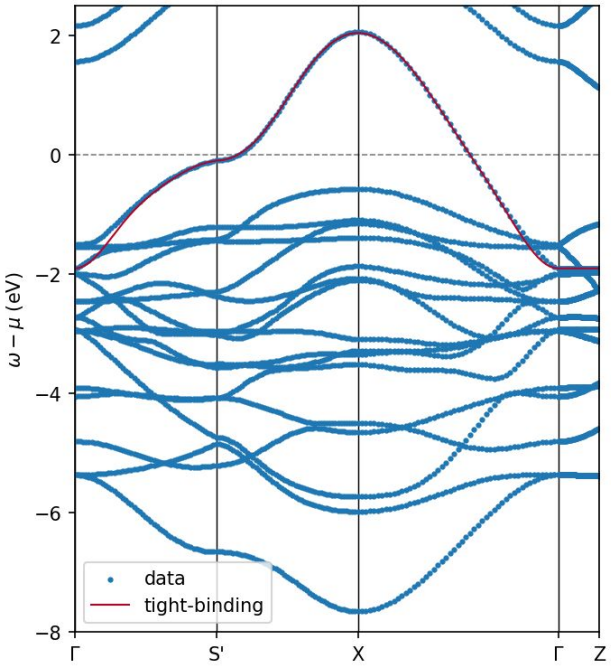
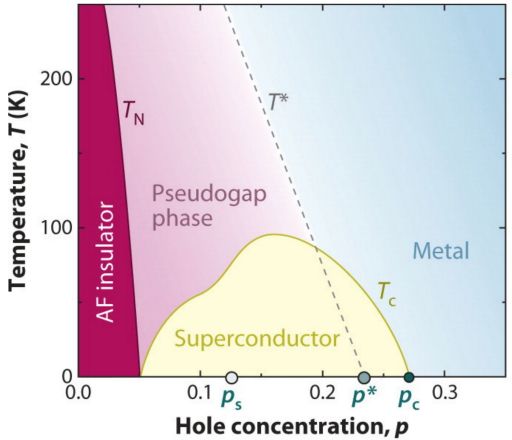
6. solid_dmft tutorial: Mott insulator La_2CuO_4





- simple 1-band model, 2D square-lattice sheets
- $1e^-$ per Cu atom, mainly d_{x2-y2} character



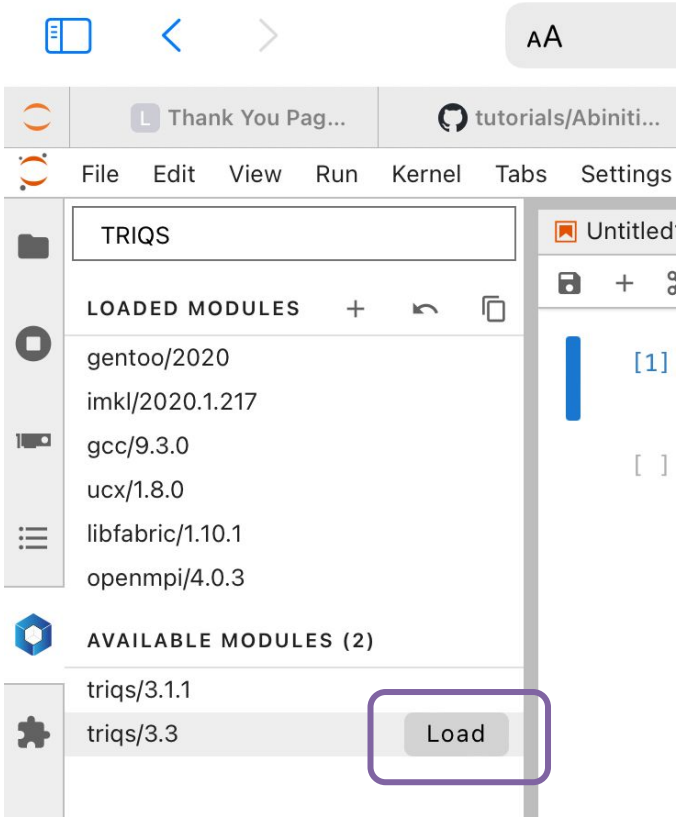
🎨 L. Taillefer, Ann. Rev. Condens. Matter Phys. 1, 51 (2010)

6. solid_dmft tutorial: Mott insulator La_2CuO_4

1. paramagnetic regime at $T \gg 2T_N = 325$ K using CTHyb
2. Mott insulating regime at $U \gg U_{MIT}$ using CTHyb
3. compare results obtained in 2. with Hubbard-I
4. use FermiSee to explore Fermi liquid parameters interactively

6. solid_dmft tutorial

- log in to: jupyter.quantum2024.ccs.usherbrooke.ca
- change number of cores to 4
- check that the jupyter kernel ist set to TRIQS 3.3 share
- on the left load the triqs/3.3 module ->
- If you are prompted to go to the terminal: click “New Launcher” -> open Other/Terminal
- use srun instead of mpirun



Job opportunities at CCQ

Intern program

- 10 weeks during summer
- undergrad - to 1st year graduate
- application in December - February

PreDoc program

- 4 months, twice annually
- 1st - 3rd year graduate
- application in September (now) for start in mid to late January 2023

PostDoc

- 2+1 years, start in September (with some flexibility)
- application starting in September (one year before)

https://www.simonsfoundation.org/flatiron/careers/?tab=job-openings&center=ccq
(bit.ly/3L3wJC1)

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Download your tutorials & TRIQS assignment

- to download your tutorials (all folders at once), open a new cell at execute:

```
%%bash
tar -czf archive.tar.gz ~/tutorials/*
```

- now you can download the created tar.gz file in your home dir via right-click
- TRIQS assignment due next week Friday, upload to:

  `/project/doc/triqs/assignment`

TRIQS tutorials feedback

We appreciate your feedback:
forms.gle/eHau3yfe3y8XVfMU8