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SEVERAL ASPECTS OF THE SELF-CONSISTENT CYCLE MIXING IN ABINIT

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Outline

- ✓ Pulay mixing
- ✓ Potential mixing vs density mixing
- ✓ Mixing within PAW
- ✓ Conclusion

SCF mixing

Self-consistent cycle

Start with V_0^{in} , $m=0$

Solve $H(V_m^{in})|\psi_n\rangle = \epsilon_n|\psi_n\rangle$

Compute new V_m^{out}

Mix $V_i^{out}, V_i^{in}, \dots$

Get new V_{m+1}^{in}

Stop if

$$V_m^{in} - V_m^{out} < \epsilon$$

Key quantity: Potential residual

$$R(V^{in}) = V^{out}(V^{in}) - V^{in}$$

Goal for a mixing scheme:

Minimize norm of potential residual

$$\langle R(V^{in}) | R(V^{in}) \rangle$$

Example of linear mixing:

$$V_{m+1}^{in} = V_m^{in} + \alpha \cdot R(V_m^{in})$$

Improvement: preconditioning $V_{m+1}^{in} = V_m^{in} + P R(V_m^{in})$

P : preconditioning matrix

See iprcl, diemix, dimeac,... ABINIT keywords

PM Anglade talk during this session

Pulay mixing – Theory 1

Pulay mixing First approach

$V_1^{in}, V_2^{in}, \dots, V_m^{in}$ have been stored

Search new optimal « mixed » potential
as linear combination of V_i^{in}

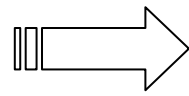
$$V_m^{mix} = \sum_{i=1}^m \alpha_i V_i^{in}$$

Assumption: linearity of potential residual

$$R(V_m^{mix}) = \sum_{i=1}^m \alpha_i R(V_i^{in})$$

Look for α_i giving the minimum $\langle R(V_m^{mix}) | R(V_m^{mix}) \rangle$ With $\sum_{i=1}^m \alpha_i = 1$

Charge conservation


$$\alpha_i = \frac{\sum_j (A_{ji})^{-1}}{\sum_{j,k} (A_{kj})^{-1}} \quad A_{ij} = \langle R(V_j^{in}) | R(V_i^{in}) \rangle$$

Pulay mixing – Theory 2

*Pulay mixing
2nd approach*

New formulation:
$$V_m^{mix} = V_m^{in} + \sum_{i=1}^{m-1} \bar{\alpha}_i (V_{i+1}^{in} - V_i^{in})$$

With new variables $\bar{\alpha}_i$

$$\bar{\alpha}_i = - \sum_{j=1}^{m-1} (\bar{A}_{ij})^{-1} \cdot \langle R(V_{j+1}^{in}) - R(V_j^{in}) | R(V_m^{in}) \rangle$$

$$\bar{A}_{ij} = \langle R(V_{j+1}^{in}) - R(V_j^{in}) | R(V_{i+1}^{in}) - R(V_i^{in}) \rangle$$

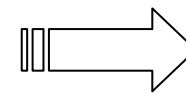
Charge conserved

$$V_{m+1}^{in} = V_m^{in} + P R(V_m^{in}) + \sum_{i=1}^{m-1} \bar{\alpha}_i [(V_{i+1}^{in} - V_i^{in}) + P (R(V_{i+1}^{in}) - R(V_i^{in}))]$$

Pulay mixing – Implementation in ABINIT

What do we need at each SCF step ?

- Previous values of \bar{A}_{ij} for $i < m, j < m$
- Previous value of V_i^{in}
- Previous values of $R(V_i^{in})$ for $i < m$
- Previous values of $P R(V_i^{in})$ for $i < m$



*(2m+2) « big »
arrays to store*

*(f_fftgr Fortran array
in scfcv)*

A « sliding » storage

Where are quantities computed ?

- Arrays allocation : **scfcv**
- Mixing driver : **newvtr, newrho**
- Residual preconditioning : **prcref**
- Pulay mixing of potentials and residuals : **scfopt**

Pulay mixing – ABINIT keywords

iscf : Integer for Self-Consistent-Field cycles

Controls the self-consistency.

Positive, non-zero values => this is the usual choice for doing the usual ground state (GS) calculations or for structural relaxation, where the potential has to be determined self-consistently. The choice between different algorithms for SCF is possible :

- =1 => get the largest eigenvalue of the SCF cycle (DEVELOP option, used with irdwfk=1 or irdwfk=1)
- =2 => SCF cycle, simple mixing of the potential
- =3 => SCF cycle, Anderson mixing of the potential
- =4 => SCF cycle, Anderson mixing of the potential based on the two previous iterations
- =5 => SCF cycle, CG based on the minim. of the energy with respect to the potential
- =7 => SCF cycle, **Pulay mixing** of the potential based on the **npulayit** previous iterations
- =12 => SCF cycle, simple mixing of the density
- =13 => SCF cycle, Anderson mixing of the density
- =14 => SCF cycle, Anderson mixing of the density based on the two previous iterations
- =15 => SCF cycle, CG based on the minim. of the energy with respect to the density
- =17 => SCF cycle, **Pulay mixing** of the density based on the **npulayit** previous iterations

npulayit : Number of PULAY ITerations for SC mixing

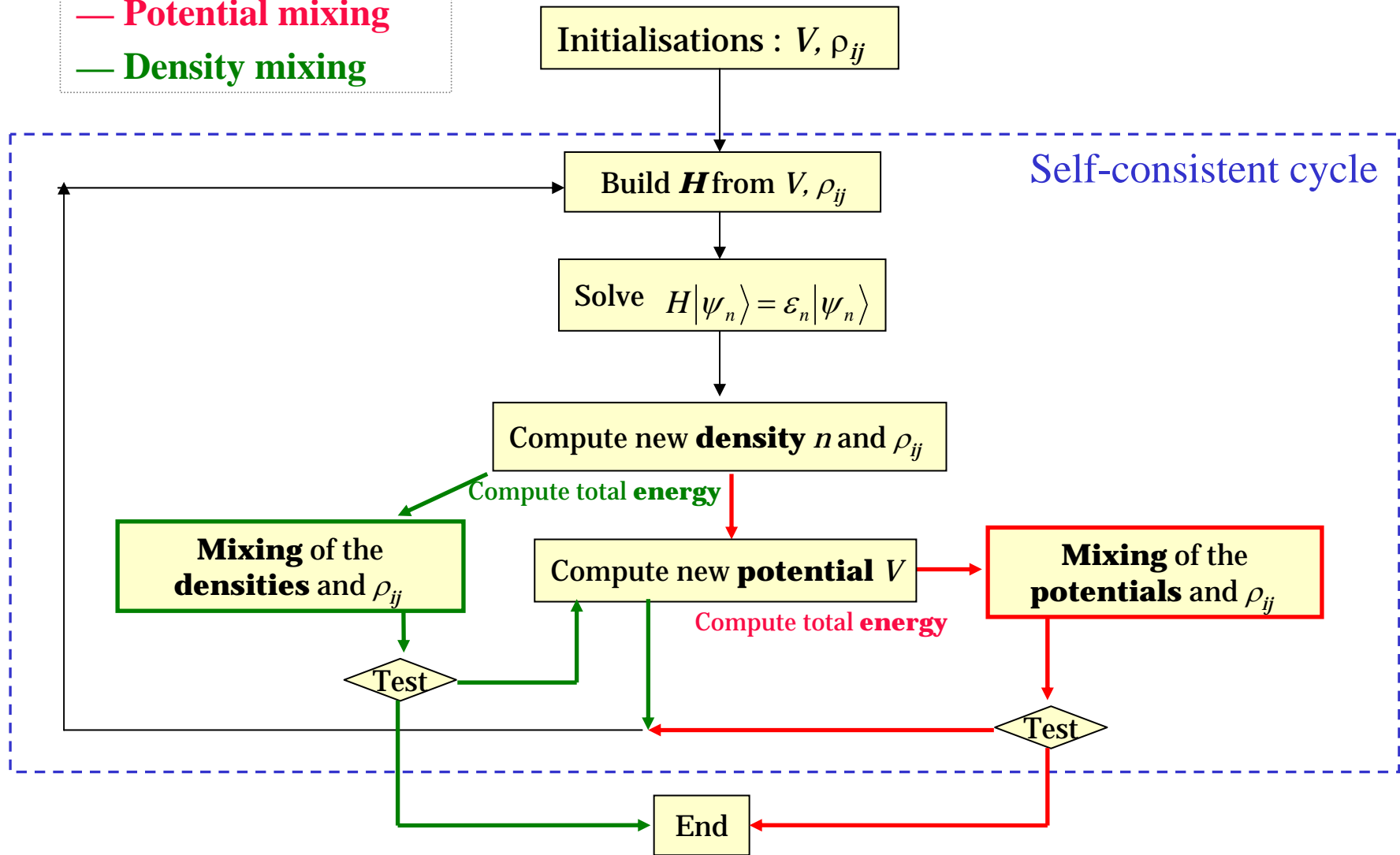
Needed only when iscf=7 or 17.

Gives the number of previous iterations involved in **Pulay mixing** (mixing during electronic SC iterations).

Default is 7

Potential mixing vs density mixing - 1

— Potential mixing
— Density mixing



Potential mixing vs density mixing - 2

Potential mixing

Total energy is computed
after potential update

Mixing is done at the end of
the iteration

*Every energy contribution
has been updated*

Perfect restart is available

Density mixing

Total energy is computed
after density update

Mixing is done in the middle
of the iteration

*Every energy contribution
has not been updated*

*Perfect restart is not
possible (if not converged)*



Has to use 2 different
decompositions of total energy

Potential mixing vs density mixing - 3

Mixing on "potential"...

« Direct » decomposition

$$E_{tot} = E_{Kin} + E_{Hartree} + E_{xc} + \int V_{loc} \cdot n + \underbrace{E_{non-local}}_{\text{Norm-conserving}} + \underbrace{E^1 - \tilde{E}^1}_{PAW}$$

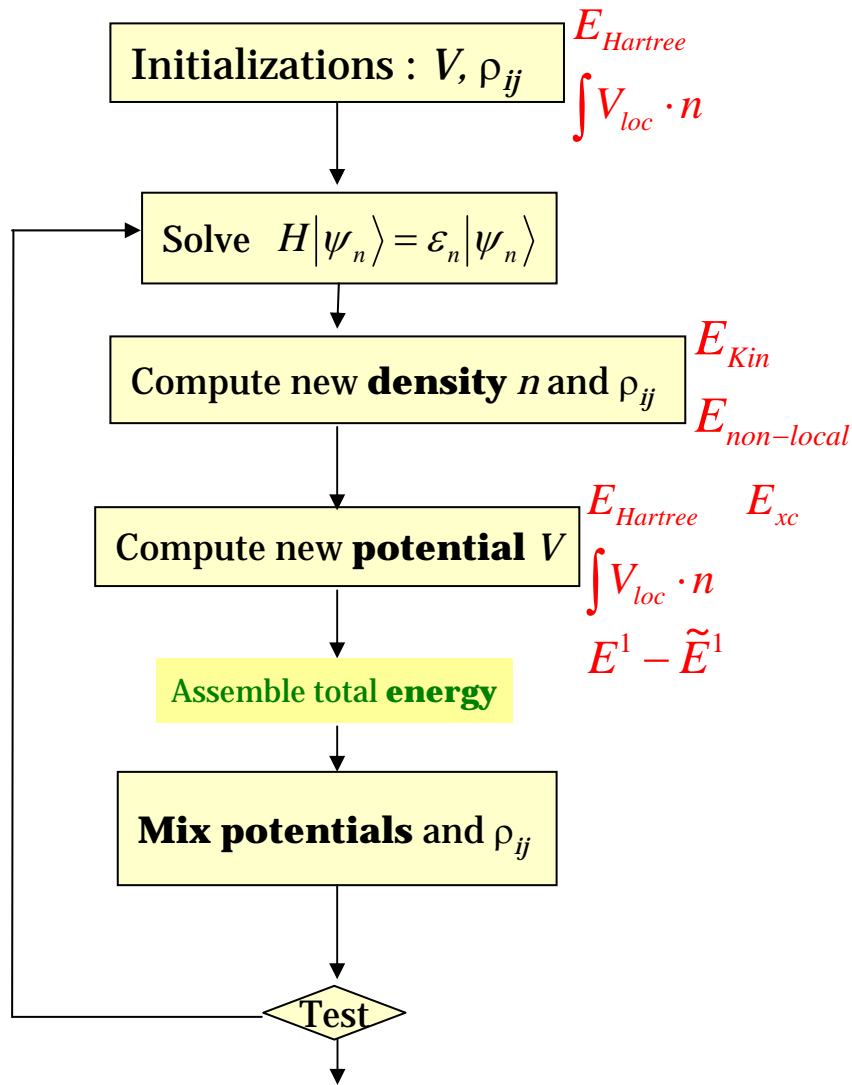
Mixing on "density"...

« Double-counting » decomposition

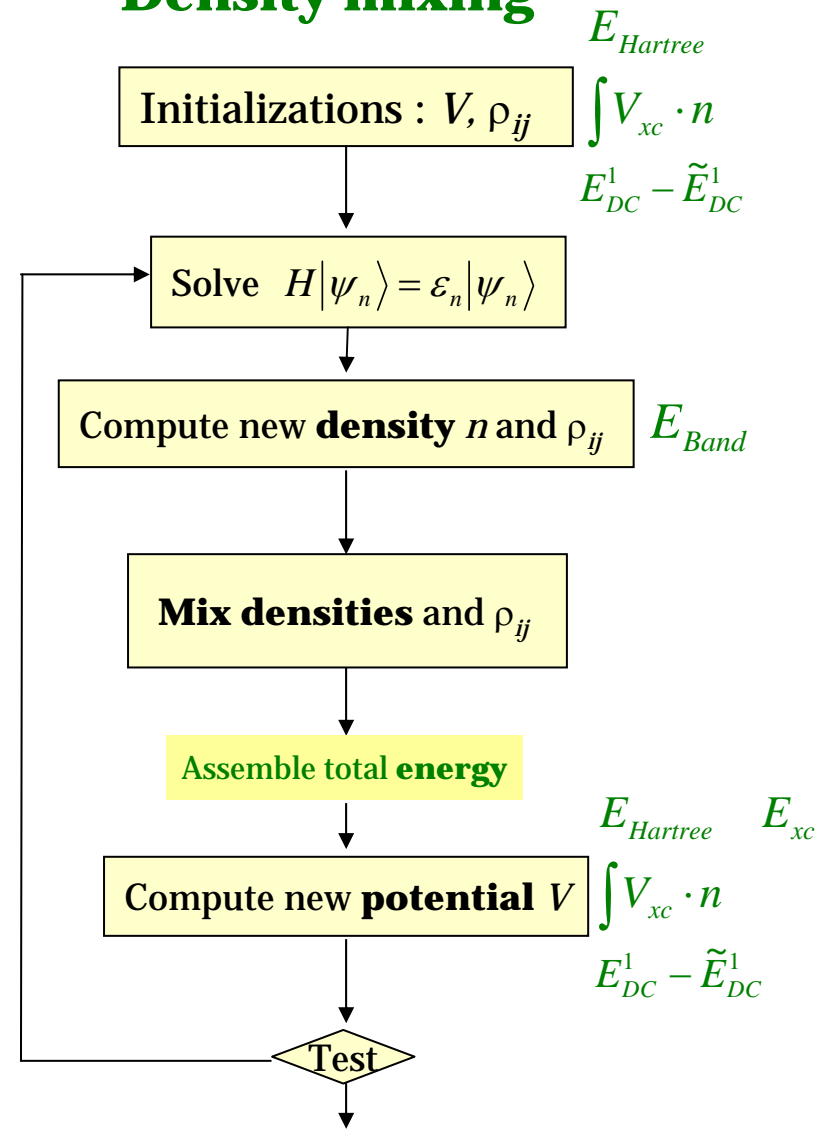
$$E_{tot}^{DC} = E_{Band} - E_{Hartree} + E_{xc} - \int V_{xc} \cdot n + \underbrace{E_{DC}^1 - \tilde{E}_{DC}^1}_{PAW}$$

Potential mixing vs density mixing - 4

Potential mixing



Density mixing



Potential mixing vs density mixing - 5

Mixing on potential is done when all energy contributions have been updated

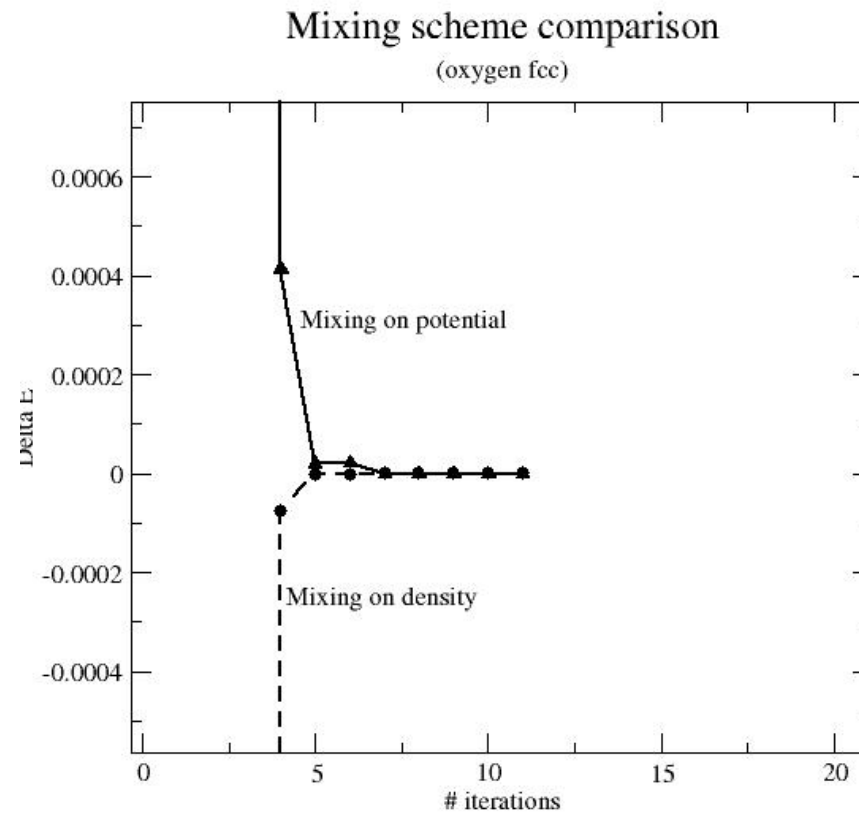


Energy is variational

Mixing on density is done when energy contributions have not been all updated



Energy is not variational (Harris-Foulkes -like)



Mixing within PAW - 1

$$\begin{aligned}
 E_{tot} &= E_{Kin} + E_{Hartree}(\tilde{n} + \hat{n}) + E_{xc}(\tilde{n} + \hat{n}) \\
 &+ \int V_{loc}(\tilde{n} + \hat{n}) \cdot (\tilde{n} + \hat{n}) + E^1(n^1) - \tilde{E}^1(\tilde{n}^1 + \hat{n}) \\
 E_{tot}^{DC} &= E_{Band} - E_{Hartree}(\tilde{n} + \hat{n}) + E_{xc}(\tilde{n} + \hat{n}) \\
 &- \int v_{xc}(\tilde{n} + \hat{n}) \cdot (\tilde{n} + \hat{n}) + E_{DC}^1(n^1) - \tilde{E}_{DC}^1(\tilde{n}^1 + \hat{n})
 \end{aligned}$$

$$\tilde{n}(\mathbf{r}) = \sum f_n \langle \tilde{\psi}_n | \mathbf{r} \rangle \langle \mathbf{r} | \tilde{\psi}_n \rangle$$

$$n^1(\mathbf{r}) = \sum_{i,j,R} \rho_{ij}^R \langle \phi_i | \mathbf{r} \rangle \langle \mathbf{r} | \phi_j \rangle$$

$$\tilde{n}^1(\mathbf{r}) = \sum_{i,j,R} \rho_{ij}^R \langle \tilde{\phi}_i | \mathbf{r} \rangle \langle \mathbf{r} | \tilde{\phi}_j \rangle$$

$$\hat{n}(\mathbf{r}) = \sum_{i,j,R} \rho_{ij}^R \hat{Q}_{ij}^L(\mathbf{r})$$

Quantities to be mixed:

$$\begin{aligned}
 &(\tilde{n} + \hat{n}) \\
 &\rho_{ij}^R
 \end{aligned}$$

Mixing within PAW - 2

- ρ_{ij} is updated at the same time as density; therefore, use of density mixing is recommended for PAW.
- ρ_{ij} and density have to be mixed simultaneously and with the SAME MIXING scheme (Pulay, Anderson, ...)
- As D_{ij} quantities (non-local terms) are updated at the same time as potential, it should be better to mix them with the potential.
 ρ_{ij} and D_{ij} play a symmetric role in total energy.

$$E_{non-local} = \sum_{ij} \rho_{ij} D_{ij}$$

Mixing within PAW - 3

- Mixing ρ_{ij} and potential is available in ABINIT and convergency of the SCF cycle is good.
- Potentials/densities are stored on the « fine » FFT grid ; this is memory consuming, especially with Pulay mixing.

It is possible to save memory:

- Mix « coarse » FFT grid contribution with Pulay scheme
- Mix « fine » FFT grid contribution with a linear scheme

(see *pawmixdg* keyword)

Mixing within PAW – ABINIT keywords

pawmixdg : PAW - MIXing is done (or not) on the (fine) Double Grid

The choice made for this variable determine on which grid the density (or potential) is mixed during the SCF cycle.

- If **pawmixdg=1** the density/potential is mixed in REAL space using the fine FFT grid (defined by pawcutdg or ngfftdg).
- If **pawmixdg=0** the density/potential is mixed in RECIPROCAL space using the coarse FFT grid (defined by ecut or ngfft). Only components of the coarse grid are mixed using the scheme defined by [iscf](#); other components are only preconditionned by diemix and simply mixed.

This option is useful to save memory and does not affect numerical accuracy of converged results. If **pawmixdg=1**, density and corresponding residual are stored for previous iterations and are REAL arrays of size nfftdg. If **pawmixdg=0**, density and corresponding residual are stored for previous iterations and are COMPLEX arrays of size nfft. The memory saving is particularly efficient when using the Pulay mixing (iscf=7 or 17).

pawlmix : PAW - maximum L used in the spherical part MIXing

pawoptmix : PAW - OPTion for the MIXing of the spherical part

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← *Only for
developers and
experienced users*

Conclusion

- Pulay mixing :
 - Efficient and simple scheme
- Mixing on potential/density:
 - Both are (nearly) equivalents
 - Prefer density mixing within PAW
- Mixing within PAW :
 - $(\tilde{n} + \hat{n})$ and ρ_{ij}^R mixings have to be consistent
 - Prefer mixing on “coarse” grid