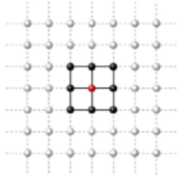
TRIQS

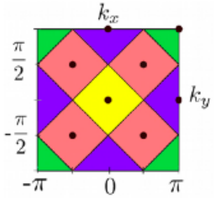
A Software Platform for Quantum Embedding

SIMONS FOUNDATION

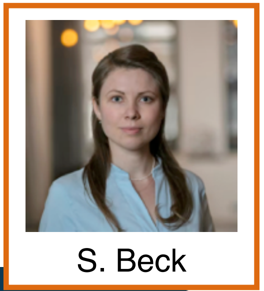
FLATIRON INSTITUTE
Center for Computational
Quantum Physics

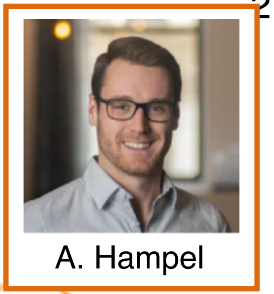


A. Georges



DMFT & Cluster Extensions


S. Beck


A. Hampel

Abinit

WANNIER90

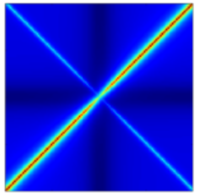
QUANTUMESPRESSO

DFT + DMFT

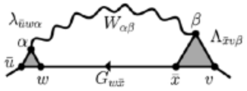
dft tools

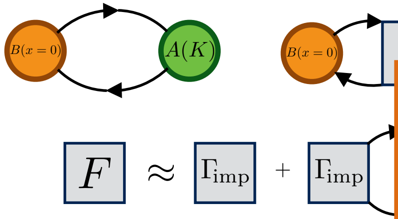
solid dmft

TRIQS



Vertex Methods





H. Strand

Impurity Solvers

ED

CTQMC

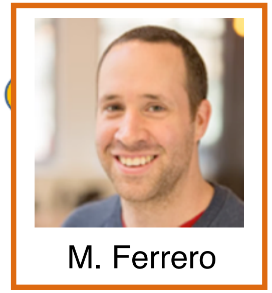
NRG

DMRG

DiagMC

PT

Non-Equilibrium


M. Ferrero

O. Parcollet et al. CPC ’15 ~ 420 Citations

TRIQS Library

- TRIQS - A **T**oolbox for **R**esearch on **I**nteracting **Q**uantum **S**ystems
  - TRIQS Library — Fundamental Building Blocks
  - Applications based on the TRIQS Library
- Open source (GPLv3 and Apache 2).
- High-level Interface in Python 3
- Low-level Backend in Modern C++

triqs.github.io

Releases 12

Version 3.1.1 Latest

O. Parcollet

A. Hampel

H. Strand

D. Kiese

P. Dumitrescu

J. Kaye

M. Ferrero

I. Krivenko

T. Ayral

D. Simon

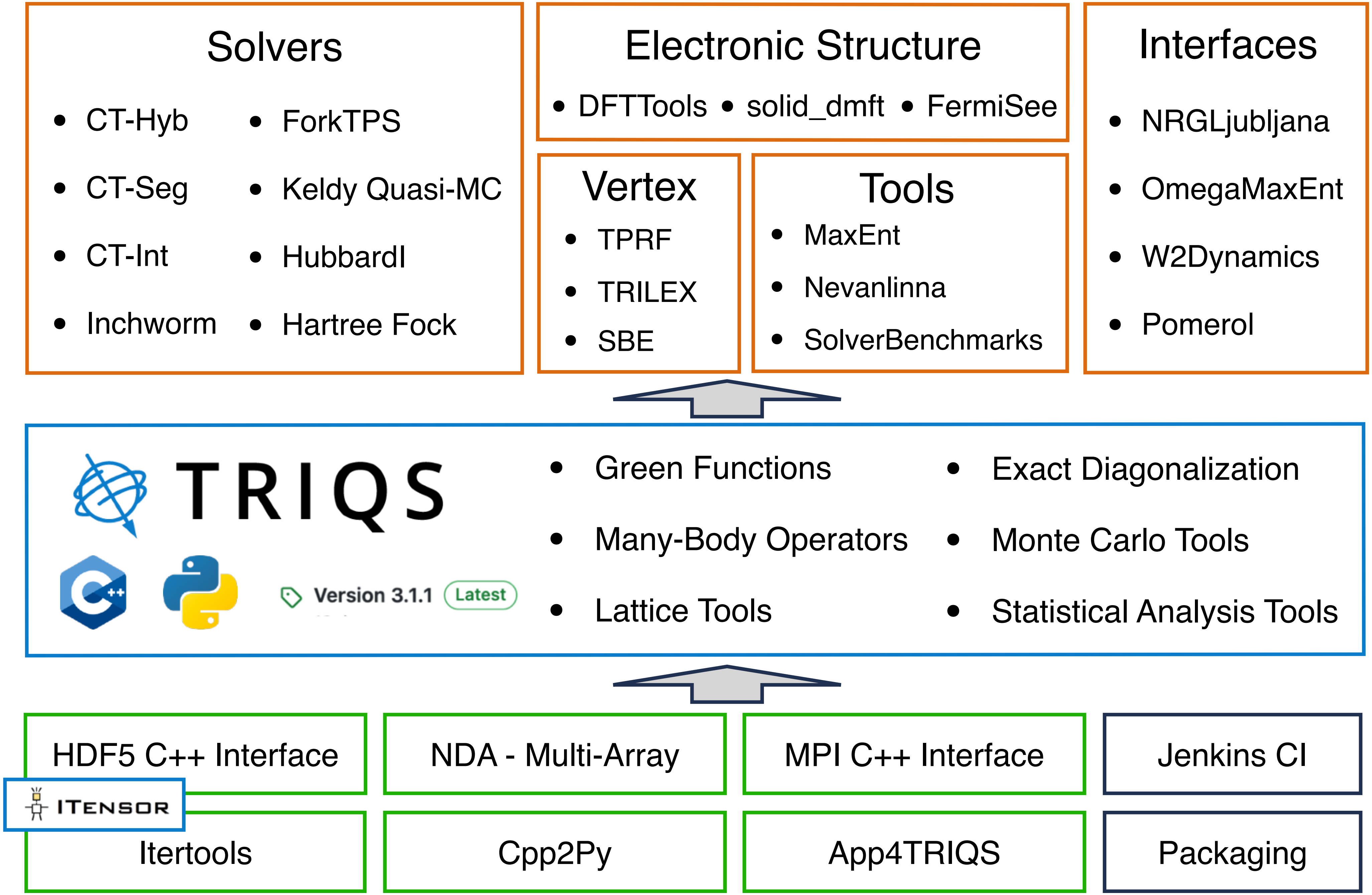
M. Zingl

A. Moutenet

S. Beck

O. Parcollet et al. CPC ’15 ~ 430 Citations

TRIQS — Software Stack



Solvers

- CT-Hyb
- CT-Seg
- CT-Int
- Inchworm
- ForkTPS
- Keldy Quasi-MC
- HubbardI
- Hartree Fock

Electronic Structure

- DFTTools
- solid_dmft
- FermiSee

Vertex

- TPRF
- TRILEX
- SBE

Tools

- MaxEnt
- Nevanlinna
- SolverBenchmarks

Interfaces

- NRGLjubljana
- OmegaMaxEnt
- W2Dynamics
- Pomerol

TRIQS

Version 3.1.1 Latest

- Green Functions
- Many-Body Operators
- Lattice Tools
- Exact Diagonalization
- Monte Carlo Tools
- Statistical Analysis Tools

HDF5 C++ Interface

NDA - Multi-Array

MPI C++ Interface

Jenkins CI

ITENSOR

Itertools

Cpp2Py

App4TRIQS

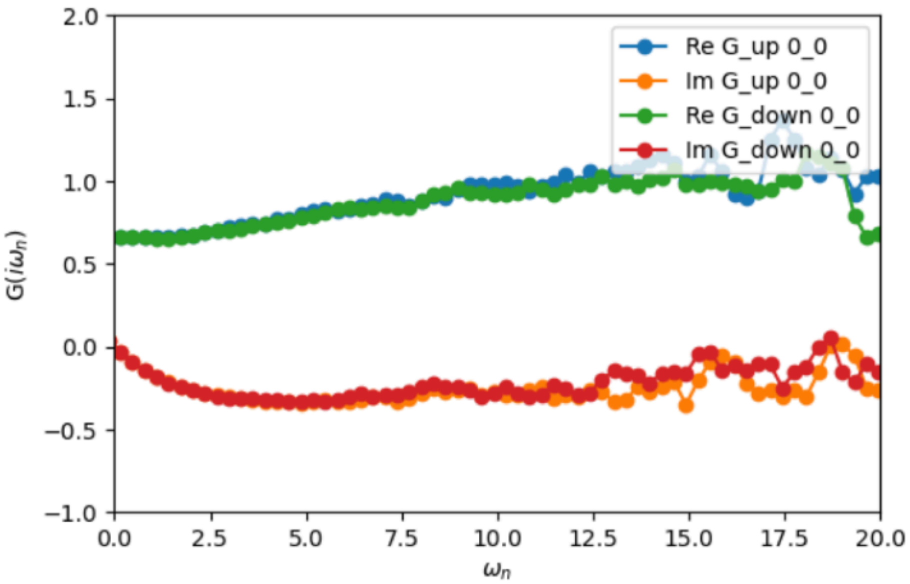
Packaging

TRIQS Applications — CT-Hyb QMC

triqs.github.io/cthyb

- Quantum Impurity Solver
- Hybridization Expansion
- Generic Multi-band/orbital Interactions
- Complex Interactions $\sum_{ijkl}\sum_{\sigma\sigma'} U^{\sigma\sigma'}_{ijkl} c^\dagger_{\sigma i} c^\dagger_{\sigma' j} c_{\sigma' k} c_{\sigma l}$

What can we measure?
$\langle \mathcal{T} c_{\sigma i}(\tau) c^\dagger_{\sigma j}\rangle$
$\langle \mathcal{T} c^\dagger_{\sigma i}(i\omega) c_{\sigma j}(i\omega') c^\dagger_{\sigma' k}(i\omega'') c_{\sigma' l}(0)\rangle$
$\langle \mathcal{T} A(\tau) B(0)\rangle$



P. Seth

I. Krivenko

M. Ferrero

H. Strand

O. Parcollet

A. Hampel

H. LaBollita

TRIQS Applications — Connection to Electronic Structure

- DFT Tools — Toolbox for Ab-Initio Calculations of Correlated Materials

  triqs.github.io/dft_tools

  M. Aichhorn et al. CPC '16 ~ 140 Citations

A. Hampel

S. Beck

M. Aichhorn

L. Pourovskii

V. Vildosola

O. Peil

M. Zingl

M. Ferrero

G. Kraberger

J. Karp

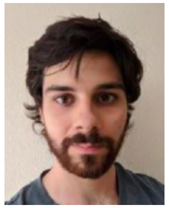
solid_dmft

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

triqs.github.io/solid_dmft/

M. Merkel et al. JoSS '22

A. Hampel


A. Carta

S. Beck

M. Merkel

TRIQS Applications — Vertex Calculations

- TPRF — The Two-particle Response Function Tool Box

  triqs.github.io/tprf

H. Strand

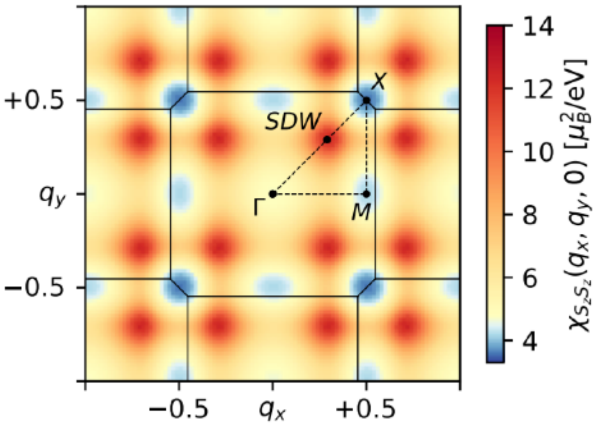
Y. in’t Veld

M. Rösner

S. Kaeser

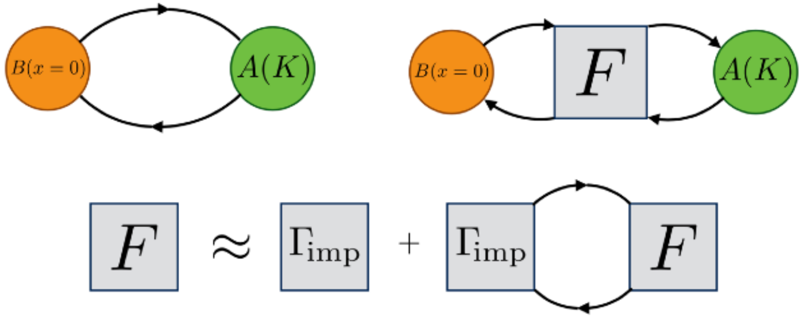
P. Hansmann

E. van Loon



H. Strand et al. PRB ’19

- Lindhard Susceptibilities
- Random-phase Approximation
- GW Approximation
- Generalized Susceptibilities
- Bethe-Salpeter Equation Solver
- Vertex-Corrected Lattice Susceptibilities



TRIQS — Packaging

triqs.github.io/triqs/latest/install.html

- Anaconda

```
conda install -c conda-forge triqs
```

Versions 3.2
Soon!

- Debian Packages for Ubuntu 20.04 and 22.04

```
apt-get install triqs
```

- Binder Notebook triqs.github.io/notebook

- Docker Image

```
docker pull flatironinstitute/triqs
docker run -p 8888:8888 flatironinstitute/triqs
```

- Singularity

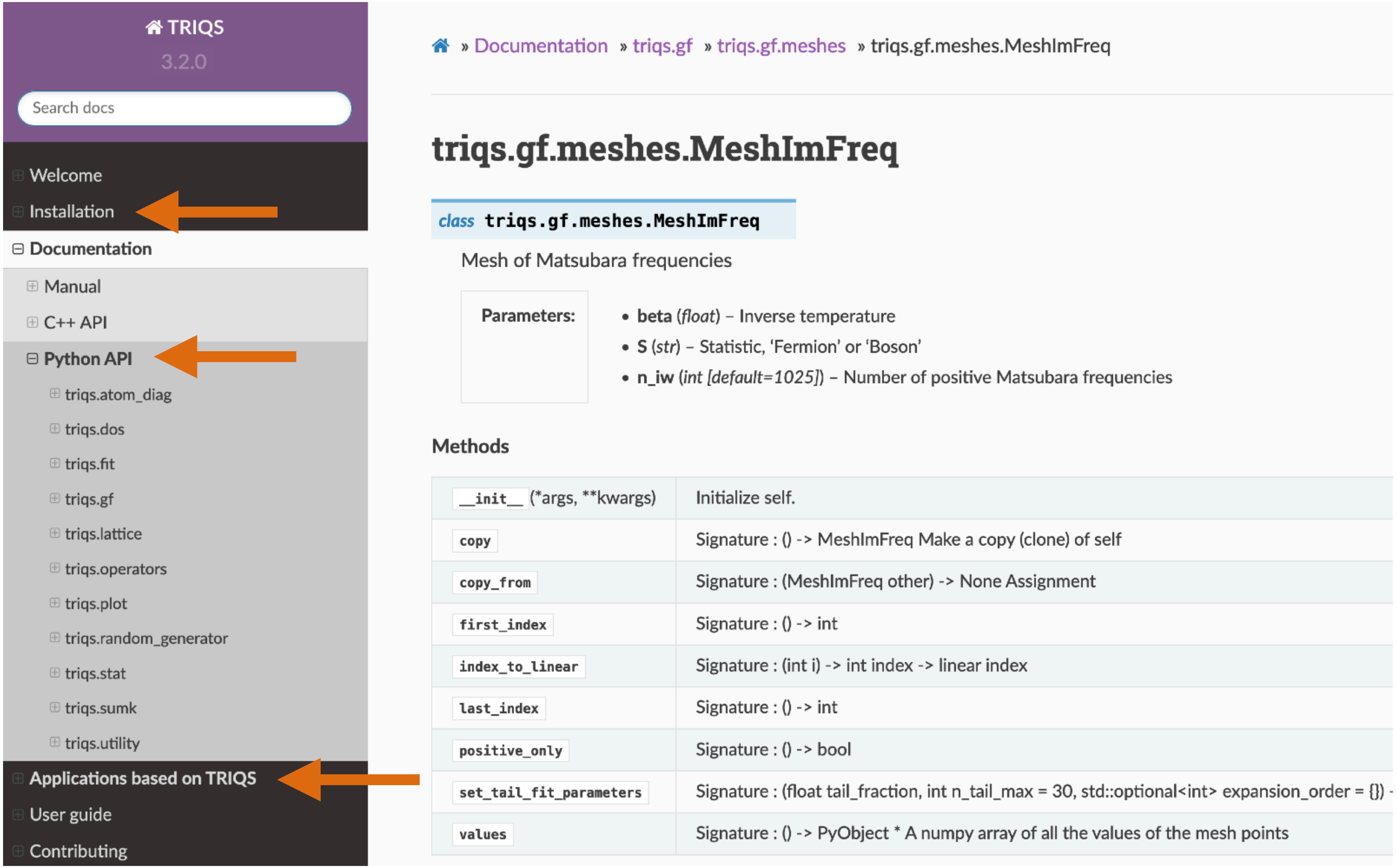
```
singularity pull docker://flatironinstitute/triqs
singularity exec triqs.sif python myscript.py
```

- EasyBuild

```
eb -r --software-name=TRIQS
```

TRIQS Documentation

triqs.github.io/triqs/3.2.x



» Documentation » triqs.gf » triqs.gf.meshes » triqs.gf.meshes.MeshImFreq

triqs.gf.meshes.MeshImFreq

class `triqs.gf.meshes.MeshImFreq`

Mesh of Matsubara frequencies

Parameters:

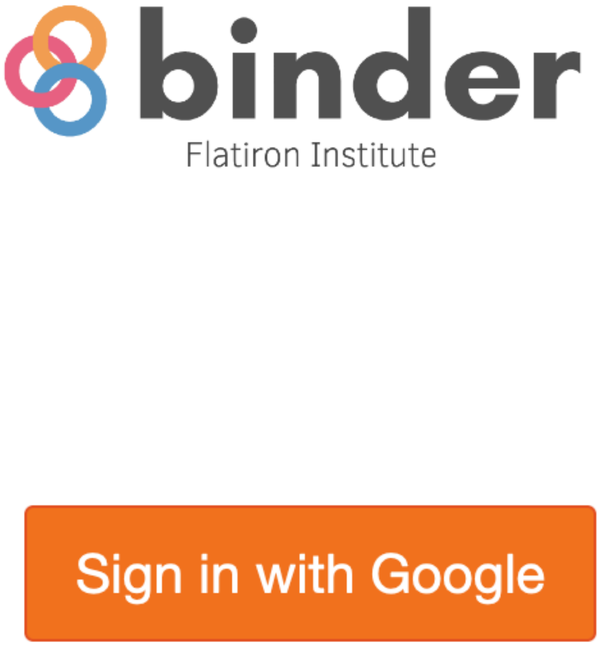
- **beta** (*float*) – Inverse temperature
- **S** (*str*) – Statistic, 'Fermion' or 'Boson'
- **n_iw** (*int [default=1025]*) – Number of positive Matsubara frequencies

Methods

`__init__`(*args, **kwargs)	Initialize self.
`copy`	Signature : () -> MeshImFreq Make a copy (clone) of self
`copy_from`	Signature : (MeshImFreq other) -> None Assignment
`first_index`	Signature : () -> int
`index_to_linear`	Signature : (int i) -> int index -> linear index
`last_index`	Signature : () -> int
`positive_only`	Signature : () -> bool
`set_tail_fit_parameters`	Signature : (float tail_fraction, int n_tail_max = 30, std::optional<int> expansion_order = {}) -
`values`	Signature : () -> PyObject * A numpy array of all the values of the mesh points

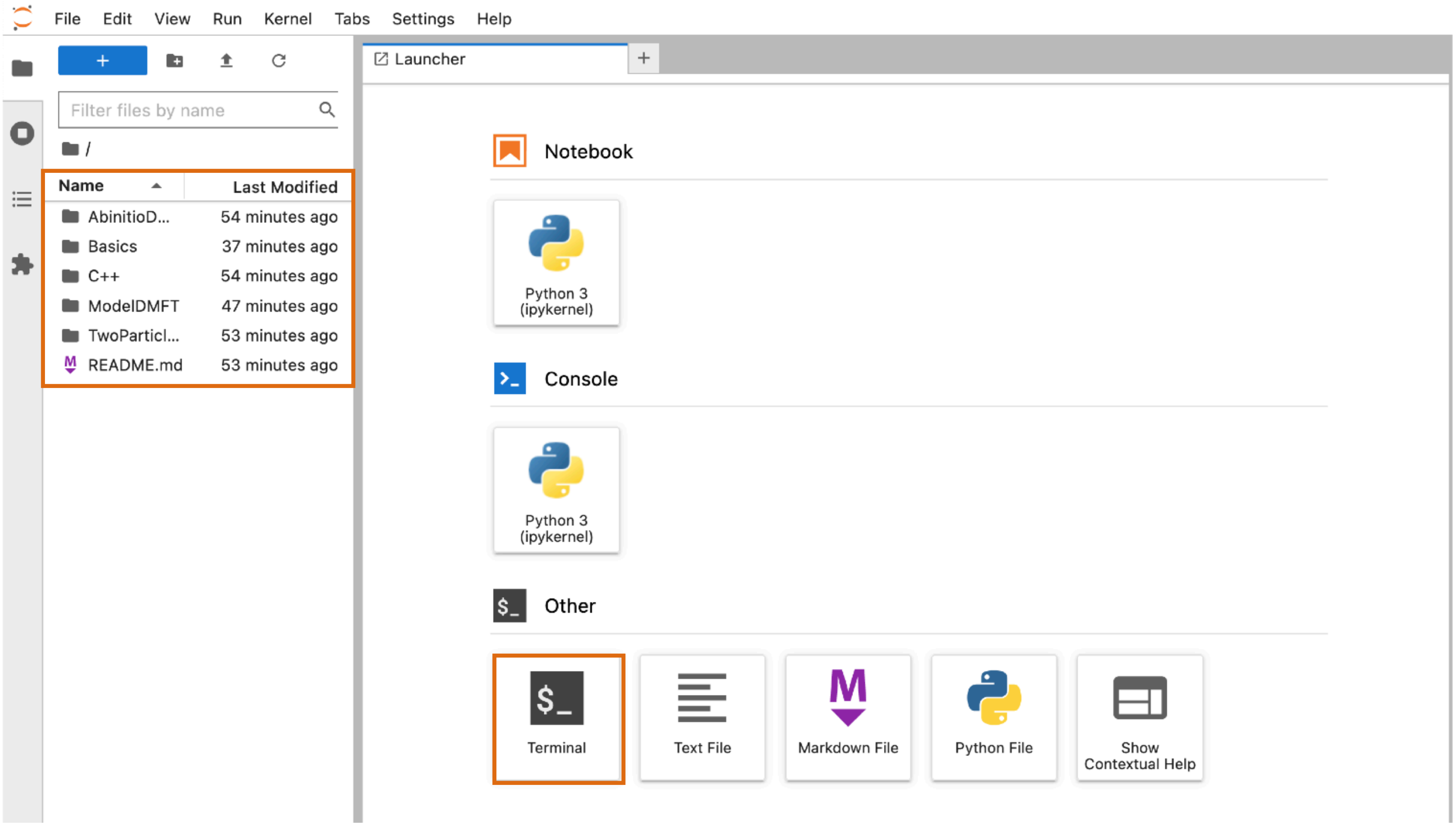
TRIQS — Getting Started

sdsc-binder.flatironinstitute.org



TRIQS — Getting Started

sdsc-binder.flatironinstitute.org



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AbinitioD...	54 minutes ago
Basics	37 minutes ago
C++	54 minutes ago
ModelDMFT	47 minutes ago
TwoParticl...	53 minutes ago
README.md	53 minutes ago

TRIQS — Getting Started

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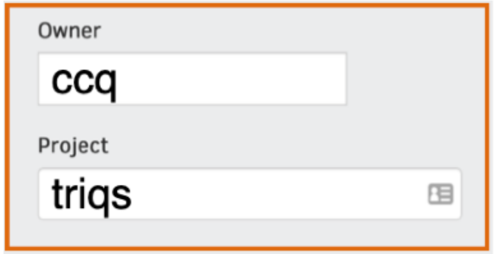
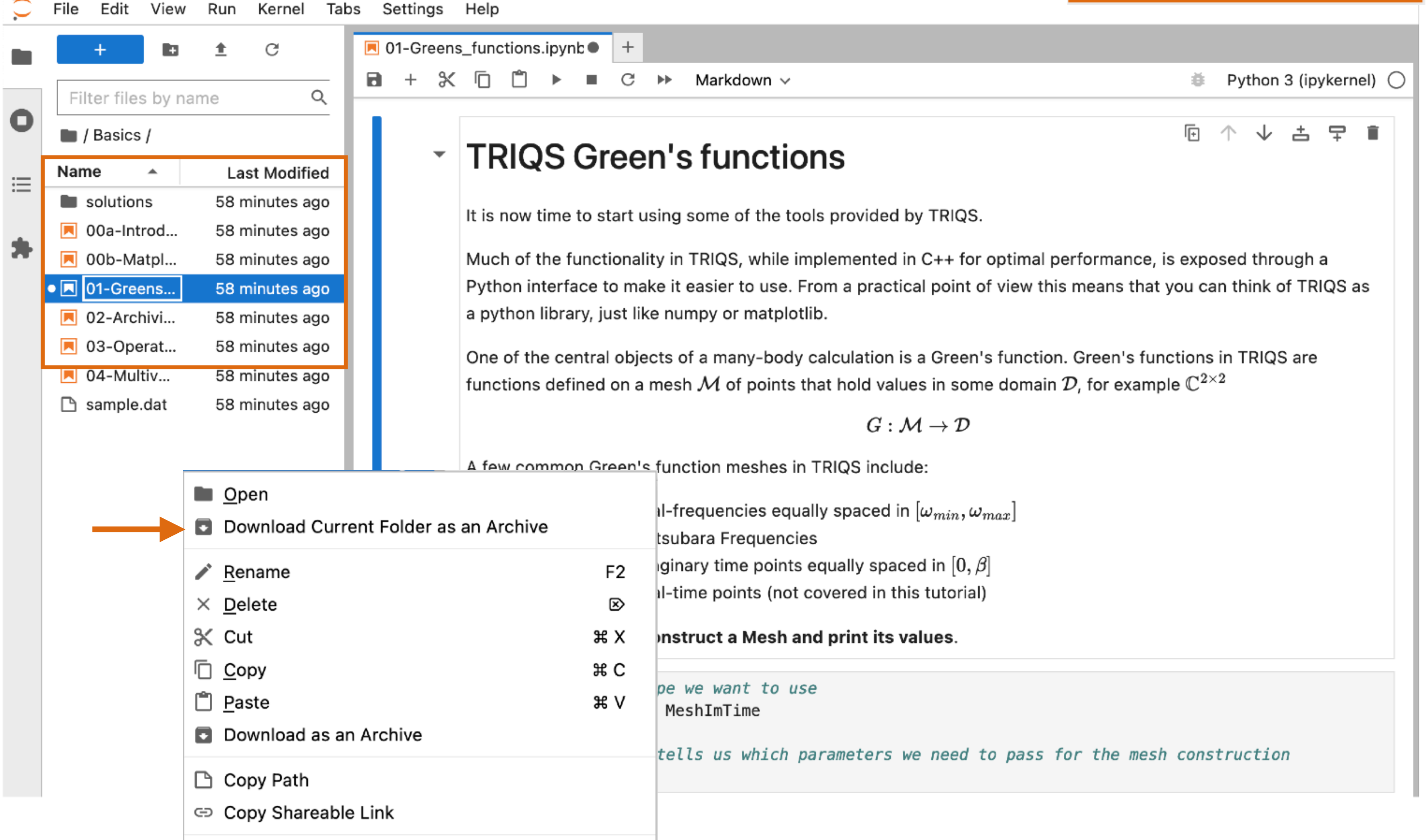


Owner
ccq

Project
triqs



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00b-Matpl...	58 minutes ago
01-Greens...	58 minutes ago
02-Archivi...	58 minutes ago
03-Operat...	58 minutes ago
04-Multiv...	58 minutes ago
sample.dat	58 minutes ago

TRIQS Green's functions

It is now time to start using some of the tools provided by TRIQS.

Much of the functionality in TRIQS, while implemented in C++ for optimal performance, is exposed through a Python interface to make it easier to use. From a practical point of view this means that you can think of TRIQS as a python library, just like numpy or matplotlib.

One of the central objects of a many-body calculation is a Green's function. Green's functions in TRIQS are functions defined on a mesh $\mathcal{M}$ of points that hold values in some domain $\mathcal{D}$, for example $\mathbb{C}^{2\times 2}$

$$G : \mathcal{M} \to \mathcal{D}$$

A few common Green's function meshes in TRIQS include:

l-frequencies equally spaced in $[\omega_{min}, \omega_{max}]$
tsubara Frequencies
ginary time points equally spaced in $[0, \beta]$
l-time points (not covered in this tutorial)

nstruct a Mesh and print its values.

```
pe we want to use
 MeshImTime

tells us which parameters we need to pass for the mesh construction
```