

Implementation of Exchange-Correlation Energy (for meta-GGA) in Abinit within the norm-conserving approach

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Abstract

The aim of this report is first to explain briefly the general procedure for calculation of exchange-correlation energy in Abinit (in case of LDA, GGA) and then to discuss the way the meta-GGA case is treated. This report could be useful to any new developers in Abinit who would like to implement in the subdirectory `/56_xc`. In this report I will essentially describe the main structures of some routines such as `rhohxc.F90`, `xcden.F90`, `xcmult.F90` and `xcpot.F90`.

Chapter 1

Rule of notations

A rule of notations (see below or at the beginning of `rhohxc.F90`, at the end of the list of *Local variables*) was proposed in version 6.5.0. In one hand, the idea is to try to keep a certain consistency with the labelling of variables. Indeed the latter have been added little by little by different developers who have their own personal notations. In a second hand, the use of a good labelling of variables facilitate the understanding when reading for the first time the code. In that sence, it is often preferable to give a variable name that sticks the much as possible to the physical quantity to which it corresponds.

The following rule of notations is only a proposal which can be off course use or not, depending on you. It can also be modified or be improved. Here below is the proposition:

- `rho` (ρ) is the electronic density
- `tau` (τ) is the kinetic energy density
- `exc` (ϵ_{xc}) is the exchange-correlation energy density per particule
- `epsxc` (ϵ_{xc}) is the exchange-correlation energy density ($\epsilon_{xc} = \rho \times \epsilon_{xc}$)
- `vxc` (v_{xc}) is the exchange-correlation potential
- `bigexc` (E_{xc}) is the exchange-correlation energy (for the moment it is still named "`enxc`")
- `m_norm` ($|m|$) is the norm of magnetization

- `g...` means the gradient (∇) of something (e.g. : `grho` means gradient of the electronic density)
- `g...2` means square norm of gradient ($|\nabla|^2$) of something (e.g. : `grho2` means square norm of gradient of the electronic density)
- `l...` means Laplacian ($\Delta \equiv \nabla^2$) of something (e.g. : `lrho` means Laplacian of electronic density)
- `d...d...` means first derivative of something with regards to something else ($\frac{\partial}{\partial}$).
- `d2...d...d...` means second derivative of ... with regards to ... and to ... ($\frac{\partial^2}{\partial^2}$)
- etc...
- `d...` without the occurrence of the second "d" means that this is an array which regroups several derivatives of the same quantity (e.g. : `depsxc` can contain $\frac{\partial \epsilon_{xc}}{\partial \rho}$ but also $\frac{\partial \epsilon_{xc}}{\partial |\nabla \rho|} \cdot \frac{1}{|\nabla \rho|}$)
- `..._b` means a block of the quantity ... (this is use in mpi loops which treat the data block by block)
- `..._updn` means that spin up and spin down are available in that array such as `data_updn(...,1)` and `data_updn(...,2)`. (if `nspden` ≥ 2 off course, otherwise if `nspden`= 1 `data_up(...,1)` contains the total quantity).
- `..._apn` in case of positrons are concerned.

to be the closest as possible with the libxc notations we also use the following variable names:

- `vxcrho` is the first derivative of the exchange-correlation energy density with regards to the electronic density ($\frac{\partial \epsilon_{xc}}{\partial \rho} \equiv \text{depsxcdrho}$).
- `vx McGrho` is the first derivative of the exchange-correlation energy density with regards to the gradient of the electronic density ($\frac{\partial \epsilon_{xc}}{|\nabla \rho|} \equiv \text{depsxcdgrho}$).
- `vxclrho` is the first derivative of the exchange-correlation energy density with regards to the Laplacian of the electronic density ($\frac{\partial \epsilon_{xc}}{\partial \Delta \rho} \equiv \text{depsxcdlrho}$).

- `vxctau` is the first derivative of the exchange-correlation energy density with regards to the kinetic energy density ($\frac{\partial \epsilon_{xc}}{\partial \tau} \equiv \text{depsxc} \tau$).

Chapter 2

Brief remind of exchange correlation equations

Let first recall the general form of the exchange-correlation energy in the case of meta-GGA. For the moment, we will consider a easier case which is a meta-GGA functional which would not depend on the kinetic energy density (τ). Nevertheless, this latter case still encompasses the LDA and GGA cases.

$$E_{xc}^{MGGA} = \int \epsilon_{xc}[\rho_\sigma(\mathbf{r}), \nabla\rho_\sigma(\mathbf{r}), \Delta\rho_\sigma(\mathbf{r})] d\mathbf{r} \quad (2.1)$$

with σ the spin index (up or down). The corresponding exchange-correlation potential is given by

$$v_{xc}^\sigma = \frac{\delta E_{xc}^{MGGA}}{\delta \rho_\sigma} = \frac{\partial \epsilon_{xc}}{\partial \rho_\sigma} - \left(\sum_{\alpha=x,y,z} \nabla_\alpha \left(\frac{\partial \epsilon_{xc}}{\partial \nabla_\alpha \rho_\sigma} \right) \right) + \Delta \left(\frac{\partial \epsilon_{xc}}{\partial \Delta \rho_\sigma} \right) \quad (2.2)$$

The total exchange-correlation energy (E_{xc}) is a simple scalar since it is the integral over the whole space ($\int d\mathbf{r}$) of a functional of density (plus eventually its gradient and its Laplacian) which itself depends on the space position (\mathbf{r}). On the contrary the potential v_{xc} is a function of the space position (\mathbf{r}) and then is a scalar field. In the above equation (Eq.??), the first term on the right hand side is the LDA contribution, the second term is the GGA contribution and the third term is the meta-GGA contribution. Note that in the code, the second term is not directly expressed in this way but with another form which is

$$\sum_{\alpha=x,y,z} \nabla_\alpha \left(\frac{\partial \epsilon_{xc}}{\partial \nabla_\alpha \rho_\sigma} \right) = \sum_{\alpha=x,y,z} \nabla_\alpha \left[\nabla_\alpha \rho_\sigma \times \left(\frac{1}{|\nabla \rho_\sigma|} \cdot \frac{\partial \epsilon_{xc}}{\partial |\nabla \rho_\sigma|} \right) \right] \quad (2.3)$$

with $|\nabla\rho_\sigma| = \left(\sum_{\alpha=x,y,z} \nabla_\alpha\rho_\sigma\right)^{1/2}$.

TO BE COMPLETED FOR THE CASE WHERE KINETIC ENERGY
DENSITY IS INVOLVED

Chapter 3

The routines structures of
rhohxc.F90, xcden.F90,
xcmult.F90 and xcpot.F90

Important inputs : electronic density (rho) and kinetic energy density (tau) Important outputs : exchange correlation energy (enxc) and potential (vxc) and kernels (second derivative (kxc) and third derivative(k3xc))
<ul style="list-style-type: none"> ● Tests the inputs and check the options ● Local variables initialization
● IF ixc == 0 (test purpose) then no XC functional
<ul style="list-style-type: none"> ● IF ixc /= 20 (most of the cases) <ul style="list-style-type: none"> ● set the value of ngrad, nspden_updn, nspden_eff, nspgrad ● allocate depsxc (if nspden==4 allocate and compute m_norm) ● allocate rhonow (will contain rho and grho) if mgga allocate lrhonow ▲ LOOP on ishift (treat the different FFT grids which are eventually shifted) <ul style="list-style-type: none"> ● call xcden() to set rhonow and lrhonow (gradient and laplacian of the electronic density is computed) (if nspden ==4 modify rhonow in consequence) ● call mkdenpos() to make the density positive (not its gradient) ● set the local variable order to 1, 2(-2) or 3, the number of derivative. ▲ LOOP on ifft (treat a block of data on the current FFT grid, npts) <ul style="list-style-type: none"> ● allocate exc_b, rho_b, rho_b_updn and vxcrho_b_updn ● call sizedvxc() to set the value of ndxvc, ngr2, nd2vxc, nvxcgrho ● allocate dvxc_b, vxmgrho_b, d2vxc_b, grho2_b_updn, lrho_b_updn, vxclrho_b_updn, tau_b_updn, vxctau_b_updn ● set (fill arrays) rho_b, rho_b_updn, grho2_b_updn, lrho_b_updn, tau_b_updn (LOOP on ipts, i.e. each FFT points of the block) ● call drivexc() to get exc_b, vxcrho_d_updn, vxmgrho_b, vxclrho_updn, vxctau_b_updn, dvxc_b, d2vxc_b ● accumulate the new block of data epsxc from exc_b and rho_b depsxc from vxcrho_b_updn (LDA contribution) dstrsxc from exc_b, rho_b, rho_b_updn, grho, vxcrho_b_updn depsxc from vxmgrho_b (GGA contribution) store data in kxc and k3xc ▼ END of LOOP on ifft <ul style="list-style-type: none"> ● copy data in dstrsxc and "copy" rhonow to rhonow_ptr (it is a pointer) ● call xcmult() to add the proper factor to gradient in rhonow_ptr (only for GGA, and metaGGA) ● call xcpot() to get/add the different components to vxc (use of rhonow_ptr and depsxc) ▼ END of LOOP on ishift <ul style="list-style-type: none"> ● normalize epsxc, dstrsxc, vxc and enxc (MPI_SUM if necessary) ● call mean_fftr() to get vxcmean from vxc (then compute also vxcavg) ● IF ixc == 20,21,22 (Fermi-Amaldi correction) THEN compute enxc et vxc from Hartree potential

Figure 3.1: Scheme of the routine `rhohxc.F90`.

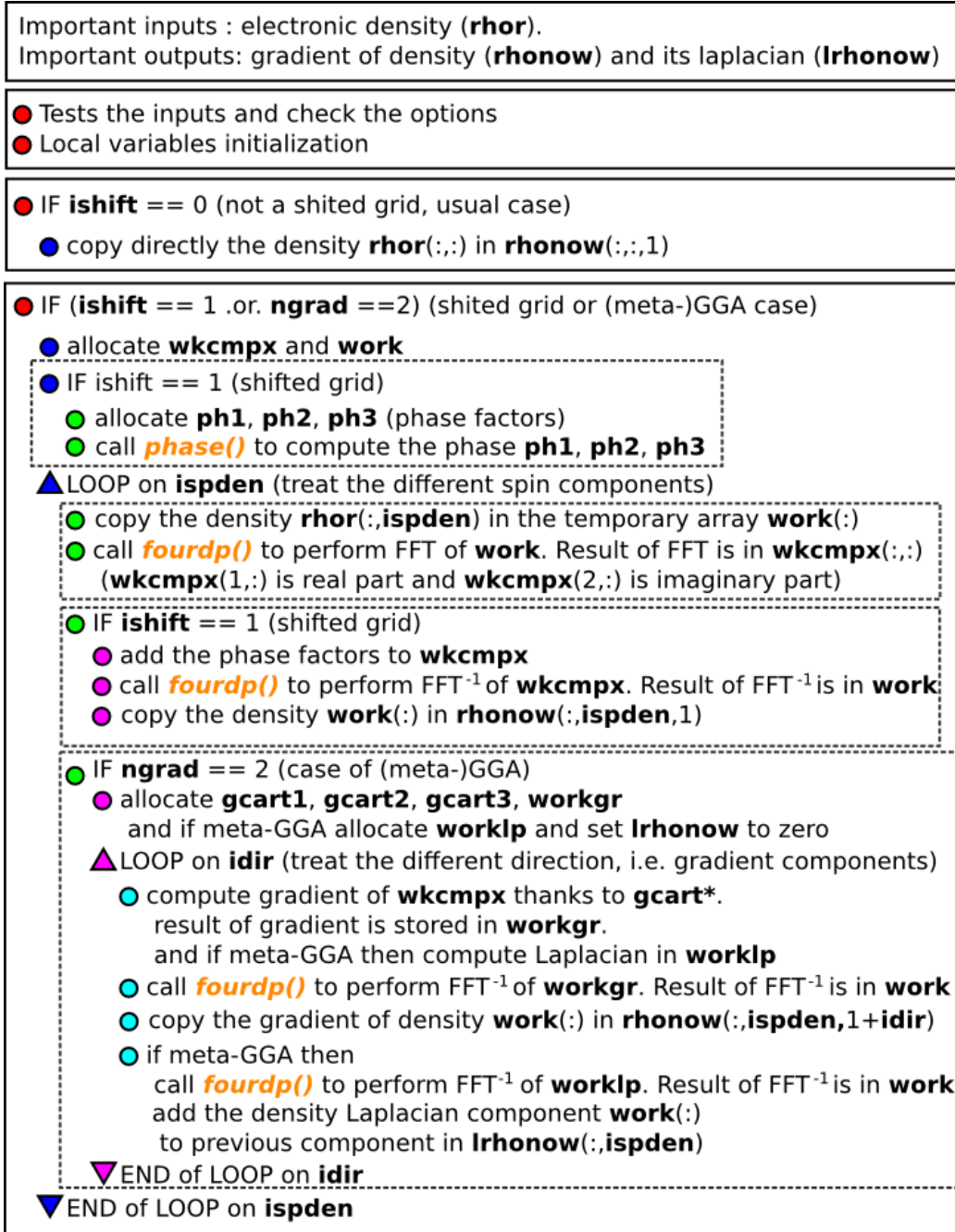


Figure 3.2: Scheme of the routine `xcden.F90`.

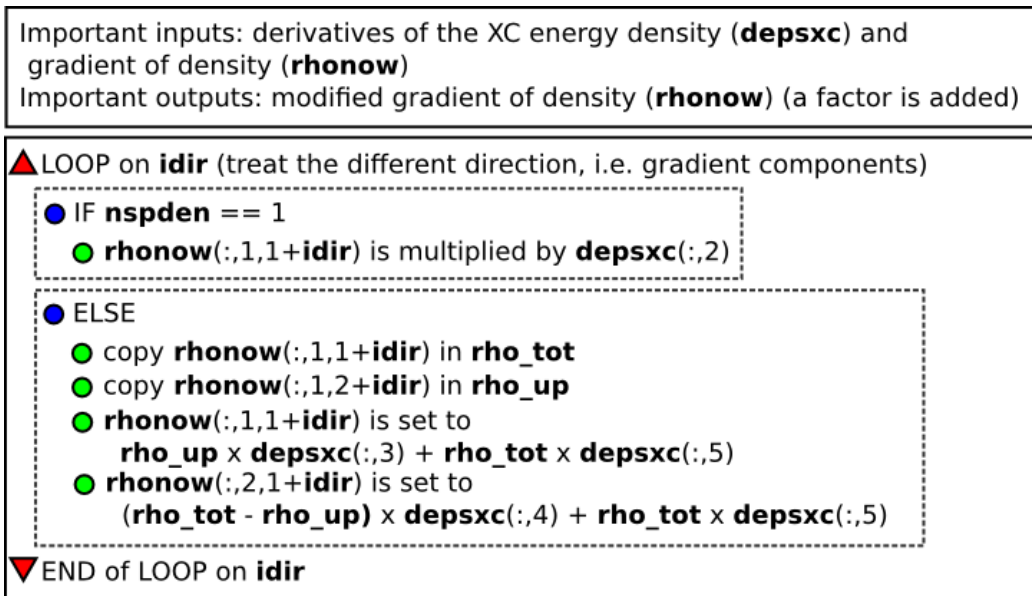


Figure 3.3: Scheme of the routine `xcmult.F90`.

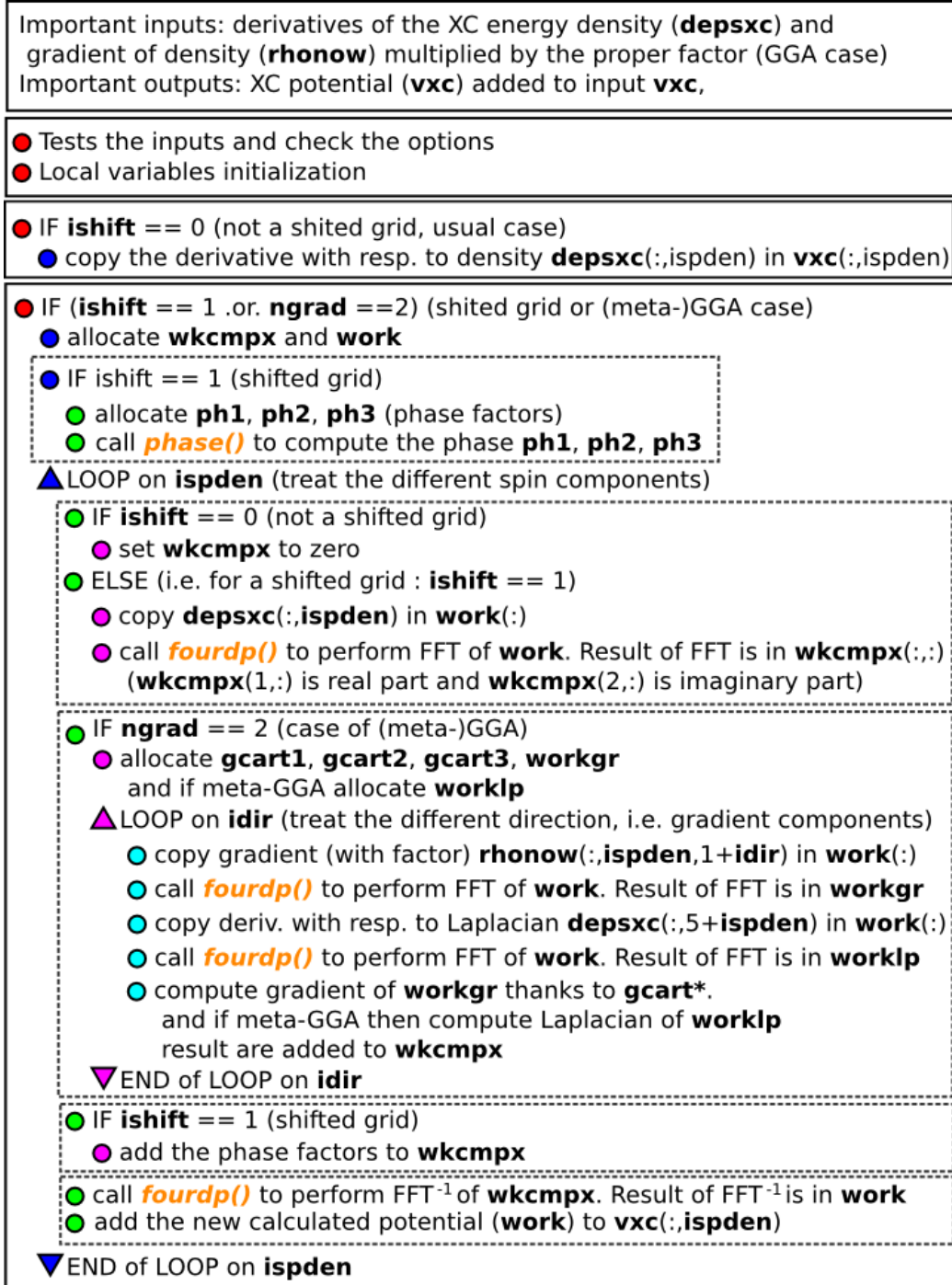


Figure 3.4: Scheme of the routine `xcpot.F90`.