Tutorial on
QSGW+DMFT:
Spin fluctuations in Ni

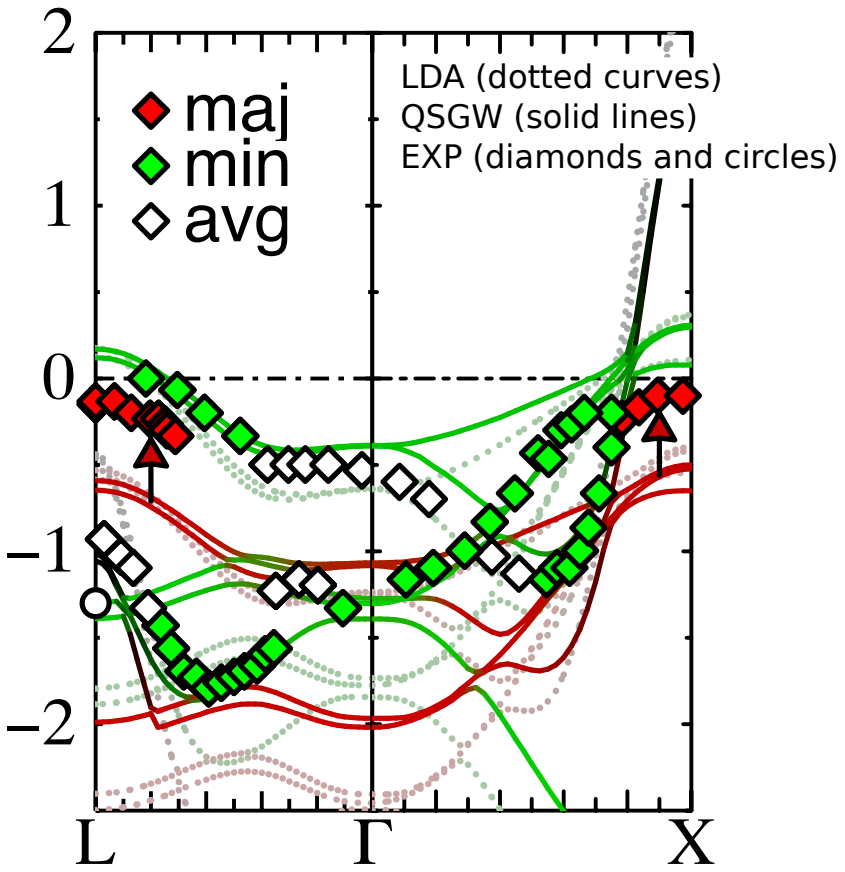
Lorenzo Sponza

Elemental Ni: an itinerant magnet

ΔE_x: exchange splitting: band shift between the two spin channels
M: magnetic moment: difference between occupation of the two spin channels

	M (Bhor)	ΔE_x @ L (eV)
LSDA	0.62	0.71
QS*GW*	0.75	0.77
Experiment	0.57	0.31

LSDA: reasonable M bad ΔE_x
QSGW: worse M worse ΔE_x



L.S., P. Pisanti, A. Vishina, D. Pashov, C. Weber, M. van Schilfgaarde, S. Acharya and G. Kotliar, Phys. Rev. B **95**, 041112(R) (2017)

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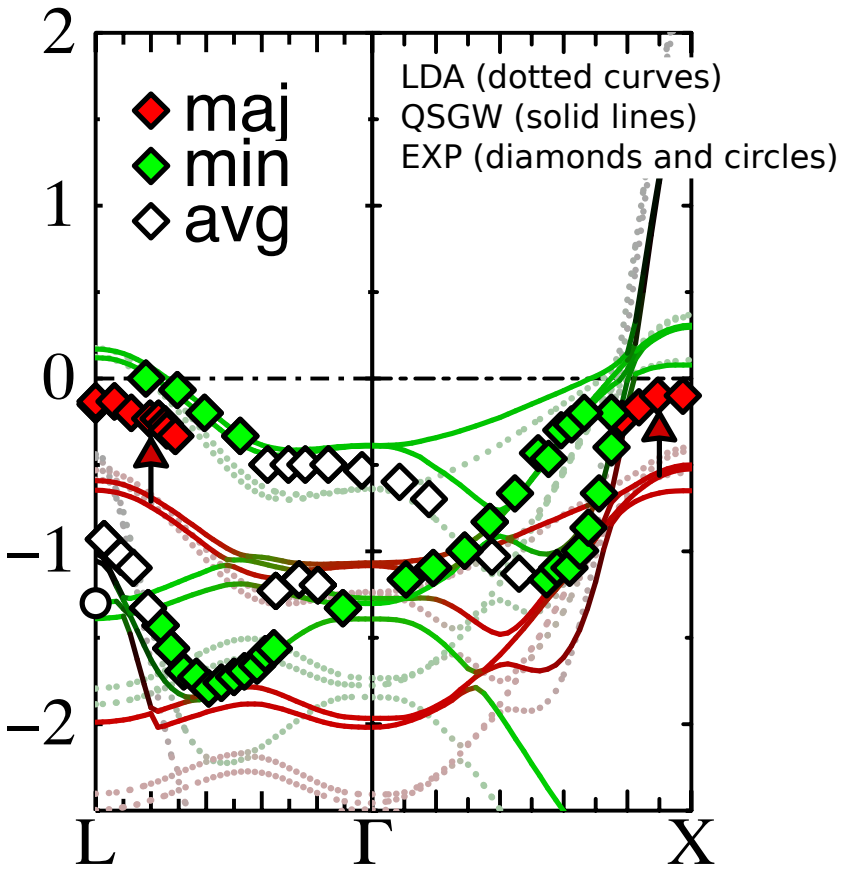
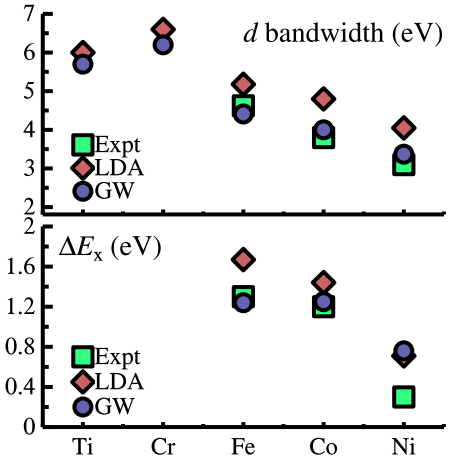
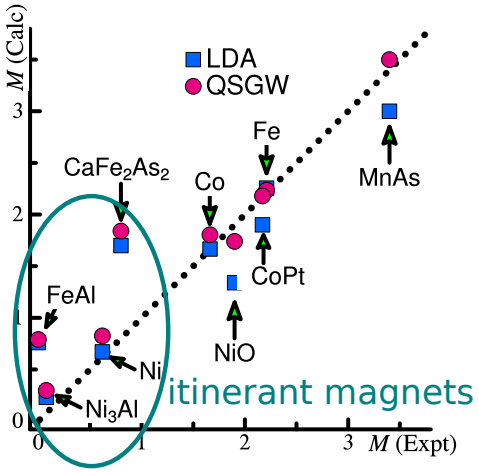


What happens?





M and ΔE_x are overestimated in itinerant magnets (QSGW and LDA)
because of the **absence of spin fluctuations**

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Elemental Ni: an itinerant magnet

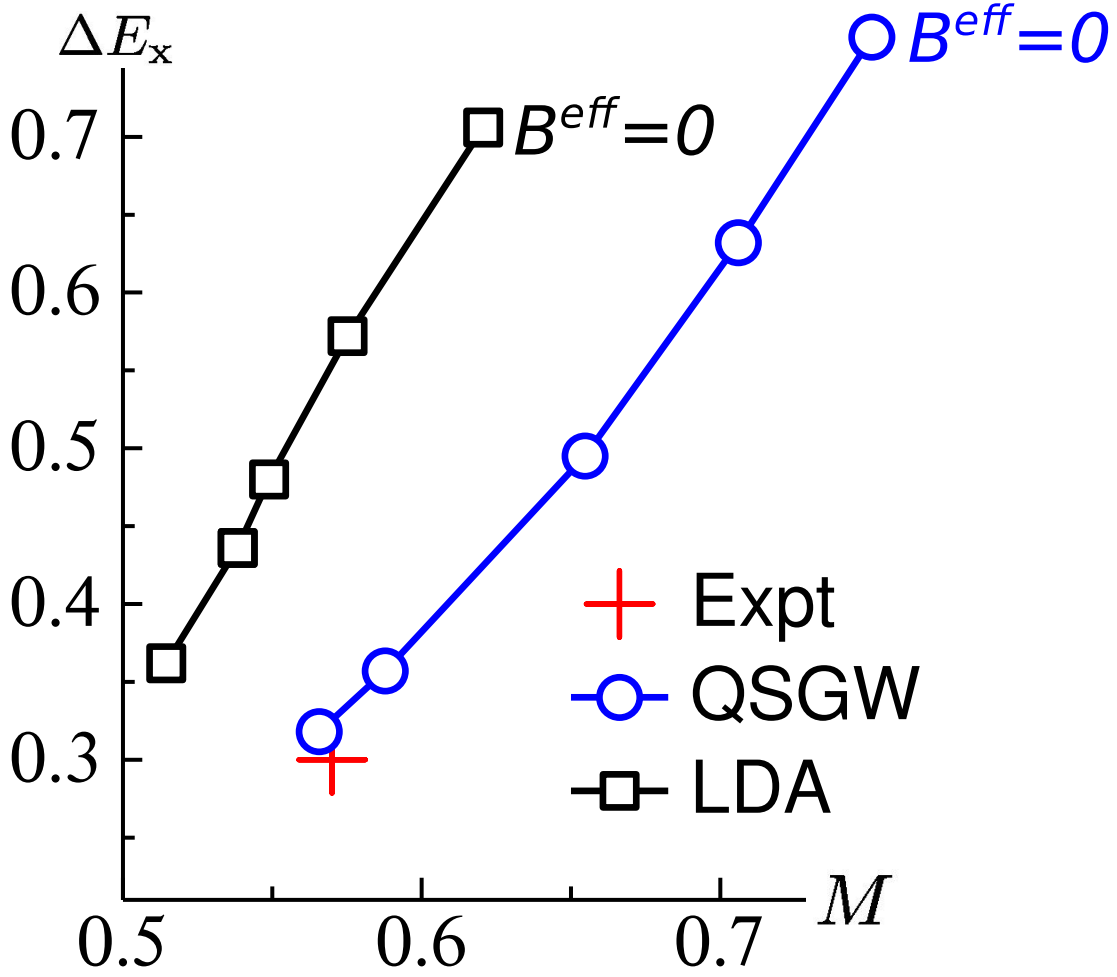
Include spin fluctuations through a **tunable external magnetic field** B^{eff}
B^{eff} is adjusted in order to reproduce the experimental *M*.

LDA + B^{eff}
No way to have good both ΔE_x and M

QSGW+B^{eff}
The B^{eff} giving the right M
gives also the right ΔE_x

	M (Bhor)	ΔE_x @ L (eV)
LSDA	0.62	0.71
QS*GW*	0.75	0.77
QS*GW*+B^{eff}	0.57	0.32
Experiment	0.57	0.31

Higher **internal consistency**
of the QSGW theory



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QSGW+B^{eff}
The B^{eff} g
gives als

Can we do this in a more ab-initio way?
Can we rely only on internal parameters?

...Let's give a try to QSGW+DMFT!

LSDA		
QSGW		
QSGW+B^{eff}	0.57	0.32
Experiment	0.57	0.31

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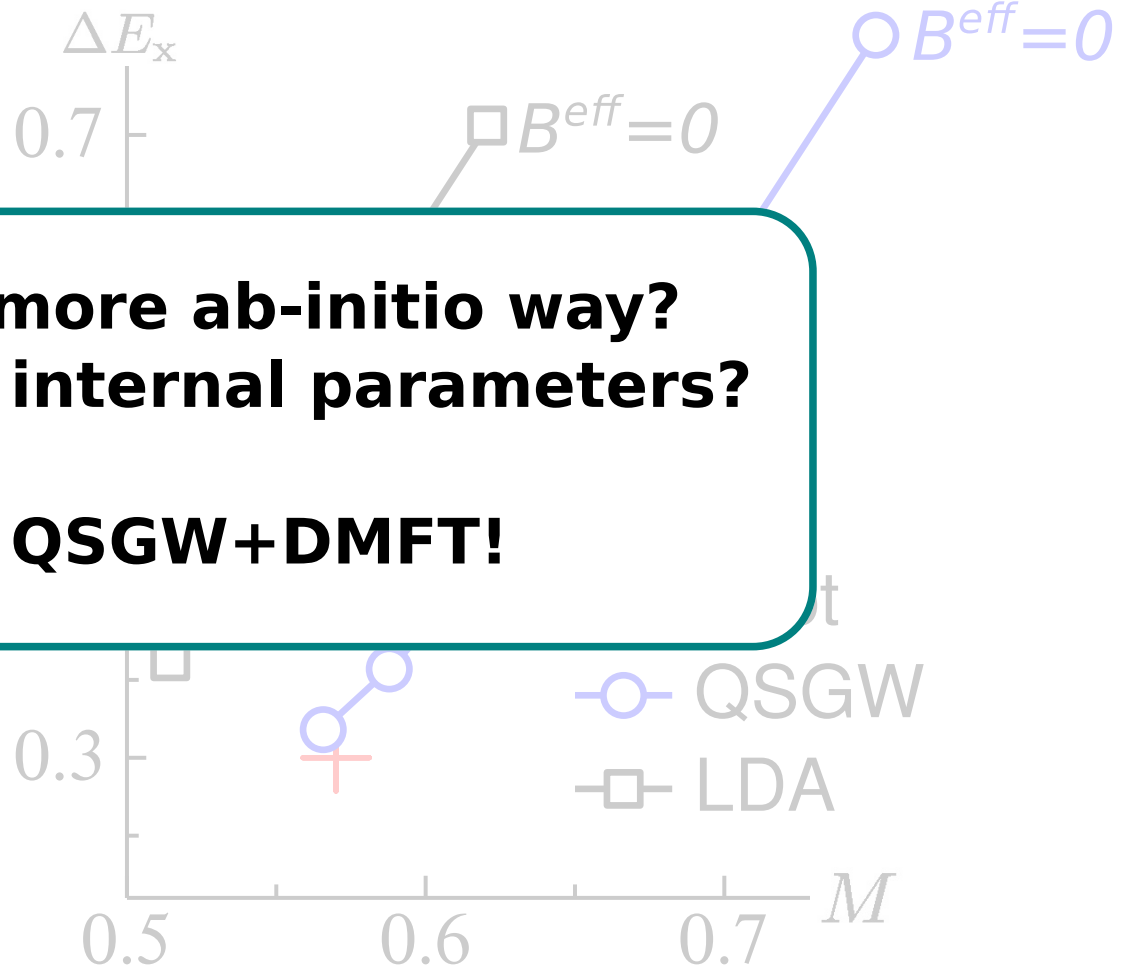

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Structure of the tutorial/hands-on session

Follow tutorials from page:

Programme of today

- Tutorial N.1: set up of the QSGW+DMFT loop
- Tutorial N.2: the DMFT loop
- Tutorial N.5: Updating the density (QSGW loop)

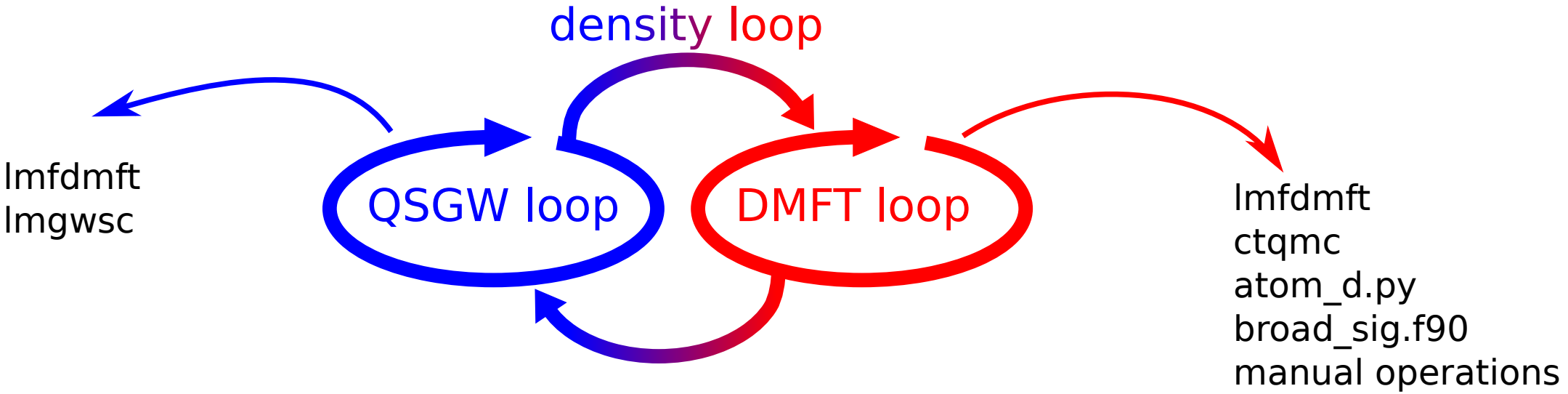
See also

- Tutorial N.3: Setting parameters of CTQMC

Optional

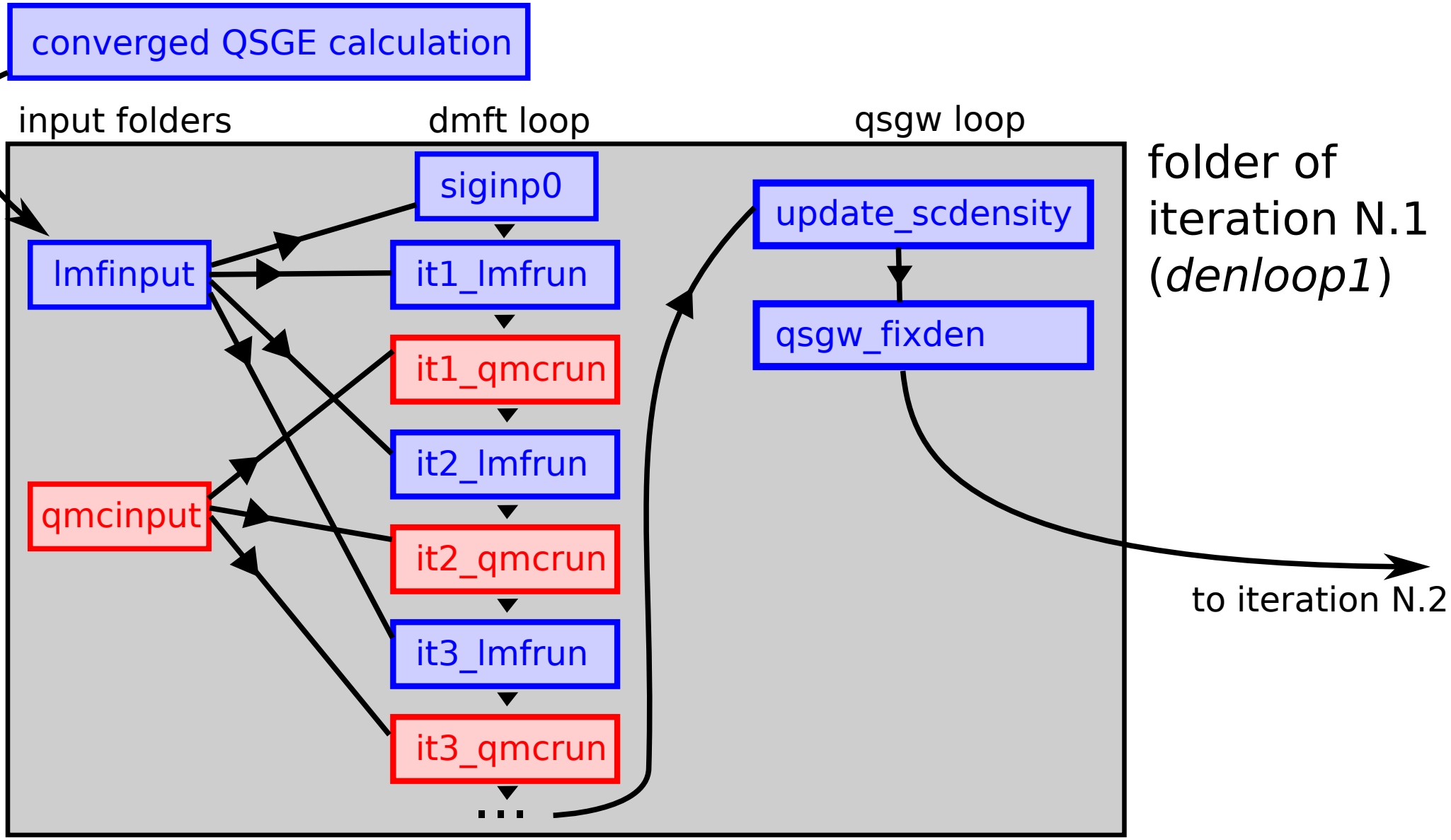
- Tutorial N.4: static limit of DMFT

Scripts and programs in the QSGW+DMFT loop



File and folders handling in the QSGW+DMFT loop

No automatization: a series of **manual operations**



Tutorial N. 1: Setting up the DMFT loop

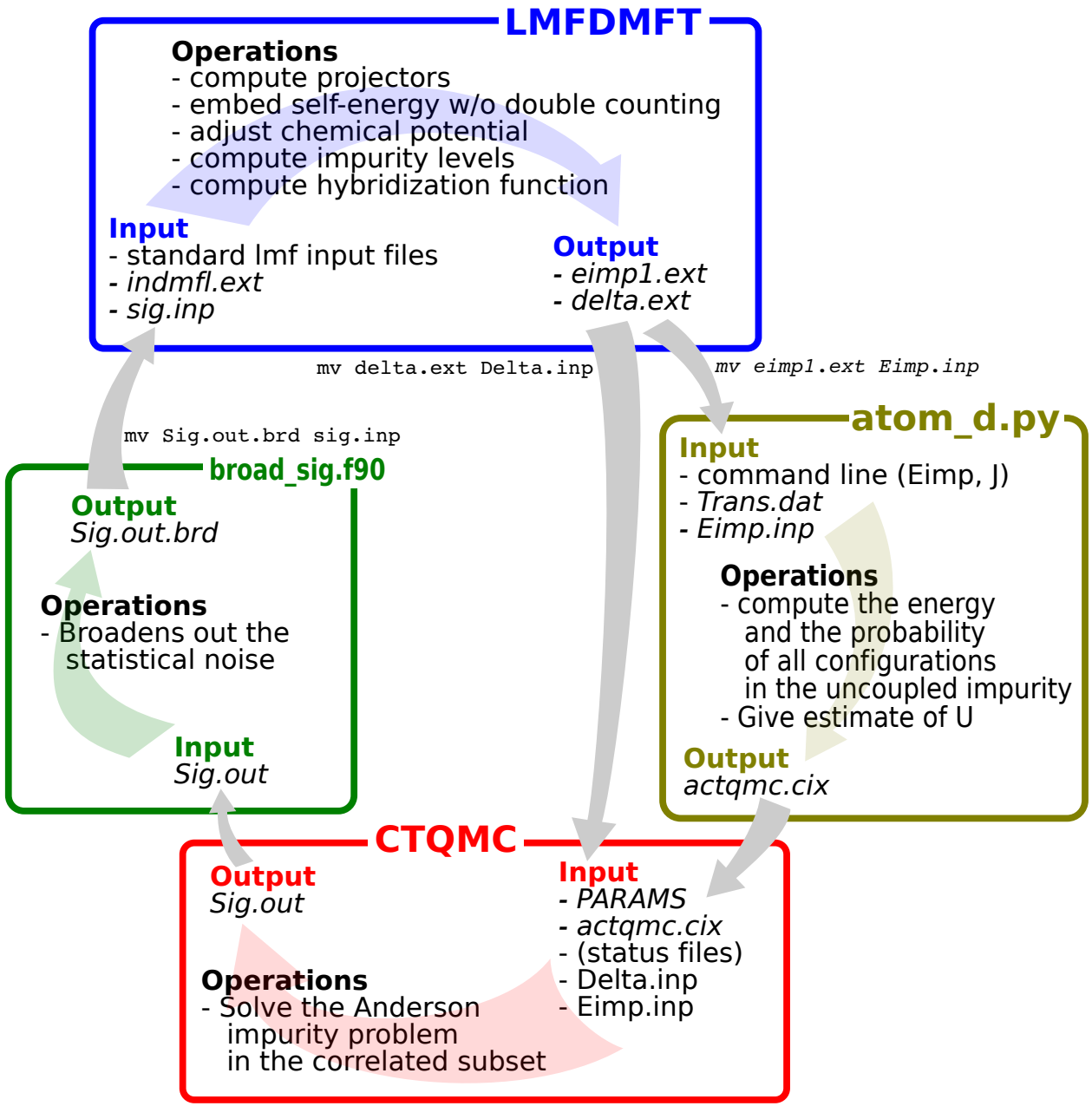
Download or ask for the USB pen

- converged QSGW → lmfinput
- input files for the CTQMC and additional programs → qmcinput

Prepare input files

- edit ctrl.ni → lmfinput
- perfrom spin-average of the self-energy → lmfinput
- compile broad_sig.x → qmcinput
- create empty impurity self-energy → siginp0

Tutorial N. 2: Running the DMFT loop



input in PARAMS

```
nf0  8.0
U    10.0
J    0.9
M    5000000.0  (~ 10 minutes)
```

Run CTQMC with a script,
run on many processors (np)

Repeat 3 or 4 iterations

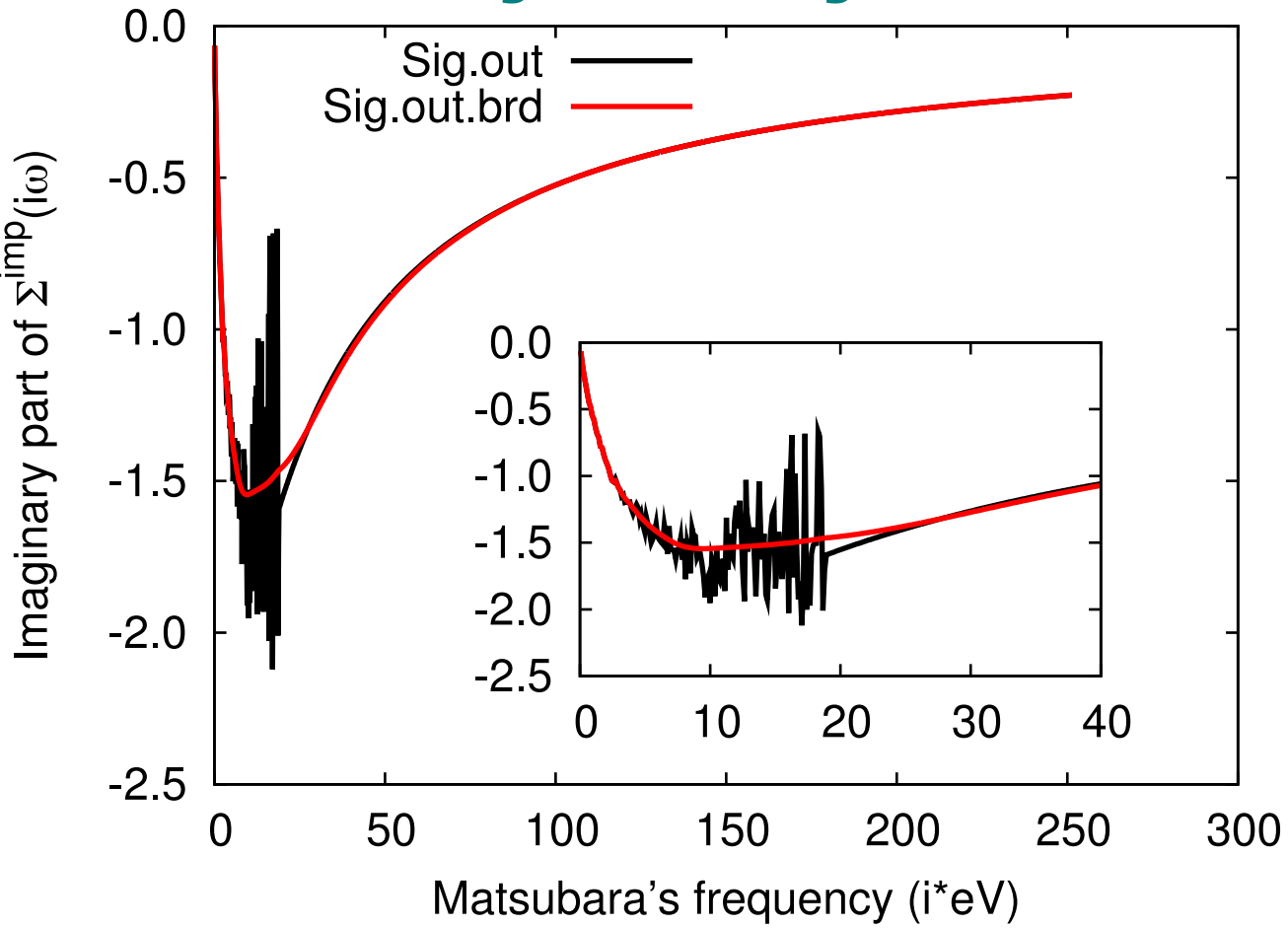
Monitor the
magnetic moment!!!
grep 'Electron charge'

Properly converged results

Actually converged results
have been obtained
with ~15 iterations,
running CTQMC on M*np=10.0E10

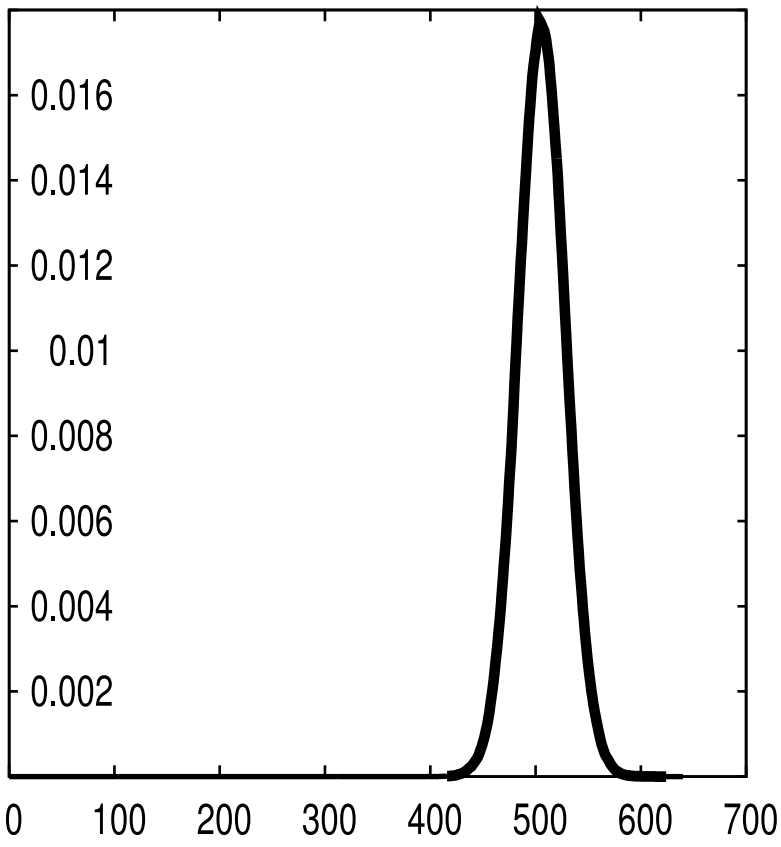
Tutorial N. 2: output of the CTQMC

Sig.out and Sig.out.brd



plot of channel 1 (column 3)
obtained with np=32

histogram.dat



Gaussian distribution
for good quality
of the MC sampling

Tutorial N. 5: QSGW loop with updated density

1) Update the denisty at fixed impurity self-energy

folder update_scdensity
lmfdmft with flag --udrs (sum over Matsubara's frequencies to get new density)
Monitor magnetic moment with grep 'Mag. moment'

DENSITY AND LDA POTENTIALS INCLUDE DMFT CORRECTIONS

2) Update QSGW self-energy at fixed density

folder qsgw_fixden
lmgwsc with flag --no-scrho

NEW QSGW POTENTIAL CONSISTENT WITH UPDATED DENSITY