Ab-initio Description of Strongly-Correlated Materials

Basics of DFT+DMFT

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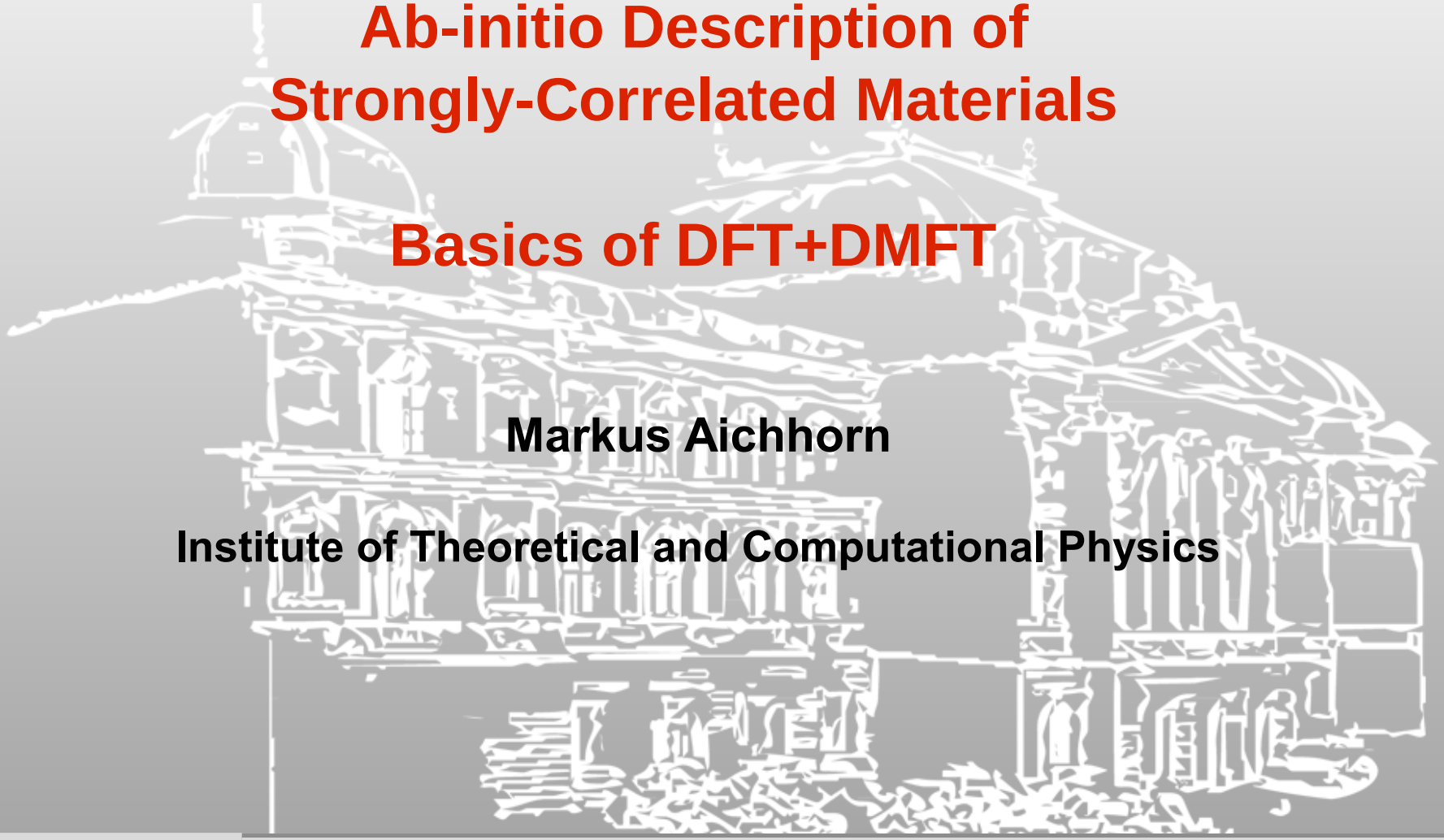
Institute of Theoretical and Computational Physics



The standard model: Density Functional Theory (DFT)

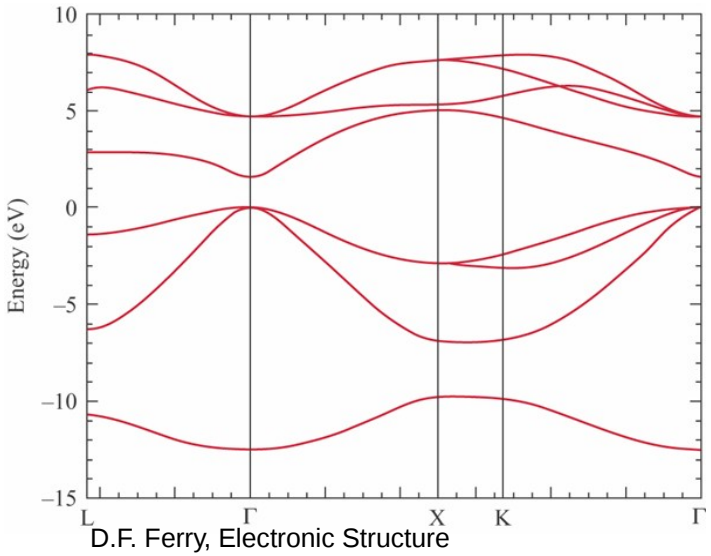
Walter Kohn
Nobel prize 98

„Ground state density determines all ground state properties“

No need for the wave function → tremendous advantage

Minimisation of energy functional $E = E[\rho]$ determines ρ_0

→ Kohn Sham equation / bands



D.F. Ferry, Electronic Structure

GaAs band structure:

Empty conduction bands

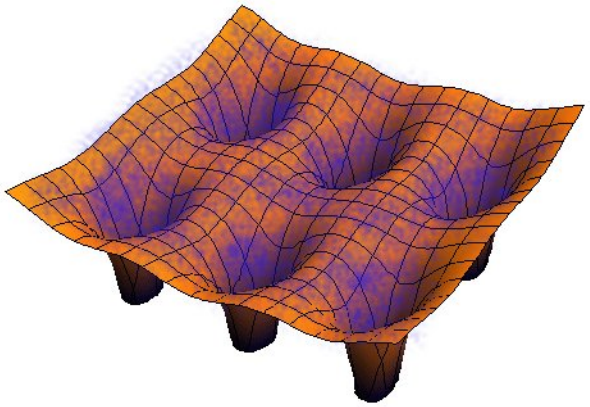
Filled valence bands

→ Semiconductor (Band Insulator)

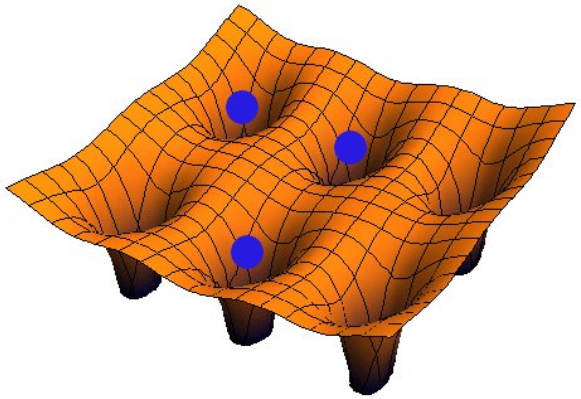
Nice agreement with real life

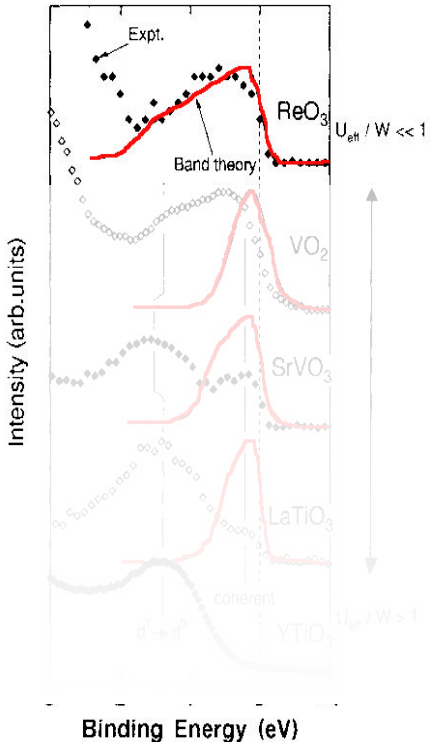
Electronic correlations

Band Theory



Localisation





Metal

Insulator

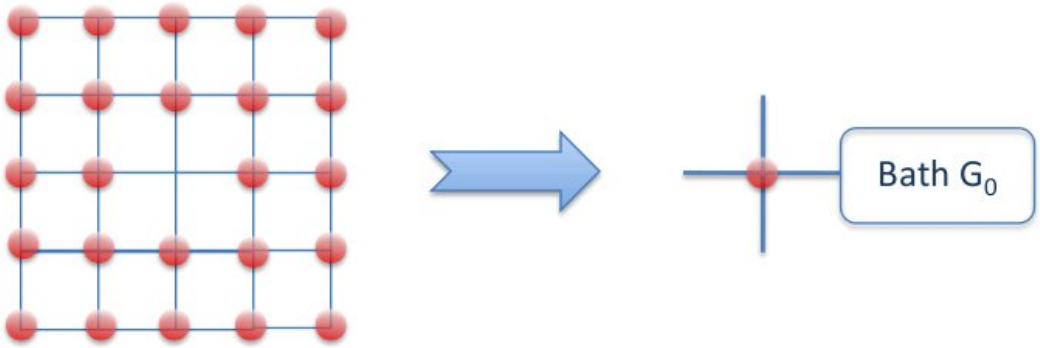
Fujimori, PRL 69, 1796 (1992)

Standard Band Theory fails!

Local Correlations: Dynamical Mean-Field Theory

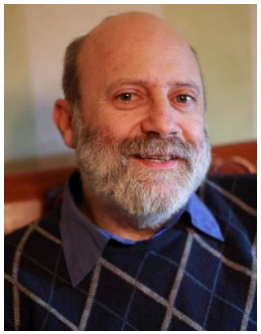
Antoine Georges

Replace full system by single atom in effective bath



crystal

effective Anderson impurity model



Gabi Kotliar

Atomic physics (local quantum fluctuations) is treated exactly

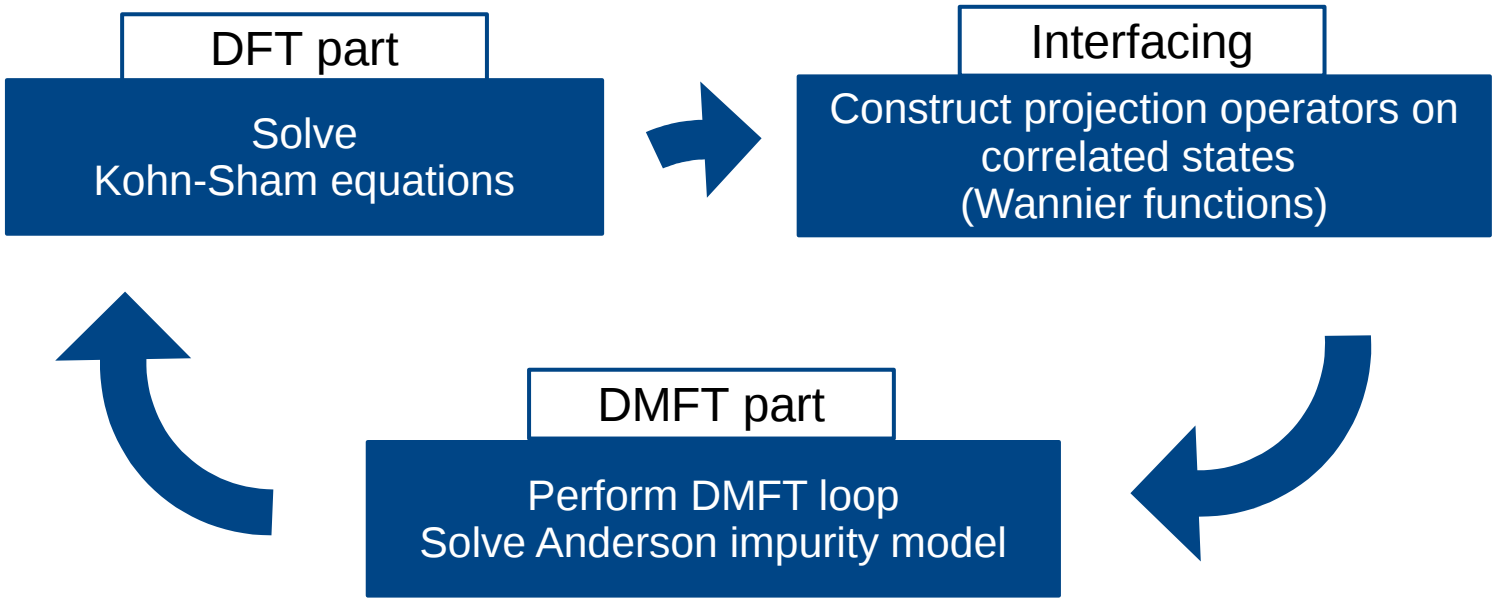
Mean-field approach: Effective bath determined self-consistently

Describes Mott metal-to-insulator transitions

A. Georges *et al.*, RMP 1996

Ab initio description: DFT + DMFT

Combine band theory (DFT) and include local atomic correlations (DMFT)



Self consistent implementation in Wien2K:

Projective Technique: M. Aichhorn et al., PRB 80, 085101 (2009)

Charge self consistency: M. Aichhorn et al., PRB 84, 054529 (2011)

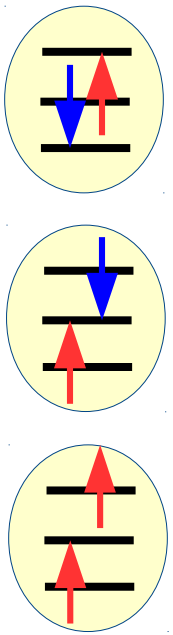
Lichtenstein *et al.* 1998; Anisimov *et al.* 1997, G. Kotliar et al., RMP 2006

Multiorbital atomic physics matters

Band theory: Electrons are waves $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$

Mott Insulator: Electrons localize!

→ Atomic structure becomes important!



$$U \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow}$$

$$U' \sum_{\alpha \neq \beta} n_{\alpha\uparrow} n_{\beta\downarrow}$$

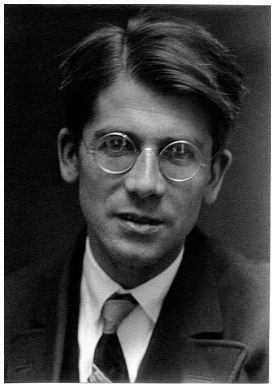
$$(U' - J) \sum_{\alpha \neq \beta} n_{\alpha\uparrow} n_{\beta\uparrow}$$

Atomic Hamiltonian

describes local physics

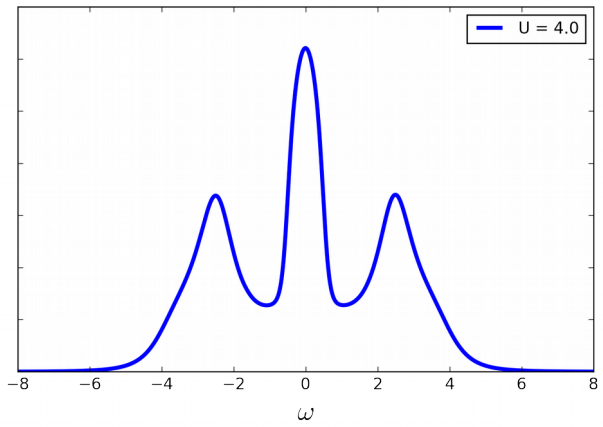
Important ingredient:

Hund's rule coupling

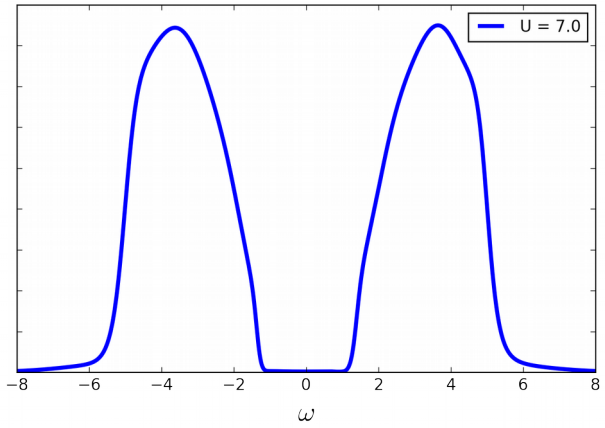


Friedrich Hund

Local Correlations: Dynamical Mean-Field Theory

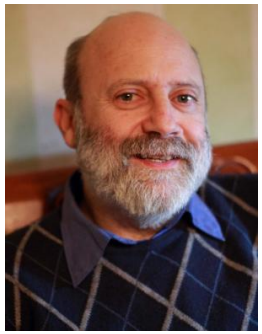


Correlated metal



Insulator

Antoine Georges

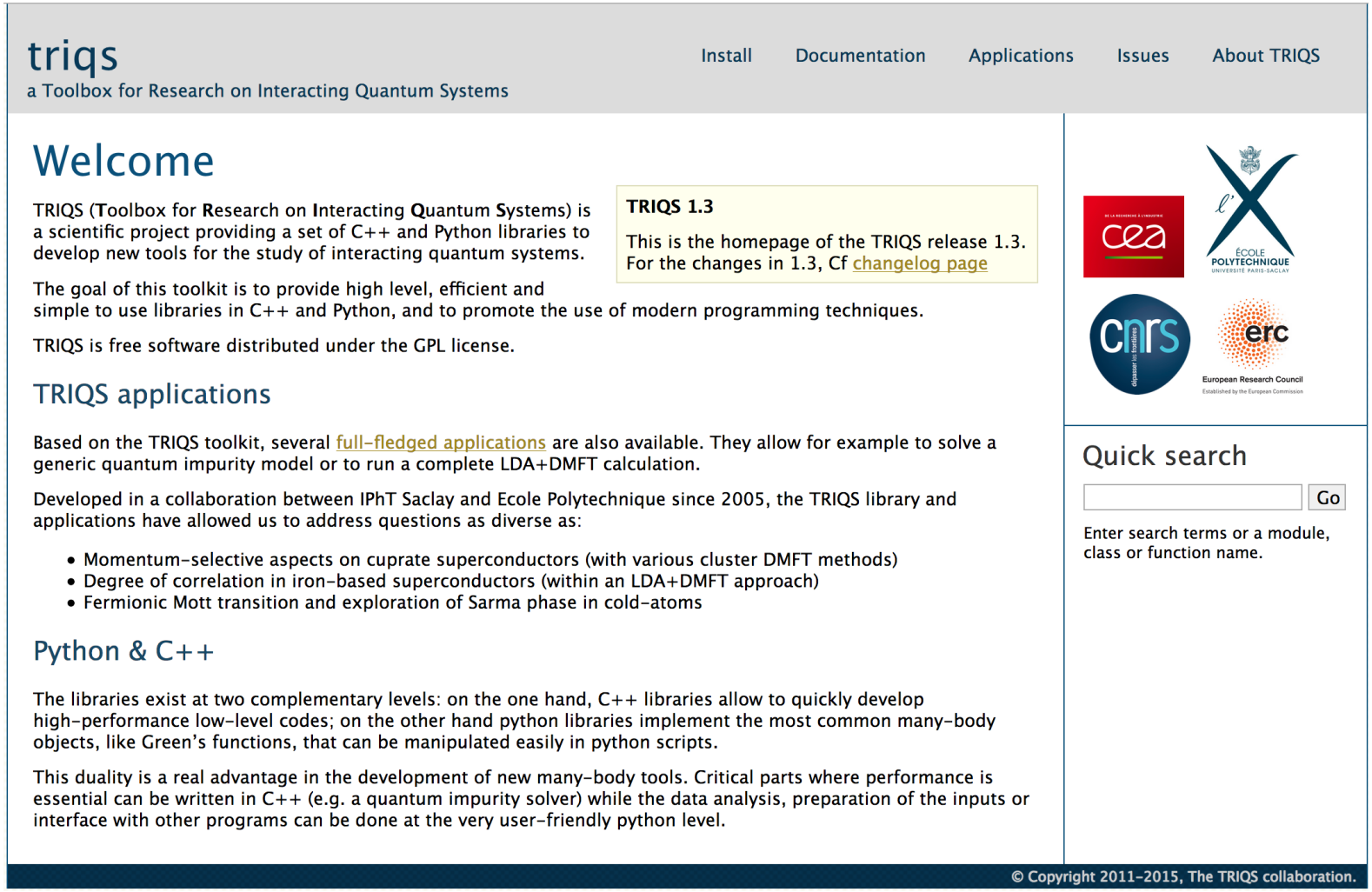


Gabi Kotliar

DMFT solution for the single-orbital Hubbard model

Exact Limiting cases:
- Noninteracting Electrons
- Atomic limit
- Infinite dimension / coordination

A. Georges *et al.*, RMP 1996



triqs
a Toolbox for Research on Interacting Quantum Systems

Install Documentation Applications Issues About TRIQS

Welcome

TRIQS (**T**oolbox for **R**esearch on **I**nteracting **Q**uantum **S**ystems) is a scientific project providing a set of C++ and Python libraries to develop new tools for the study of interacting quantum systems.

TRIQS 1.3

This is the homepage of the TRIQS release 1.3.
For the changes in 1.3, Cf changelog page

The goal of this toolkit is to provide high level, efficient and simple to use libraries in C++ and Python, and to promote the use of modern programming techniques.

TRIQS is free software distributed under the GPL license.

TRIQS applications

Based on the TRIQS toolkit, several full-fledged applications are also available. They allow for example to solve a generic quantum impurity model or to run a complete LDA+DMFT calculation.

Developed in a collaboration between IPhT Saclay and Ecole Polytechnique since 2005, the TRIQS library and applications have allowed us to address questions as diverse as:

- Momentum-selective aspects on cuprate superconductors (with various cluster DMFT methods)
- Degree of correlation in iron-based superconductors (within an LDA+DMFT approach)
- Fermionic Mott transition and exploration of Sarma phase in cold-atoms

Python & C++

The libraries exist at two complementary levels: on the one hand, C++ libraries allow to quickly develop high-performance low-level codes; on the other hand python libraries implement the most common many-body objects, like Green's functions, that can be manipulated easily in python scripts.

This duality is a real advantage in the development of new many-body tools. Critical parts where performance is essential can be written in C++ (e.g. a quantum impurity solver) while the data analysis, preparation of the inputs or interface with other programs can be done at the very user-friendly python level.

Quick search
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M. Aichhorn *et al.*, CPC 204, 200–208 (2016)
O. Parcollet *et al.*, CPC 196, 398–415 (2015)