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IMPLEMENTATION OF THE PAW FORMALISM IN ABINIT

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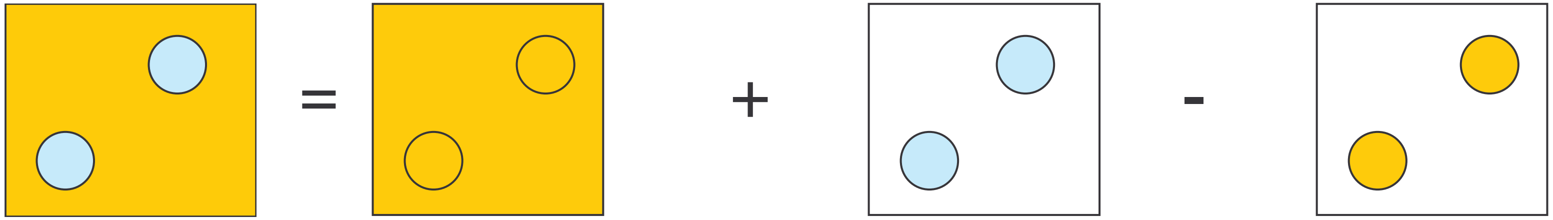
The PAW method - summary

Wavefunction:

$$\left|\psi_n\right\rangle = \left|\tilde{\psi}_n\right\rangle + \sum_i \left(\left|\phi_i\right\rangle - \left|\tilde{\phi}_i\right\rangle\right)\left\langle \tilde{p}_i \middle| \tilde{\psi}_n\right\rangle = \tau\left|\tilde{\psi}_n\right\rangle$$



Operators:

$$\langle A\rangle = \sum_n f_n \left\langle \Psi_n \middle| A \middle| \Psi_n \right\rangle = \sum_n f_n \left\langle \tilde{\Psi}_n \middle| \tau^* A \tau \middle| \tilde{\Psi}_n \right\rangle$$

Density:

$$n(\mathbf{r}) = \tilde{n}(\mathbf{r}) + \sum_R \left(n_R^1(\mathbf{r}) - \tilde{n}_R^1(\mathbf{r})\right)$$

Energy:

$$E = \tilde{E} + \sum_R \left(E_R^1 - \tilde{E}_R^1\right)$$

The PAW hamiltonian - summary

We have to solve: $\tilde{H}\,\tilde{\Psi}_n = \varepsilon_n S\,\tilde{\Psi}_n$

with

$$\boxed{\tilde{H} = \frac{dE}{d\tilde{n}} = -\frac{1}{2}\Delta + \tilde{v}_{eff} + \sum_{i,j} \left| \tilde{p}_i \right\rangle D_{ij} \left\langle \tilde{p}_j \right|}$$

and

$$S = 1 + \sum_{R,ij} \left| \tilde{p}_i^R \right\rangle \left(\left\langle \phi_i^R \middle| \phi_j^R \right\rangle - \left\langle \tilde{\phi}_i^R \middle| \tilde{\phi}_j^R \right\rangle \right) \left\langle \tilde{p}_j^R \right|$$

where

$$\tilde{v}_{eff} = v_H\left[\tilde{n} + \hat{n} + \tilde{n}_{Zc}\right] + v_{xc}\left[\tilde{n} + \hat{n} + \tilde{n}_c\right]$$

$$\begin{aligned}
D_{i,j} = {} & \sum_L \int \tilde{v}_{eff}(\mathbf{r}) Q_{ij}^L(\mathbf{r})\, d\mathbf{r} \\
& + \left\langle \phi_i \middle| -\frac{\Delta}{2} + v_H\left[n^1 + n_{Zc}\right] + v_{xc}\left[n^1 + n_c\right] \middle| \phi_j \right\rangle \\
& - \left\langle \tilde{\phi}_i \middle| -\frac{\Delta}{2} + v_H\left[\tilde{n}^1 + \hat{n} + \tilde{n}_{Zc}\right] + v_{xc}\left[\tilde{n}^1 + \hat{n} + \tilde{n}_c\right] \middle| \tilde{\phi}_j \right\rangle \\
& - \sum_L \int \tilde{v}_{eff}^1(\mathbf{r}) \hat{Q}_{ij}^L(\mathbf{r})\, d\mathbf{r}
\end{aligned}$$

<u>Other formulation</u> (implemented in ABINIT):

$$D_{ij} = D_{ij}^0 + \sum_{kl} \rho_{kl} E_{ijkl} + D_{ij}^{xc} + \sum_L \int \tilde{v}_{eff}(\mathbf{r}) \hat{Q}_{ij}^L(\mathbf{r})\, d\mathbf{r}$$

$$\rho_{i,j} = \sum_n f_n \left\langle \tilde{\Psi}_n \middle| \tilde{p}_j \right\rangle \left\langle \tilde{p}_i \middle| \tilde{\Psi}_n \right\rangle$$

Toward PAW in ABINIT…

- ABINIT has been first developped is the framework of NORM-CONSERVING pseudopotentials

- To take full benefit of PAW formalism it was necessary to use ULTRASOFT pseudopotentials.
  …implying the introduction of a « compensation charge » in the formalism.

- Implement PAW in ABINIT is long task:
  - The first stage was to introduce PAW formalism into « ground state » part of ABINIT.
  - This is fully available from ABINIT v4.6.x.
  - Translation of « Response function » part of ABINIT is in progress…

Modifications of *H* in ABINIT needed by PAW

From…

Norm conserving

$$\tilde{H}\,\tilde{\Psi}_i = \varepsilon_i\,\tilde{\Psi}_i$$

$$\tilde{H} = \frac{dE}{d\tilde{n}} = -\frac{1}{2}\Delta + \tilde{v}_{eff} + \sum_i \left| p_i \right\rangle D_i^0 \left\langle p_i \right|$$ ⊠

D_i^0 is constant (KB energy)

i over quantum numbers *l*,*n*

…to…

PAW

$$\tilde{H}\,\tilde{\Psi}_i = \varepsilon_i S\,\tilde{\Psi}_i$$ (*)

⊠ $$S = 1 + \sum_{R,ij} \left| \tilde{p}_i^R \right\rangle S_{ij}^R \left\langle \tilde{p}_j^R \right|$$

$$\tilde{H} = \frac{dE}{d\tilde{n}} = -\frac{1}{2}\Delta + \tilde{v}_{eff} + \sum_{i,j} \left| \tilde{p}_i \right\rangle D_{ij} \left\langle \tilde{p}_j \right|$$ ⊠

$D_{i,j}$ is updated at each iteration

i over quantum numbers *l*,*n* and *m*

⊠ *symbol points out similar quantities*

(*) Two generalized eigenvalue algorithm have been implemented:

- ✓ Generalized conjugate gradient by Payne, Teter, Allan… (**`cgwf.F90`**)
- ✓ Locally optimal block preconditionned conjugate gradient (**`lobpcgwf.F90`**) (possibility of parallelization over bands)

Modifications of *E* in ABINIT needed by PAW

From…

Norm conserving

$$E^{total} = E^{Ewald} + E^{K} + E^{local}\left[\tilde{n}\right] + E^{Hartree}\left[\tilde{n}\right] + E^{xc}\left[\tilde{n} + \tilde{n}_c\right] + E^{non-local}$$

Non-local energy term

☒ $$E^{Non-local} = \sum_{n,k} f_{nk} \sum_{\mathrm{R},ln} \left\langle \tilde{\Psi}_{nk} \middle| \tilde{p}_{ln}^{\mathrm{R}} \right\rangle E_{ln}^{\mathrm{KB}} \left\langle \tilde{p}_{ln}^{\mathrm{R}} \middle| \tilde{\Psi}_{nk} \right\rangle$$

…to…

PAW

$$E^{total} = E^{Ewald} + E^{K} + E^{local}\left[\tilde{n} + \hat{n}\right] + E^{Hartree}\left[\tilde{n} + \hat{n}\right] + E^{xc}\left[\tilde{n} + \hat{n} + n_c\right] + E^{PAW}$$

« Spherical part » of energy

$$E^{PAW} = \sum_{R}\left(E_R^1 - \tilde{E}_R^1\right) = \sum_{R}\left(\left(E_R^{K\,1} + E_R^{H\,1} + E_R^{xc\,1}\right) - \left(\tilde{E}_R^{K\,1} + \tilde{E}_R^{H\,1} + \tilde{E}_R^{xc\,1}\right)\right)$$

Modifications of *n (density)* in ABINIT needed by PAW

From…

Norm conserving

$$n^{total}(r)=\tilde{n}(r)=\sum_{n,k} f_{nk}\left|\tilde{\Psi}_{nk}\right|^2$$

…to…

PAW

$$n^{total}(r)=\tilde{n}(r)+\sum_{R}\left(n_R^1(r)-\tilde{n}_R^1(r)\right)$$

$$=\sum_{n,k} f_{nk}\left|\tilde{\Psi}_{nk}\right|^2+\sum_{R}\sum_{i,j}\rho_{ij}^R\left(\left\langle\phi_i^R\middle|\phi_j^R\right\rangle-\left\langle\tilde{\phi}_i^R\middle|\tilde{\phi}_j^R\right\rangle\right)$$

⌧ $$\rho_{ij}^R=\sum_{n,k} f_{nk}\left\langle\tilde{\Psi}_{nk}\middle|\tilde{p}_i^R\right\rangle\left\langle\tilde{p}_j^R\middle|\tilde{\Psi}_{nk}\right\rangle$$

Analogous to a non-local energy term

Ultrasoft pseudization implies:

$$\int n^{total}(r)\cdot dr=\int\tilde{n}(r)\cdot dr+\int\hat{n}(r)\cdot dr$$

Compensation charge

Norm-conserving vs ultrasoft PAW

Norm conserving		PAW	
Wave functions expressed on plane waves	$\tilde{\Psi}_{nk}$	Wave functions expressed on plane waves (only part of total WF)	$\tilde{\Psi}_{nk}$
Total density	$\tilde{n}(r)$	Total density	$\tilde{n}(r)+\hat{n}(r)$
Total energy	$E^{total} = \tilde{E}$	Total energy	$E^{total} = \tilde{E} + E^{PAW}$
KB energies	E_{nl}^{KB}	Psp strengths	$D_{lmn,l'm'n'}^{R}$
One FFT grid		Two FFT grids *(see later)* One radial grid for spheres	

[...]

Conventions in spherical part formulation

- Partial waves and projectors: $\phi_{lmn}(\mathbf{r}) = \frac{\phi_{\ln}(r)}{r} S_{lm}(\hat{r})$

  where $S_{lm}(\hat{r})$ are the **real** spherical harmonics

- Real Gaunt coefficients are: $RG^{LM}_{l_i m_i, l_j m_j} = \int_\Omega S_{l_i m_i}(\hat{r}) S_{LM}(\hat{r}) S_{ljmj}(\hat{r}) d\Omega$

- *Important relations:* $e^{i\mathbf{k}.\mathbf{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l S_{lm}(\hat{r}) S_{lm}(\hat{k}) j_l(kr)$

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} S_{lm}(\hat{r}) S_{lm}(\hat{r}')$$

Example of formal calculation

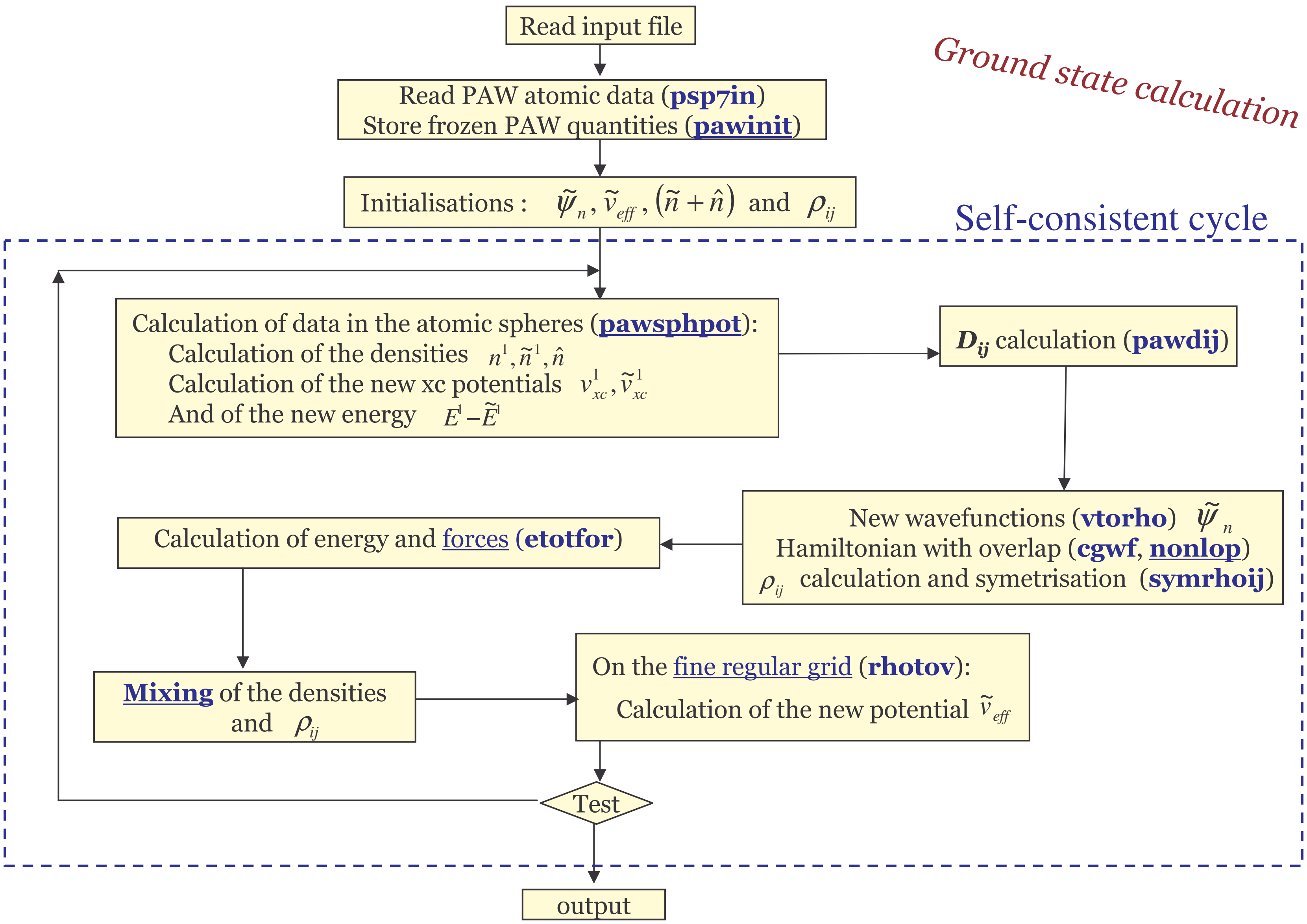
$$\langle \phi_i | v_H(n^1) | \phi_j \rangle = \iint_R \phi_i^*(\mathrm{r}) \frac{n^1(\mathrm{r}')}{|\mathrm{r}-\mathrm{r}'|} \phi_j(\mathrm{r}') d\mathrm{r} d\mathrm{r}'$$

$$= \iint_R \frac{\phi_i(r)}{r} S_{l_i m_i}(\hat{r}) \left(\sum_{i'j'} \rho_{i'j'} \frac{\phi_{i'}(r')}{r'} S_{l_{i'} m_{i'}}(\hat{r}') \frac{\phi_{j'}(r')}{r'} S_{l_{j'} m_{j'}}(\hat{r}') \right) \left(\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} S_{lm}(\hat{r}) S_{lm}(\hat{r}') \right) \frac{\phi_j(r)}{r} S_{l_j m_j}(\hat{r}) r^2 dr d\Omega r'^2 \, dr' d\Omega'$$

$$= \sum_l \sum_m \sum_{i'j'} \rho_{i'j'} RG^{lm}_{l_i m_i, l_j m_j} RG^{lm}_{l_{i'} m_{i'}, l_{j'} m_{j'}} V^l_{l_i, l_j, l_{i'}, l_{j'}}$$

with $V^l_{l_i, l_j, l_{i'}, l_{j'}} = \int_0^R \int_0^R \frac{4\pi}{2l+1} \phi_{l_i}(r) \phi_{l_j}(r) \phi_{l_{i'}}(r') \phi_{l_{j'}}(r') \frac{r_<^l}{r_>^{l+1}} dr dr'$

PAW in ABINIT – overview



Ground state calculation

Read input file

Read PAW atomic data (**psp7in**)
Store frozen PAW quantities (**pawinit**)

Initialisations : $\tilde{\psi}_n, \tilde{v}_{eff}, (\tilde{n}+\hat{n})$ and ρ_{ij}

Self-consistent cycle

Calculation of data in the atomic spheres (**pawsphpot**):
Calculation of the densities $n^1, \tilde{n}^1, \hat{n}$
Calculation of the new xc potentials $v^1_{xc}, \tilde{v}^1_{xc}$
And of the new energy $E^1 - \tilde{E}^1$

$\boldsymbol{D_{ij}}$ calculation (**pawdij**)

New wavefunctions (**vtorho**) $\tilde{\psi}_n$
Hamiltonian with overlap (**cgwf**, **nonlop**)
ρ_{ij} calculation and symetrisation (**symrhoij**)

Calculation of energy and forces (**etotfor**)

Mixing of the densities
and ρ_{ij}

On the fine regular grid (**rhotov**):
Calculation of the new potential $\tilde{v}_{eff}$

Test

output

Efficiency

In ABINIT we choose to…

- ☺ Have good ultrasoft PAW atomic data (downloadable on web site)
- ☺ Store as much frozen atomic data as possible (see pawinit)
- ☺ Use several adapted radial grids (see psp7in)
- ☺ Exploit symetries to compute only the non-zero radial moments of the densities (see pawdens)
- ☺ Develop the radial XC potentials in moments and compute only the first ones (see pawxcm)
- ☺ Exploit symetries of the system to symetrize ρ_{ij} (see symrhoij)
- ☺ Mix effectively the spherical part of the density (mix ρ_{ij})
- ☺ Have efficient algorithms to solve generalized eigenproblem

Accuracy

In ABINIT you can…

- ☺ Have good ultrasoft PAW atomic data (downloadable on web site)
- ☺ Adjust sharpness of grids in real space (spheres) or reciprocal space *pawntheta, pawnphi* *mqgriddg*
- ☺ Choose to compute XC potential exactly (LDA only) or with a development over few moments *pawxcdev*
- ☺ Use two adjustable Fourier grids: *ecut, ecutdg* *nfft, nfftdg*
  - a « coarse » grid for wave functions development
  - a « fine » grid (double grid) for densities description inside spheres
- ☺ Choose order of development of densities in spherical harmonics *pawlcutd*
- ☺ And also use all adjustable convergence parameters (same as in *norm-conserving* case)…

How does a PAW calculation work in ABINIT ?

- **At first order** *Mandatory*
  - Only change all the pseudopotential files
- **At second order** *Always*
  - Test the convergency of the fine grid (ecutdg or ngfftdg)
- **At third order** *Rarely*
  - (De)activate second order expansion of XC potentials (pawxcdev) and eventually adjust sharpness of spherical grids (pawntheta, pawnphi)
  - Cut or not spherical harmonics expansion (lcutd)
  - Adjust sharpness of grid used to express atomic data in reciprocal space (pawmqgrid)
  - Use only main part of ρ_{ij} in mixing scheme of SC cycle (pawlmix)
  - *… and other adjustable parameters (see PAW chapter of input variables manual)*

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Initial storage of frozen atomic data (*pawinit*)

Initialization of some starting values for several arrays used by PAW calculation

1-Initialize data related to angular mesh (Gaunt coefficients, ...)

2-Tabulate normalized shape function *g(r)* (for compensation charge)

3-Compute:

$$q_{ij}^{lm} = \int_R \left[\phi_i^*(\mathbf{r})\phi_j(\mathbf{r}) - \tilde{\phi}_i^*(\mathbf{r})\tilde{\phi}_j(\mathbf{r}) \right] r^l S_{lm}(\hat{r}) d\mathbf{r} = RG_{l_i m_i, l_j m_j}^{lm} \int_{\mathbf{0}}^{\mathbf{R}} \left(\phi_{\mathbf{i}}(r)\phi_{\mathbf{j}}(r) - \tilde{\phi}_{\mathbf{i}}(r)\tilde{\phi}_{\mathbf{j}}(r) \right) r^l dr$$

$$s_{ij} = \sqrt{4\pi} q_{ij}^{00}$$

$E_{ij,kl}$ *Involved in computation of Hartree potential inside spheres*

5-Compute Ex-correlation energy for the core density

>

Computation of data inside PAW spheres (*pawsphpot*)

- Calculation of spherical densities (pawdens)

$$n(r,\theta,\varphi)=\sum_{LM} n_{LM}(r)S_{LM}(\theta,\varphi)$$

Compute : $n^1_{LM}(r),\ \tilde{n}^1_{LM}(r),\ \hat{n}_{LM}(r)$

- Possibility to compute $n(r,\theta,\phi)$ or $n_{LM}(r)$
- Possibility to compute all LM moments or only the first ones (having the main contribution)

- Calculation of the spherical potentials (pawxc & pawxcm)

$$v_{xc}(r,\theta,\varphi)=\sum_{LM} v^{xc}_{LM}(r)S_{LM}(\theta,\varphi)=v_{xc}\left[n_0(\vec{r})\right]+\left[n(\vec{r})-n_0(\vec{r})\right]\frac{dv_{xc}}{dn}\left[n_0\right]+\frac{\left[n(\vec{r})-n_0(\vec{r})\right]^2}{2}\frac{d^2v_{xc}}{dn^2}\left[n_0\right]$$

$$\downarrow \qquad\qquad\qquad\qquad \downarrow$$

Direct computation
on spherical grid
(LDA only)

OR

Development in moments
stopped at first moment

Accurate
CPU expensive

Approximated

≥

The non local operator *(nonlop)*

The nonlocal operator has the form $v_{NL} = \sum_{R,lmn,l'm'n'} \left| \tilde{p}^{R}_{lmn} \right\rangle \mathbf{O}^{R}_{lmn,l'm'n'} \left\langle \tilde{p}^{R}_{l'm'n'} \right|$

$$v_{NL}(\mathrm{G},\mathrm{G}') = \sum_{R,lmn,l'm'n'} \left\langle \mathrm{G} \middle| \tilde{p}^{R}_{lmn} \right\rangle \mathbf{O}^{R}_{lmn,l'm'n'} \left\langle \tilde{p}^{R}_{l'm'n'} \middle| \mathrm{G}' \right\rangle$$

$$= (4\pi)^2 \sum_{R} e^{iR(G'-G)} \sum_{lmn,l'm'n'} \left[H^{R}_{lmn}(\mathrm{G})\right] \mathbf{O}^{R}_{lmn,l'm'n'} \left[H^{R}_{l'm'n'}(\mathrm{G}')\right]^{*}$$

$$H^{\mathbf{R}}_{lmn}(\mathbf{G}) = (-i)^{l} S_{lm}(\hat{G}) \int_{0}^{R} j_{l}(Gr)\, \tilde{p}^{\mathbf{R}}_{ln}(r)\, r dr$$

As mentionned by symbols ⌧, several quantities have this form:

- If $O^{R}_{lmn,l'm'n'} = D^{R}_{ij}$, we get the non-local part of Hamiltonian
- If $O^{R}_{lmn,l'm'n'} = S^{R}_{ij}$, we get operator **S**
- If $O^{R}_{lmn,l'm'n'} = 1$, we get ρ^{R}_{ij}

All these quantities are computed in the same routine (nonlop)

How to retrieve norm-conserving expression

$$v_{NL}(G,G') = (4\pi)^2 \sum_{R} e^{iR(G'-G)} \sum_{lmn} H^{R}_{lmn}(\mathrm{G}) E^{KB}_{ln} \left[H^{R}_{lmn}(\mathrm{G}')\right]^{*}$$

$$= (4\pi)^2 \sum_{R} e^{iR(G'-G)} \sum_{ln} \left[(\cancel{-i})^{l} \int_{0}^{R} j_{l}(Gr)\, \tilde{p}^{R}_{ln}(r)\, r dr \right] E^{KB}_{ln} \left[(\cancel{-i})^{l} \int_{0}^{R} j_{l'}(G'r)\, \tilde{p}^{R}_{l'n'}(r)\, r dr \right]^{*} \sum_{m} S_{lm}(\hat{G}) S_{lm}(\hat{G}')$$

$$= (4\pi)^2 \sum_{R} e^{iR(G'-G)} \sum_{l,n} f^{R}_{nl}(G) \cdot E^{KB}_{ln} \cdot f^{R}_{nl}(G') \cdot \left[\frac{2l+1}{4\pi} P_{l}(\cos\theta_{G,G'}) \right]$$

≥

Forces

Forces in PAW have been implemented as sum of the following terms:

$$\mathbf{F}_1 = -\int (\tilde{n} + \hat{n})(\mathbf{r}) \frac{\partial v_H(\tilde{n}_{Zc})}{\partial \mathbf{R}} d\mathbf{r}$$

$$\mathbf{F}_{xc} = -\int v_{xc}[\tilde{n} + \hat{n} + \tilde{n}_c] \frac{\partial \tilde{n}_c}{\partial \mathbf{R}} d\mathbf{r}$$

In pawcorloc

$$\mathbf{F}_2 = -\sum_{ijlm} \int \tilde{v}_{eff}(\mathbf{r}) \rho_{ij} q_{ij}^{lm} \frac{\partial\left[g_l(|\mathbf{r}-\mathbf{R}|) S_{lm}(r-R)\right]}{\partial \mathbf{R}} d\mathbf{r}$$

In pawgrnhat

In nhatgrid

$$\mathbf{F}_3 = -\sum_{ij} \sum_{n} \frac{\partial \rho_{ij}^n}{\partial \mathbf{R}} \left[D_{ij} - \varepsilon_n \sqrt{4\pi} q_{ij}^{00}\right]$$

In nonlop

In pawmkrhoij

Stress tensor

Stresses in PAW have been implemented as sum of the following terms:

$$\sigma_{\alpha\beta} = \frac{1}{\Omega}\frac{\partial E}{\partial \varepsilon_{\alpha\beta}} = \underbrace{kinstr + ewstr + lpstr(\tilde{n}+\hat{n}) + harstr(\tilde{n}+\hat{n}) + strxc(\tilde{n}+\hat{n}+\tilde{n}_c) + strsii}_{\text{Norm}-\text{conserving like terms}}$$

$$+\sigma_1+\sigma_2+\sigma_3+\sigma_4$$

$$\sigma_1 = \frac{1}{\Omega}\delta_{\alpha\beta}\int \tilde{v}_{eff}(\mathbf{r})\hat{n}(\mathbf{r})d\mathbf{r}$$

In pawgrnhat

$$\sigma_2 = \frac{1}{\Omega}\sum_{ij}\rho_{ij}\sum_{lm}\int \tilde{v}_{eff}(\mathbf{r})q_{ij}^{lm}\frac{\partial(g_l S_{lm})}{\partial \varepsilon_{\alpha\beta}}d\mathbf{r}$$

In nhatgrid

$$\sigma_3 = \frac{1}{\Omega}\sum_{ijn}\frac{\partial \rho_{ij}^{n}}{\partial \varepsilon_{\alpha\beta}}(D_{ij} - \varepsilon_n\sqrt{4\pi}q_{ij}^{00})$$

In pawmkrhoij

In nonlop

$$\sigma_4 = \frac{1}{\Omega}\delta_{\alpha\beta}\int v_{xc}[\tilde{n}+\hat{n}+\tilde{n}_c]\tilde{n}_c d\mathbf{r} + \frac{1}{\Omega}\int v_{xc}[\tilde{n}+\hat{n}+\tilde{n}_c]\frac{\partial \tilde{n}_c}{\partial \varepsilon_{\alpha\beta}}d\mathbf{r}$$

In pawcorloc

Mixing during electronic iterations

Mixing is available either on $\tilde{v}_{eff}$ or on $\tilde{n}+\hat{n}$.
In PAW, mixing on densities seems to be more suitable.

The spherical part (ρ_{ij} quantities) has also to mixed !
Their mixing scheme is adjusted on the density (or potential) mixing scheme.

	Mixing on potential	**Mixing on densities**
Simple mixing	*iscf=2*	*iscf=12*
Anderson mixing	*iscf=3*	*iscf=13*
Anderson mixing (order 2)	*iscf=4*	*iscf=14*
Conjugate-gradient mixing	*iscf=5*	*Not yet available*
Pulay mixing	*iscf=7*	*iscf=17*

Exemple, with a simple mixing:

$$n_{n+1}^{mix}(r) = n_n^{in}(r) + \alpha \cdot \underbrace{\left(n_n^{out}(r) - n_n^{in}(r)\right)^{PC}}_{resid_n^{PC}(r)}$$

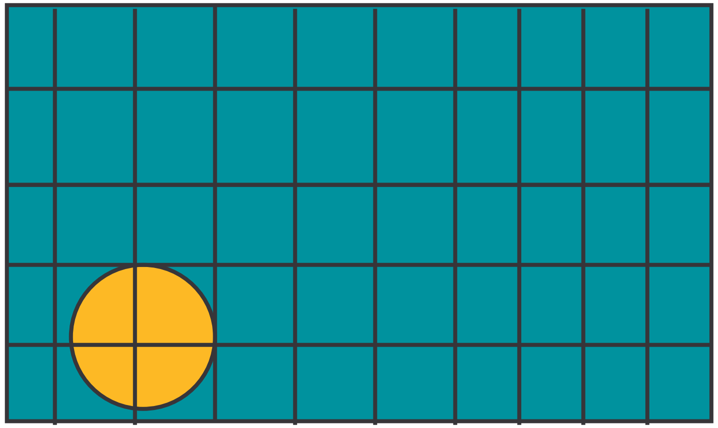
$$\left[\rho_{ij}\right]_{n+1}^{mix} = \left[\rho_{ij}\right]_n^{in} + \alpha \cdot \underbrace{\left(\left[\rho_{ij}\right]_n^{out} - \left[\rho_{ij}\right]_n^{in}\right)^{PC}}_{resid\left[\rho_{ij}\right]_n^{PC}}$$

PC means « preconditionned »

≥

The fine regular grid

- A coarse grid is used to obtain wavefunctions $\tilde{\Psi}_n$
- We need $\hat{n}$ on the regular and on the radial grid
- For accuracy, a fine grid is used to compute $\tilde{v}_{eff} = v_H[\tilde{n} + \hat{n} + \tilde{n}_{Zc}] + v_{xc}[\tilde{n} + \hat{n} + \tilde{n}_c]$



If only the « coarse » FFT grid is used, not enough points are in PAW spheres

See variable pawecutdg

« Double FFT » technique is used to transfer densities (potentials) between grids:

$$\tilde{n}_{coarse}(\vec{r}) \xrightarrow{FFT} \tilde{n}_{coarse}(\vec{G}) \longrightarrow \tilde{n}_{fine}(\vec{G}) \xrightarrow{FFT} \tilde{n}_{fine}(\vec{r})$$

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Conclusion

- What is done in ABINIT v4.6.x:
  - Calculation of the total energy, forces and stresses
  - Atomic data generators

- What is to be done:
  - Calculation of linear response
  - Spin orbit coupling
  - Detailed Latex Documentation

- What is to be improved
  - Introduce PAW formalism in the whole GS code (some restrictions still remain)
  - Parallelize (on atoms ?)