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 ($\epsilon_{xc} = \rho \times \varepsilon_{xc}$)

- `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 ... ($\frac{\partial^2}{\partial\,\partial}$)

- etc...

- `d...` without the occurence 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 ($\frac{\partial\epsilon_{xc}}{\partial\rho} \equiv$ `depsxcdrho`).

- `vxcgrho` is the first derivative of the exchange-correlation energy density with regards to the gradient of the electronic density ($\frac{\partial\epsilon_{xc}}{|\nabla\rho|} \equiv$ `depsxcdgrho`).

- `vxclrho` is the first derivative of the exchange-correlation energy density with regards to the Laplacian of the electronic density ($\frac{\partial\epsilon_{xc}}{\partial\Delta\rho} \equiv$ `depsxcdlrho`).

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

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.

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

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

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

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

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

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**))

● Tests the inputs and check the options
● Local variables initialization

● IF **ixc** == 0 (test purpose) then no XC functional

● IF **ixc** /= 20 (most of the cases)
  ● 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)
      ● 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**)
        ● 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**, **vxcgrho_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**, **vxcgrho_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 **vxcgrho_b** (GGA contribution)
          store data in **kxc** and **k3xc**
    ▼END of LOOP on **ifft**
    ● copy data in **strsxc** 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**
  ● normalize **epsxc**, **strsxc**, **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`.

Important inputs : electronic density (**rhor**).
Important outputs: gradient of density (**rhonow**) and its laplacian (**lrhonow**)

● Tests the inputs and check the options
● Local variables initialization

● IF **ishift** == 0 (not a shited grid, usual case)

  ● copy directly the density **rhor**(:,:) in **rhonow**(:,:,1)

● IF (**ishift** == 1 .or. **ngrad** ==2) (shited grid or (meta-)GGA case)

  ● allocate **wkcmpx** and **work**
  ● IF ishift == 1 (shifted grid)

    ● allocate **ph1**, **ph2**, **ph3** (phase factors)
    ● call *phase()* to compute the phase **ph1**, **ph2**, **ph3**
  ▲LOOP on **ispden** (treat the different spin components)

    ● copy the density **rhor**(:,**ispden**) in the temporary array **work**(:)
    ● call *fourdp()* to perform FFT of **work**. Result of FFT is in **wkcmpx**(:,:)
      (**wkcmpx**(1,:) is real part and **wkcmpx**(2,:) is imaginary part)

    ● IF **ishift** == 1 (shifted grid)
      ● add the phase factors to **wkcmpx**
      ● call *fourdp()* to perform FFT^{-1} of **wkcmpx**. Result of FFT^{-1} is in **work**
      ● copy the density **work**(:) in **rhonow**(:,**ispden**,1)

    ● IF **ngrad** == 2 (case of (meta-)GGA)
      ● allocate **gcart1**, **gcart2**, **gcart3**, **workgr**
        and if meta-GGA allocate **worklp** and set **lrhonow** to zero
      ▲LOOP on **idir** (treat the different direction, i.e. gradient components)
        ● compute gradient of **wkcmpx** thanks to **gcart***.
          result of gradient is stored in **workgr**.
          and if meta-GGA then compute Laplacian in **worklp**
        ● call *fourdp()* to perform FFT^{-1} of **workgr**. Result of FFT^{-1} is in **work**
        ● copy the gradient of density **work**(:) in **rhonow**(:,**ispden**,1+**idir**)
        ● if meta-GGA then
          call *fourdp()* to perform FFT^{-1} of **worklp**. Result of FFT^{-1} is in **work**
          add the density Laplacian component **work**(:)
          to previous component in **lrhonow**(:,**ispden**)
      ▼END of LOOP on **idir**
  ▼END of LOOP on **ispden**

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

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Important inputs: derivatives of the XC energy density (**depsxc**) and
 gradient of density (**rhonow**)
Important outputs: modified gradient of density (**rhonow**) (a factor is added)

▲ LOOP on **idir** (treat the different direction, i.e. gradient components)

● IF **nspden** == 1
  ○ **rhonow**(:,1,1+**idir**) is multiplied by **depsxc**(:,2)

● ELSE
  ○ copy **rhonow**(:,1,1+**idir**) in **rho_tot**
  ○ copy **rhonow**(:,1,2+**idir**) in **rho_up**
  ○ **rhonow**(:,1,1+**idir**) is set to
    rho_up x **depsxc**(:,3) + **rho_tot** x **depsxc**(:,5)
  ○ **rhonow**(:,2,1+**idir**) is set to
    (**rho_tot** - **rho_up**) x **depsxc**(:,4) + **rho_tot** x **depsxc**(:,5)

▼ END of LOOP on **idir**

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

Important inputs: derivatives of the XC energy density (**depsxc**) and
 gradient of density (**rhonow**) multiplied by the proper factor (GGA case)
Important outputs: XC potential (**vxc**) added to input **vxc**,

● Tests the inputs and check the options
● Local variables initialization

● IF **ishift** == 0 (not a shited grid, usual case)
  ● copy the derivative with resp. to density **depsxc**(:,ispden) in **vxc**(:,ispden)

● IF (**ishift** == 1 .or. **ngrad** ==2) (shited grid or (meta-)GGA case)
  ● allocate **wkcmpx** and **work**

  ● IF ishift == 1 (shifted grid)
    ○ allocate **ph1**, **ph2**, **ph3** (phase factors)
    ○ call *phase()* to compute the phase **ph1**, **ph2**, **ph3**

  ▲LOOP on **ispden** (treat the different spin components)

    ○ IF **ishift** == 0 (not a shifted grid)
      ● set **wkcmpx** to zero
    ○ ELSE (i.e. for a shifted grid : **ishift** == 1)
      ● copy **depsxc**(:,**ispden**) in **work**(:)
      ● call *fourdp()* to perform FFT of **work**. Result of FFT is in **wkcmpx**(:,:)
        (**wkcmpx**(1,:) is real part and **wkcmpx**(2,:) is imaginary part)

    ○ IF **ngrad** == 2 (case of (meta-)GGA)
      ● allocate **gcart1**, **gcart2**, **gcart3**, **workgr**
        and if meta-GGA allocate **worklp**
      ▲LOOP on **idir** (treat the different direction, i.e. gradient components)
        ○ copy gradient (with factor) **rhonow**(:,**ispden**,1+**idir**) in **work**(:)
        ○ call *fourdp()* to perform FFT of **work**. Result of FFT is in **workgr**
        ○ copy deriv. with resp. to Laplacian **depsxc**(:,5+**ispden**) in **work**(:)
        ○ call *fourdp()* to perform FFT of **work**. Result of FFT is in **worklp**
        ○ compute gradient of **workgr** thanks to **gcart***.
          and if meta-GGA then compute Laplacian of **worklp**
          result are added to **wkcmpx**
      ▼END of LOOP on **idir**

    ○ IF **ishift** == 1 (shifted grid)
      ● add the phase factors to **wkcmpx**

    ○ call *fourdp()* to perform FFT^{-1} of **wkcmpx**. Result of FFT^{-1} is in **work**
    ○ add the new calculated potential (**work**) to **vxc**(:,**ispden**)
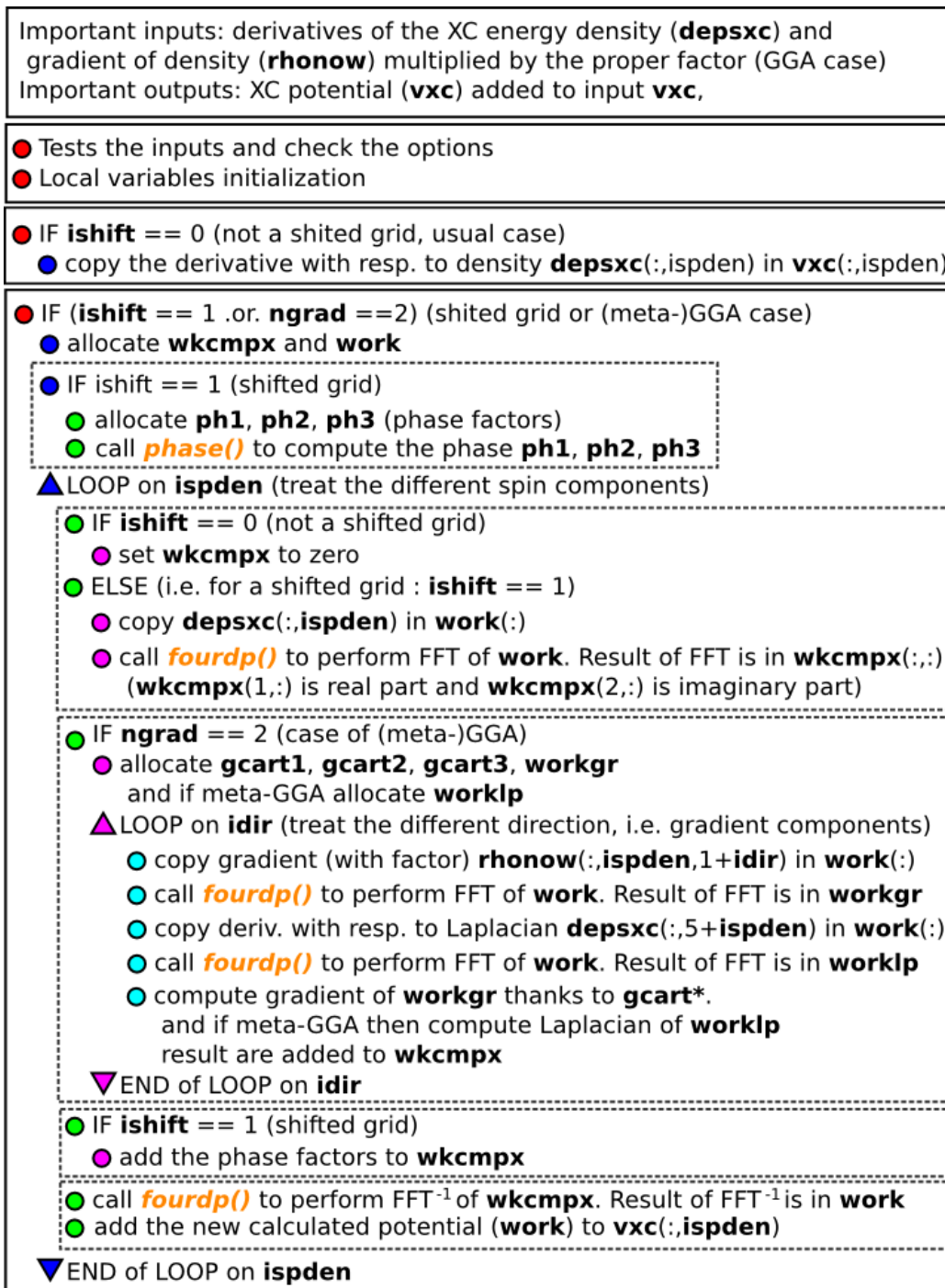
  ▼END of LOOP on **ispden**

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