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Input variables to use DFT+DMFT in ABINIT

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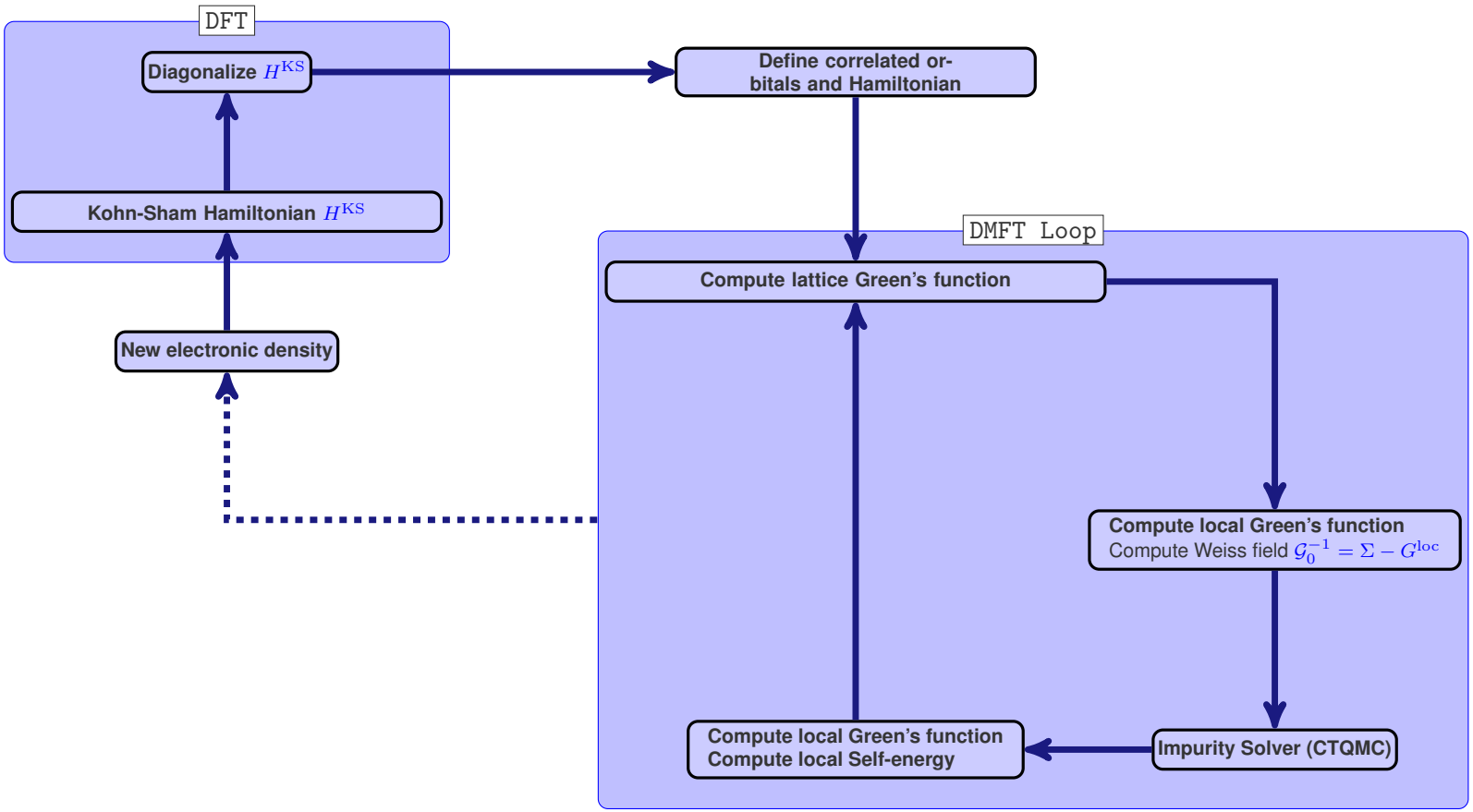
International Summer School on Computational Quantum Material 2018

The DFT+DMFT scheme (usedmft=1)



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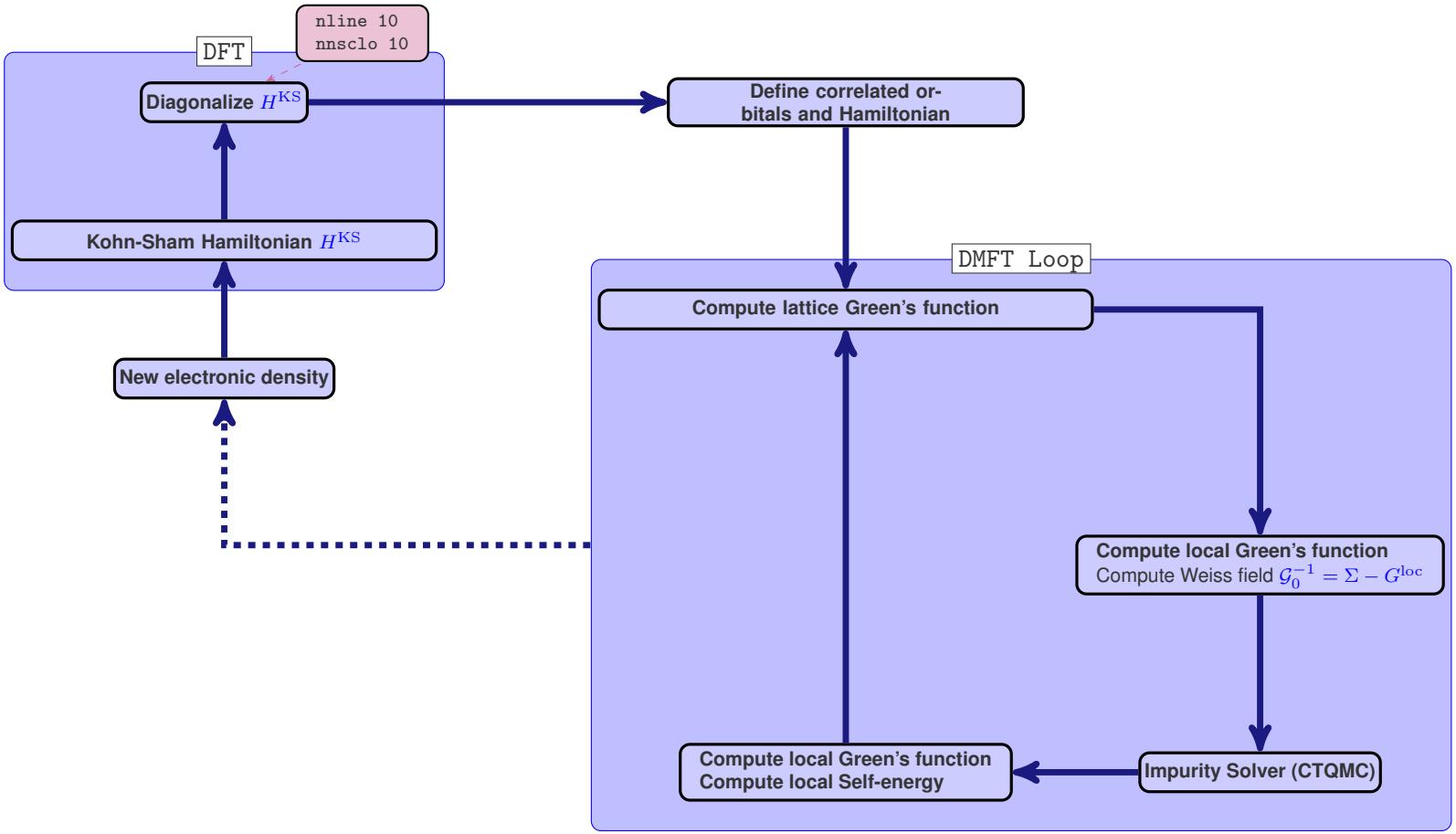

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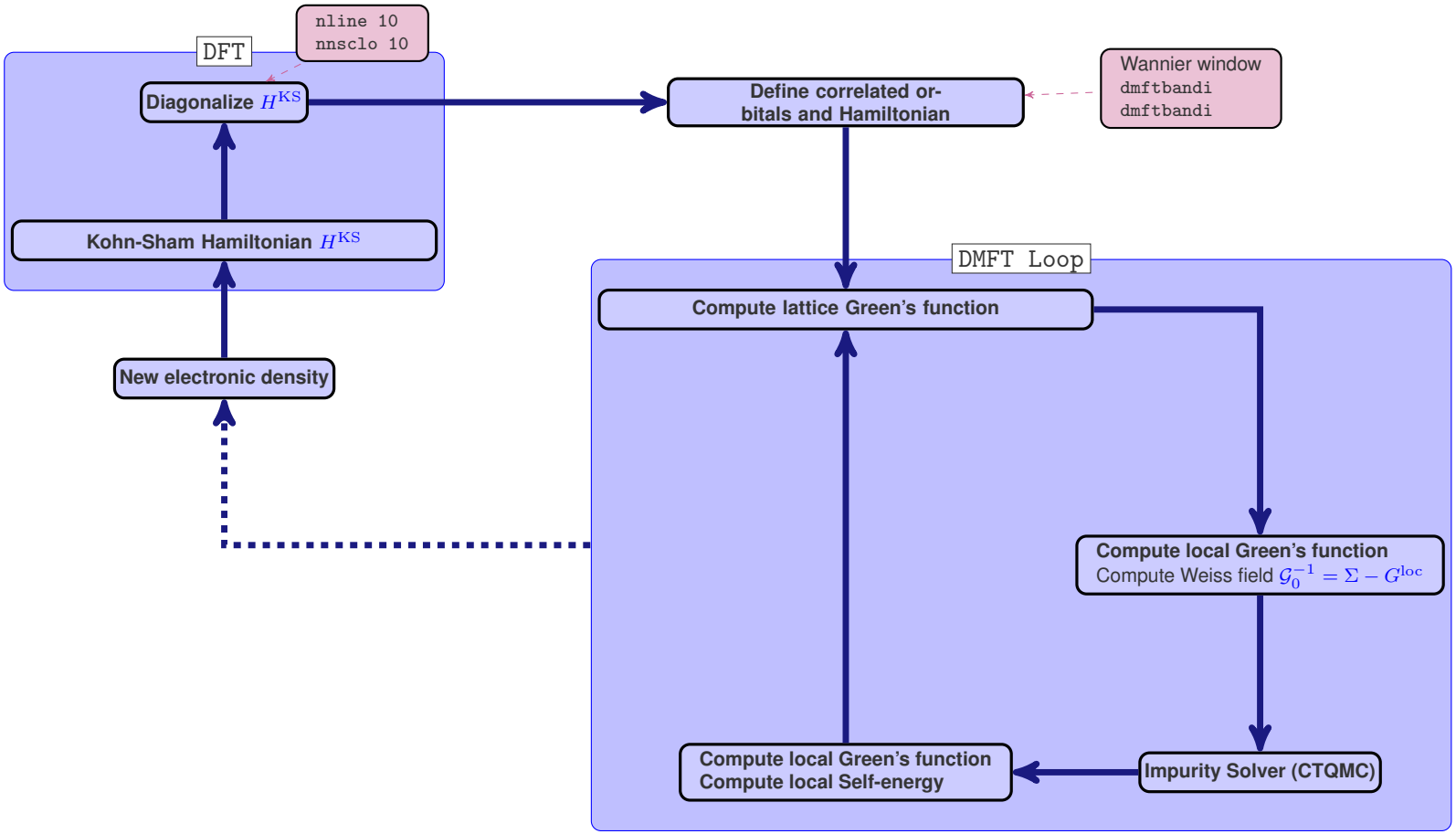

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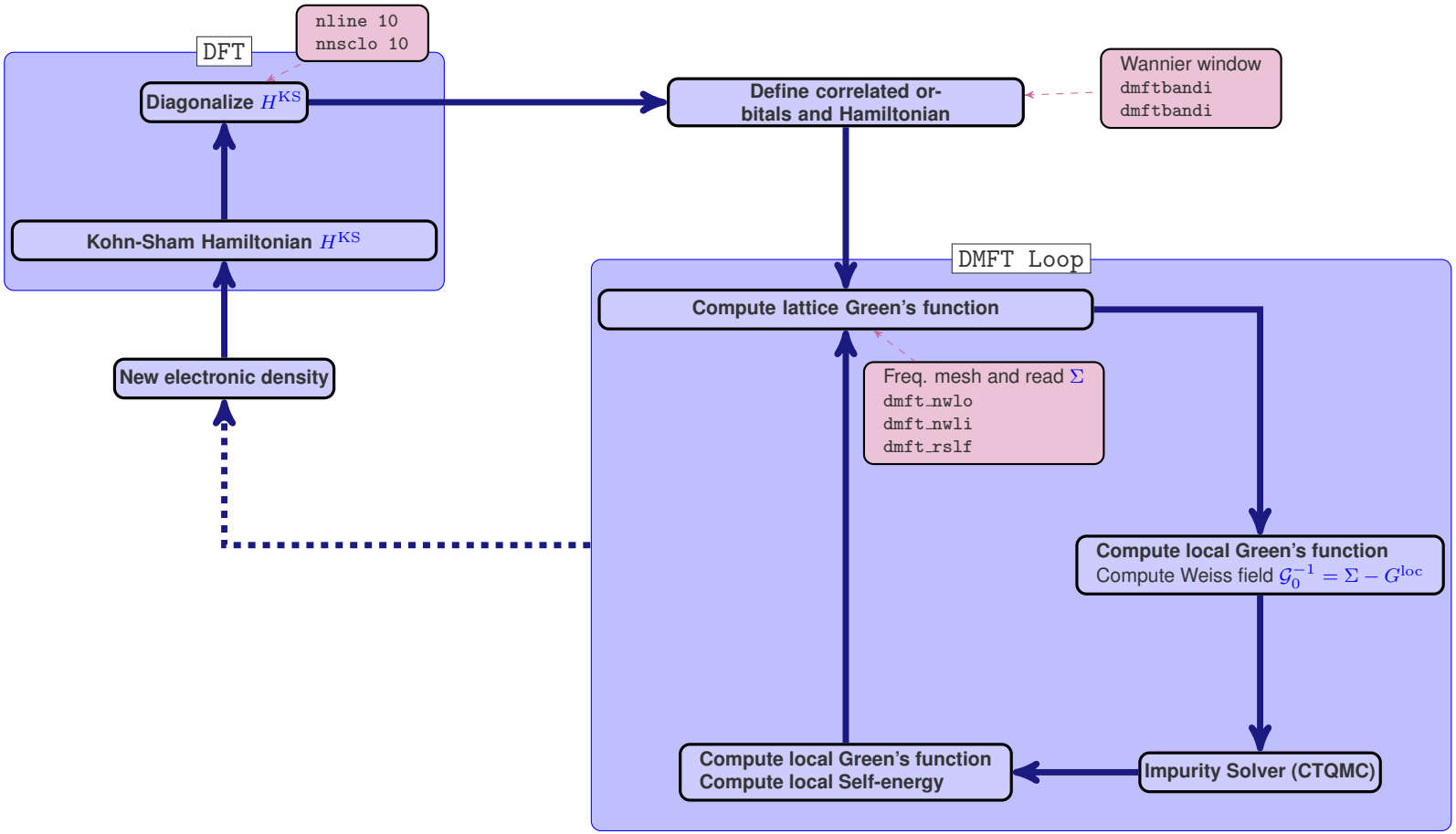

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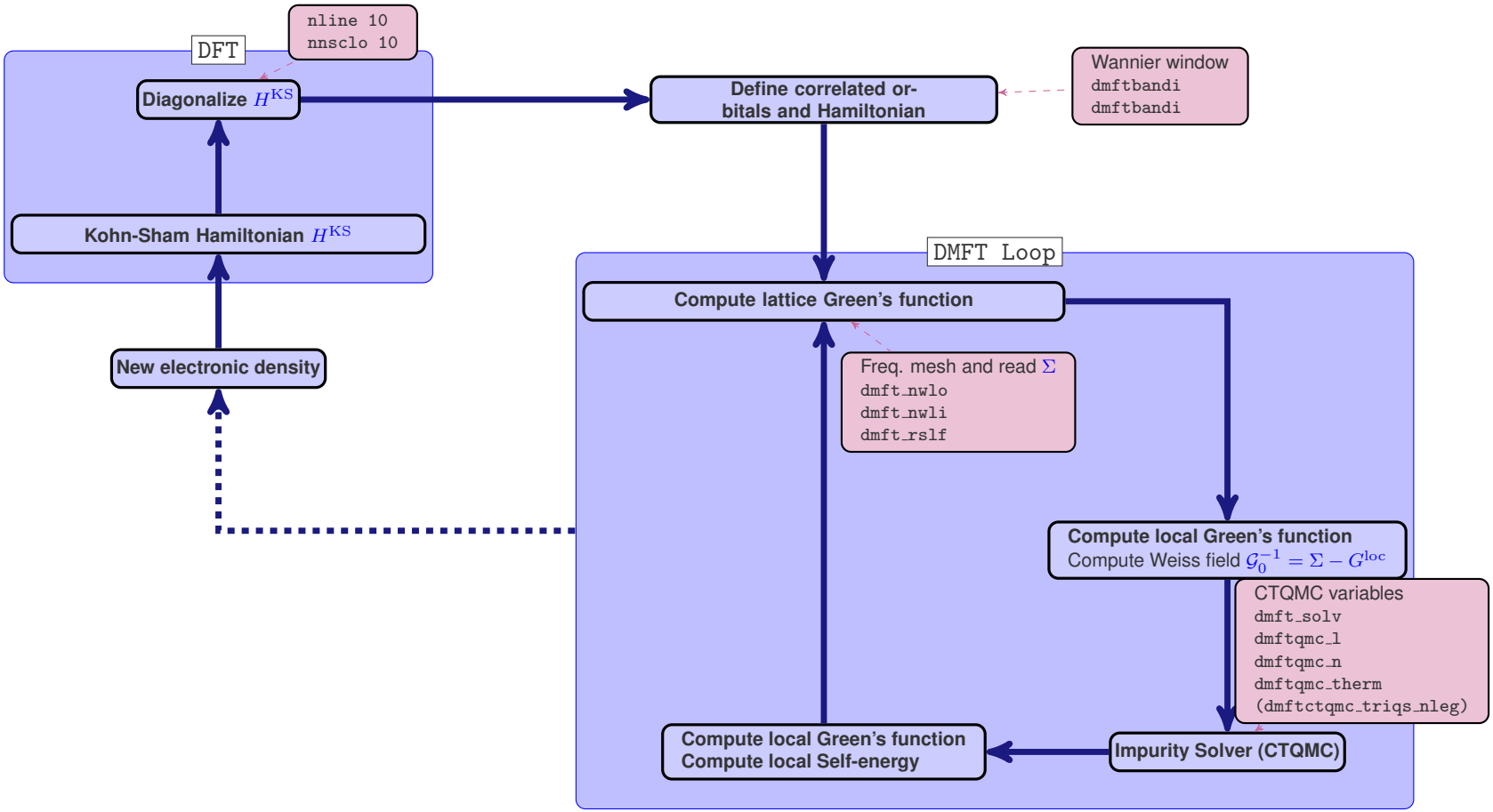

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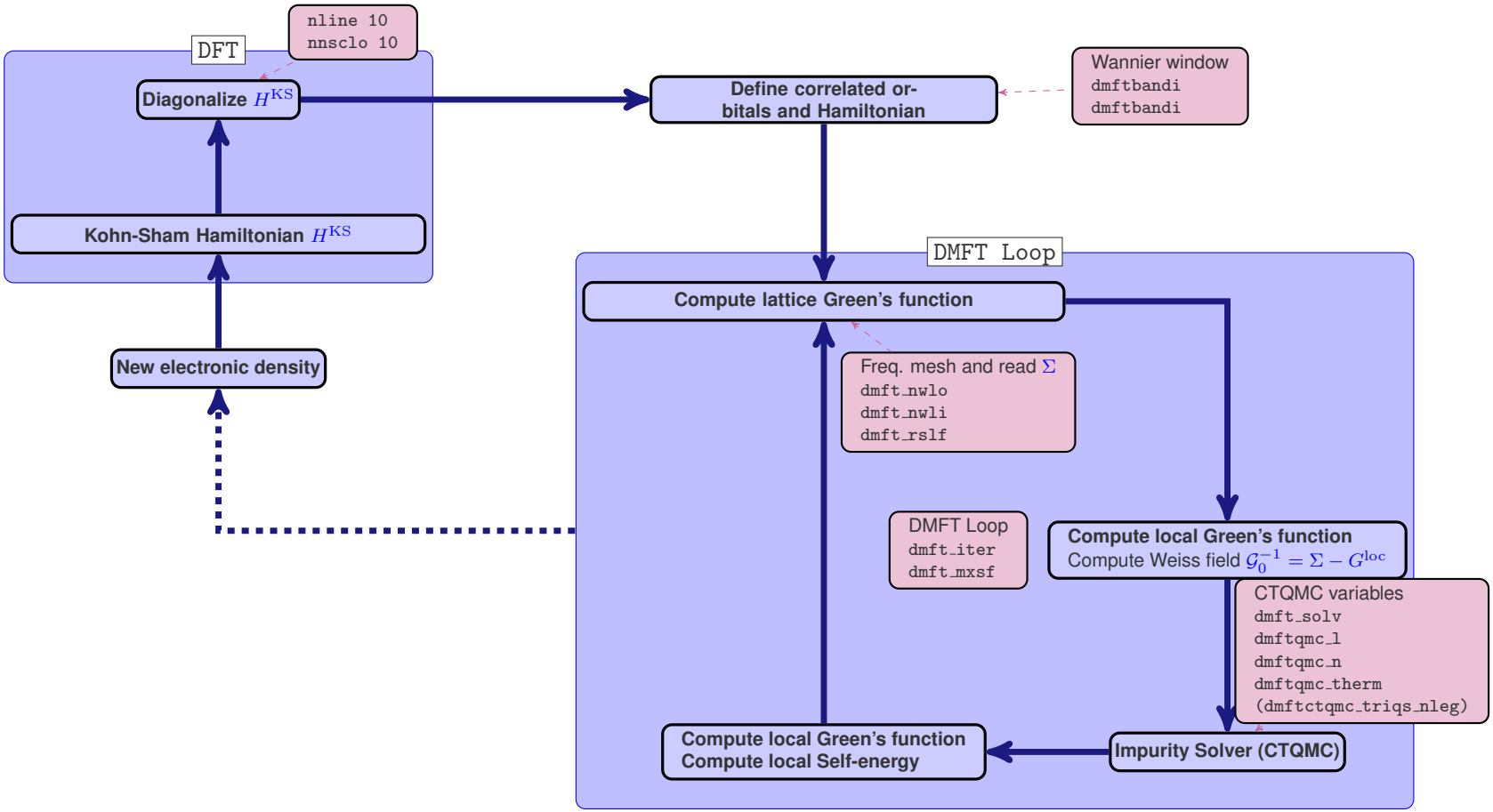

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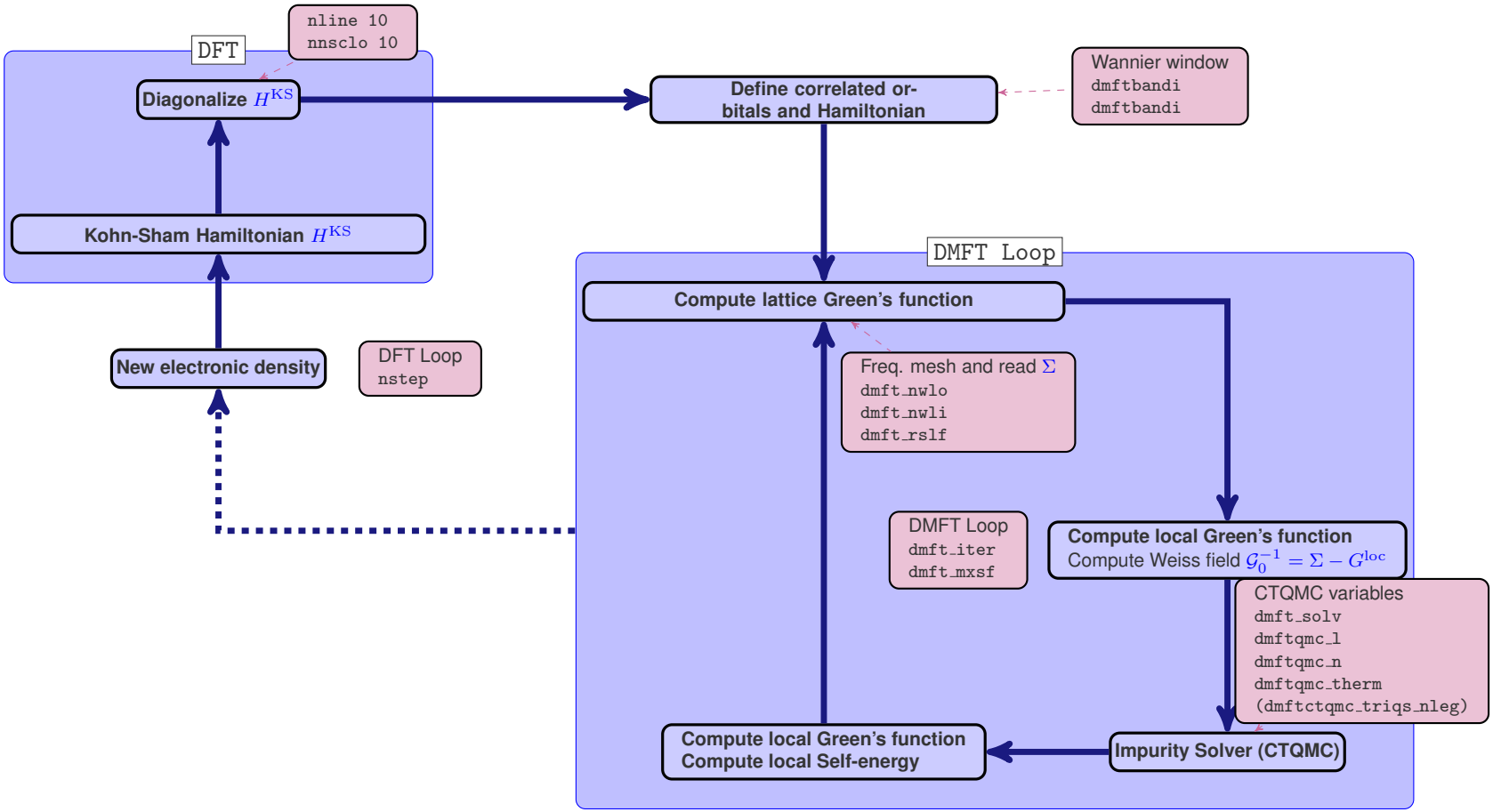
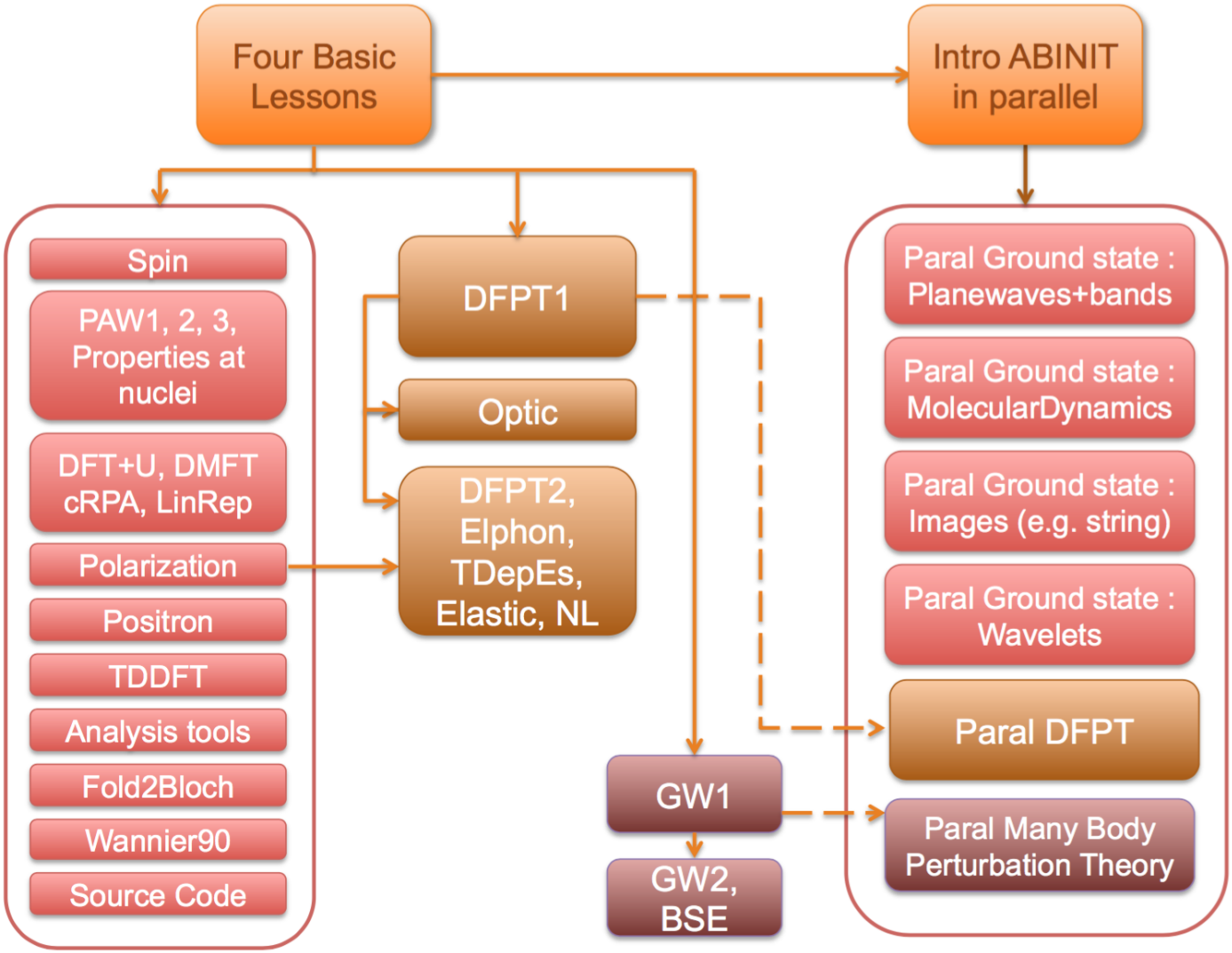


The DFT+DMFT variables

```
# == LDA+DMFT
usedmft1    0        # Do a first calculation in DFT without DMFT
nline      10        # Diagonalise correctly the Hamiltonian
nnsclo     10        # Diagonalise correctly the Hamiltonian
usedmft2    1        # Activate DFT+DFT
dmftbandi  21        # Select bands for Wannier construction
dmftbandf  23        # Select bands for Wannier construction
#dmft_nwlo 200       # Log frequency mesh (not used with TRIQS)
dmft_nwli  100       # Linear Mastubara frequency mesh
dmft_iter   1        # Number of DMFT iterations
dmft_rslf   0        # Activate reading of self-energy on disk
dmft_mxsf   0.7      # Anderson Mixing of the self-energy
dmft_dc     1        # Double counting (1: FLL, 2: AMF)
dmft_t2g    1        # Special value for t2g only calculation.

# == CTQMC
dmft_solv         5     # Solver for Anderson Impurity Model
                        #  1: Hartree Fock
                        #  2: Hubbard I (for density density interactions)
                        #  5: ABINIT CTQMC     (for density density interactions)
                        #  8: ABINIT CTQMC     (for density density interactions
                        #                       with off diagonal hybridizaton (soon available))
                        #  6: TRIQS CTQMC    (for density density interactions)
                        #  7: TRIQS CTQMC    (for general interactions)
dmftqmc_l       201     # Number of time slices for the calculation of Green's function
                        # dmftqmc_l must be larger than 2*dmft_nwli
dmftqmc_n      2.d5     # Number of CTQMC steps
dmftqmc_therm 10000     # Number of thermalization steps
dmft_tolfreq      0.01 # As log grid is not used, required precision is reduced.
dmftctqmc_triqs_nleg 30 # Number of Legendre polynomial to describe the Green's function.
```

ABINIT DMFT and cRPA tutorials



Two DMFT tutorial are available

- DMFT using the CTQMC code of ABINIT (see web site)
- DMFT using the CTQMC code of TRIQS
  - Coupling between ABINIT and CTHyb TRIQS has been done by Valentin Planes and updates by Olivier Gingras recently.
  - Available in your home directory.

Lesson on DFT+DMFT

A DFT+DMFT calculation for $SrVO_3$.

This lesson aims at showing how to perform a DFT+DMFT calculation using Abinit.

You will not learn here what is DFT+DMFT. But you will learn how to do a DFT+DMFT calculation and what are the main input variables controlling this type of calculation.

It might be useful that you already know how to do PAW calculations using ABINIT but it is not mandatory (you can follow the two lessons on PAW in ABINIT, PAW1 and PAW2. Also the DFT+U lesson in ABINIT might be useful to know some basic variables common to DFT+U and DFT+DMFT.

This lesson should take one hour to complete (especially if you have access to several processors).

1 The DFT+DMFT method: summary and key parameters

The DFT+DMFT method aims at improving the description of strongly correlated systems. Generally, these highly correlated materials contain rare-earth metals or transition metals, which have partially filled *d* or *f* bands and thus localized electrons. For further information on this method, please refer to *[Georges1996]* and *[Kotliar2006]*. For an introduction to Many Body Physics (Green's function, Self-energy, imaginary time, and Matsubara frequencies), see e.g. *[Coleman2015]* and *[Tremblay2017]*.

Several parameters (both physical and technical) needs to be discussed for a DFT+DMFT calculation.

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Calculation of U and J using cRPA

Using the constrained RPA to compute the U and J in the case of $SrVO_3$.

This lesson aims at showing how to perform a calculation of *U* and *J* in Abinit using cRPA. This method is well adapted in particular to determine *U* and *J* as they can be used in DFT+DMFT. The implementation is described in *[Amadon2014]*.

It might be useful that you already know how to do PAW calculations using ABINIT but it is not mandatory (you can follow the two lessons on PAW in ABINIT (PAW1, PAW2)). The DFT+U tutorial in ABINIT (DFT+U) might be useful to know some basic variables about correlated orbitals.

The first GW tutorial in ABINIT (GW) is useful to learn how to compute the screening, and how to converge the relevant parameters (energy cutoffs and number of bands for the polarizability).

This lesson should take two hours to complete (you should have access to more than 8 processors).

1 The cRPA method to compute effective interaction: summary and key parameters

The cRPA method aims at computing the effective interactions among correlated electrons. Generally, these highly correlated materials contain rare-earth metals or transition metals, which have partially filled *d* or *f* bands and thus localized electrons. cRPA relies on the fact that screening processes can be decomposed in two steps: Firstly, the bare Coulomb interaction is screened by non correlated electrons to produce the effective interaction *W r*.

Secondly, correlated electrons screened this interaction to produce the fully screening interaction

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