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PAW IMPLEMENTATION IN ABINIT AND ATOMIC DATA GENERATION

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Summary

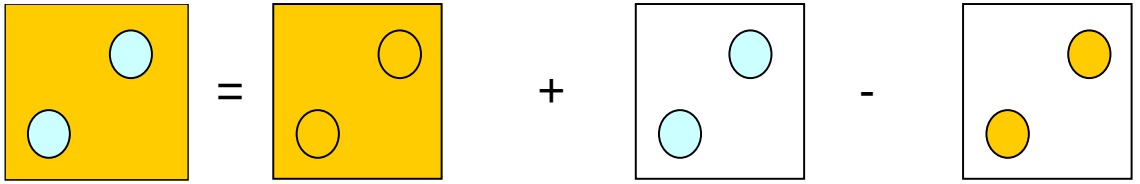
- PAW implementation in ABINIT: State of the art

- PAW atomic data generators for ABINIT

PAW implementation in ABINIT- state of the art

$$|\Psi_n\rangle = |\tilde{\Psi}_n\rangle + \sum_i \left(|\phi_i\rangle - |\tilde{\phi}_i\rangle \right) \langle \tilde{p}_i | \tilde{\Psi}_n \rangle$$

Wave functions:



Hamiltonian: $H\tilde{\psi}_n = \varepsilon_n S\tilde{\psi}_n$

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

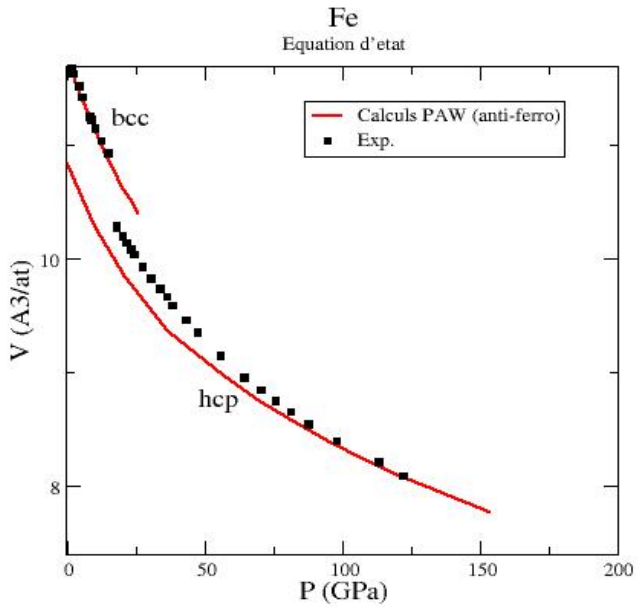
Electronic density → Ground state properties

Energy Forces Stresses

- P. Blöchl, Phys. Rev. B **50**, 17953 (1994)

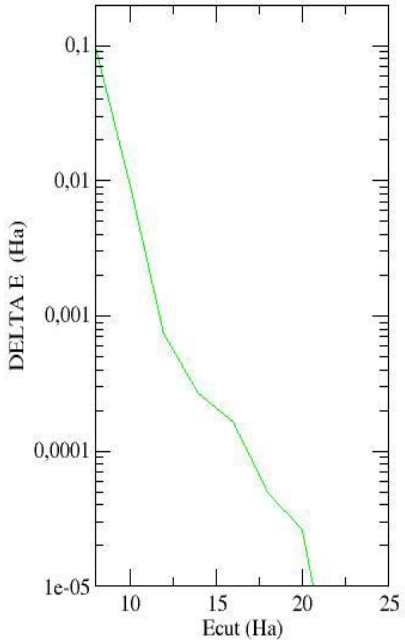
PAW implementation in ABINIT- state of the art

Iron equation of state:



A. Dewaele, P. Loubeyre, F. Ocelli, M. Mezouar,
P.I. Dorogokupets, M. Torrent,
PRL, 97, 215504 (2005)

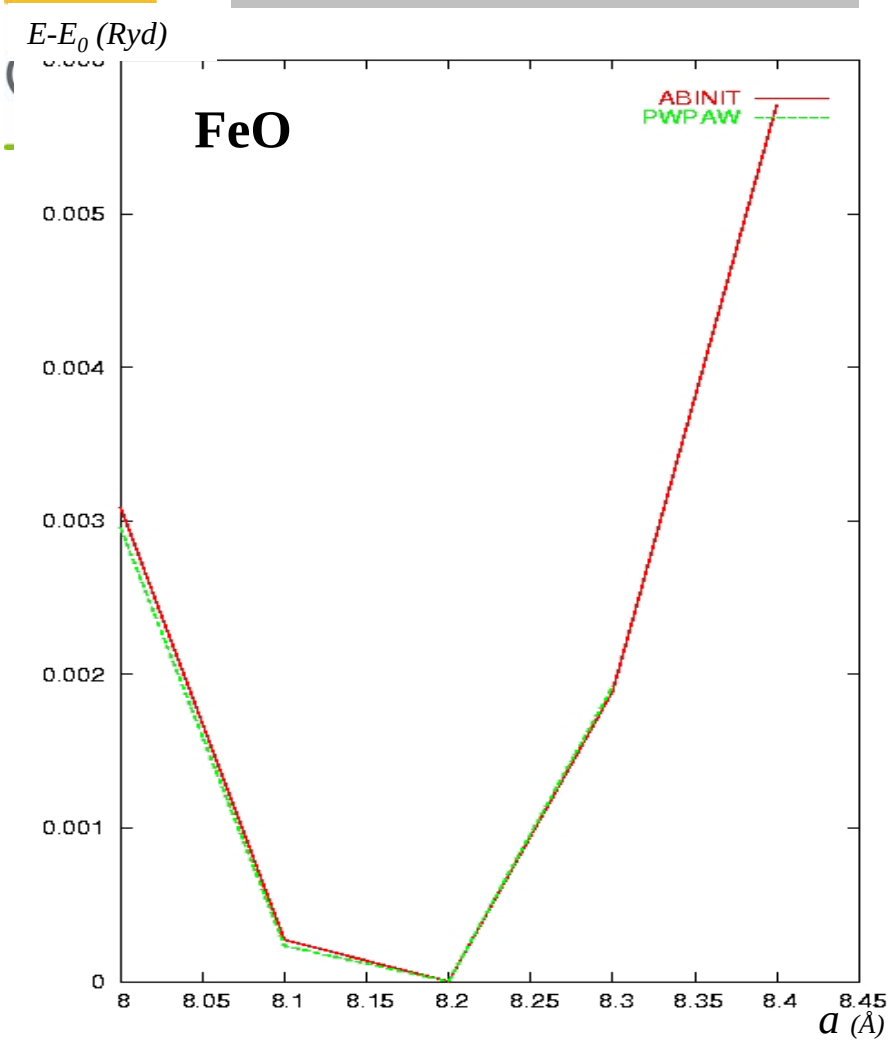
Cutoff convergency

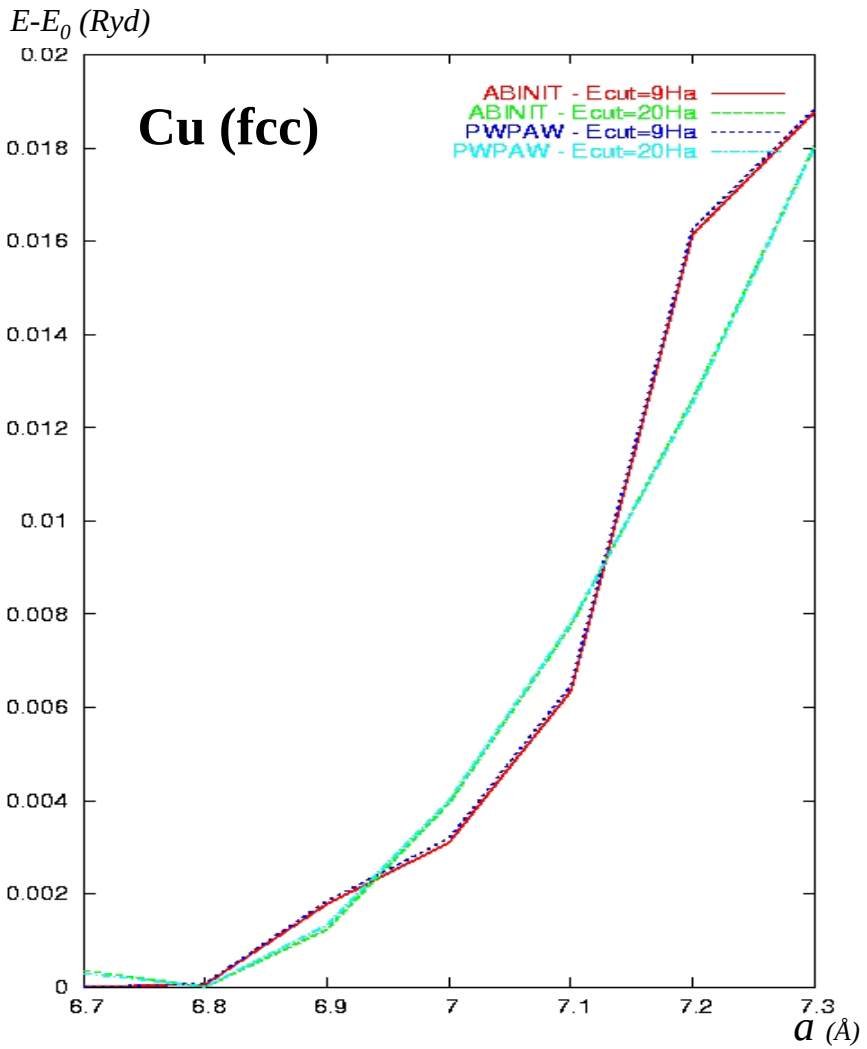


PAW implementation in ABINIT- state of the art

PWPAW using $\bar{v}$
vs ABINIT using $v_H(\tilde{n}_{ZC})$

No significative difference between results even when convergence not reached





PAW implementation in ABINIT- state of the art

New developments:

- GS parallelisation	F. Bottin talk
- XML format for atomic data	
- LDA + U	B. Amadon talk
- Wannier functions	
- Electrical conductivity	S. Mazevet talk
- Core level absorption	
- Linear response (phonons)	M. Torrent talk

PAW implementation in ABINIT- state of the art

How to develop a new functionality in the PAW framework?

General way:

apply the PAW transformation to the formula you want to code

$$M = \langle \Psi | A | \Psi \rangle = \langle \tilde{\Psi} | \tilde{A} | \tilde{\Psi} \rangle \qquad \text{with} \qquad \tilde{A} = A + \sum_{i,j} | p_i \rangle \left(\langle \phi_i | A | \phi_j \rangle - \langle \tilde{\phi}_i | A | \tilde{\phi}_j \rangle \right) \langle p_j |$$

where A is a local operator

Examples:

Wannier functions: $A = e^{-i\vec{b}\vec{r}}$

Conductivity: $A = \langle \Psi_n | \nabla | \Psi_m \rangle$

Linear response

PAW implementation in ABINIT- state of the art

Approximate way: case of localized wavefunctions

When the wavefunction Ψ_n is localized in the PAW sphere, the quantity

$M = \langle \Psi_n | A | \Psi_m \rangle$ is to be calculated only in the sphere, in which $\tilde{\Psi} = \sum_i \langle p_i | \tilde{\Psi} \rangle \tilde{\phi}_i$ if the partial wave basis is complete.

In this case, $M \approx \sum_{i,j} \langle \tilde{\Psi}_n | p_i \rangle \langle \phi_i | A | \phi_j \rangle \langle p_j | \tilde{\Psi}_m \rangle$

Examples: Core level absorption, LDA+U (localized operator)

The key quantity is: $\langle \tilde{\Psi} | p_i \rangle$ It can be calculated calling ctocproj.F90, in outscfcv.F90 for instance

You can easily develop in the PAW framework !

The PAW method

APPROXIMATIONS :

- Frozen core approximation
- The partial wave basis is truncated
- The plane wave basis is truncated

ADVANTAGES :

- Total density of the system is computed ➢ no transferability problem
- Plane wave cutoff equivalent to ultra-soft pseudopotentials (no norm-conserving constraint)
- The PAW method is as précise as an all electron method. Convergency can be controlled.
- It can be shown that ultrasoft and norm-conserving methods are approximations of the PAW method.

ATOMIC DATA:

We need the following atomic data: $\{\phi_i\}, \{\tilde{\phi}_i\}, \{\tilde{p}_i\}, V_H[\tilde{n}_{Zc}], n_c, \tilde{n}_c$

Building atomic data for PAW

USPP

Ultrasoft pseudopotential generator

Written by David Vanderbilt

Rutgers, The State University of New Jersey

Add a "plugin" into USPP…

Only have to use USPP to produce a file for Abinit

- Fully documented by D. Vanderbilt…
- Set of input files downloadable on D. Vanderbilt's site…

Downloadable on abinit.org

AtomPAW

PAW atomic data generator for "PWPAW"

Written by Natalie Holzwarth and coworkers

Dept. of Physics, Wake Forest University

Launch AtomPAW and a converter separately… *Atompaw2abinit*

.Fully documented by M.Torrent

Downloadable on abinit.org

New versions have been updated

Building atomic data for PAW

	USPP	ATOMPAW
Step 1: Choose a radial grid	Log	Log, lin
Step 2: All electron atomic calculation	Schrod. , Scal. Rel.	Schrod. , Scal. Rel.

- Atomic Schrödinger equation: $n_c(r), V_{ae}(r)$
- Choose an energy set $\{\varepsilon_i\}$ and radii $\{r_i\}$ and invert the Schrödinger equation: $\{\phi_i(r)\}$

Step 3: Pseudize the local potential

V_{loc} and V_{ae} join in r_{loc} — TM, polynom | TM, polynom, bessel

Step 4: Choose a scheme to obtain pseudowavefunctions and projectors

- The Vanderbilt scheme:
  - $\tilde{\phi}_i$ and ϕ_i join in r_i — polynom | polynom, bessel
  - Get auxilliary functions $|\chi_i\rangle = -[-\nabla^2 + V_{loc} - \varepsilon_i]|\tilde{\varphi}_i\rangle$
  - Get projectors from auxilliary functions by $|\tilde{p}_i\rangle = \sum_j (B)^{-1}_{ij} |\chi_j\rangle$ with $\beta_{ij} = \langle \tilde{\varphi}_i | \chi_j \rangle$
- The Blöchl scheme:
  - Choice of shape function *k(r)*
  - Get preliminary pseudo functions by $\left[-\nabla^2 + V_{loc} - \varepsilon_i - C_i k(r)\right]|\tilde{\varphi}_i^0\rangle = 0$
  - Get preliminary projectors by $|\tilde{p}_i^0\rangle = \left[-\nabla^2 + V_{loc} - \varepsilon_i\right]|\tilde{\varphi}_i^0\rangle$
  - *Gram-Schmidt* orthogonalization to get $|\tilde{\varphi}_i\rangle$, $|\tilde{p}_i\rangle$

Building atomic data for PAW

USPP | ATOMPAW

Step 5: Pseudize the core density

n_c and $\tilde{n}_c$ join in r_{core}

polynom | polynom

Step 6: Compute $v_H[\tilde{n}_{Zc}]$ by unscreening V_{loc}

$$v_H(\tilde{n}_{ZC}) = v_{loc} - v_H(\tilde{n} + \hat{n} + \tilde{n}_c) - v_{xc}(\tilde{n} + \hat{n} + \tilde{n}_c)$$

Choose a shape function for $\hat{n}$

num | sinc, gauss, bessel

Atomic data validation

Accuracy

The PAW calculation must give the same physical results as a reference all electron calculation

Efficiency

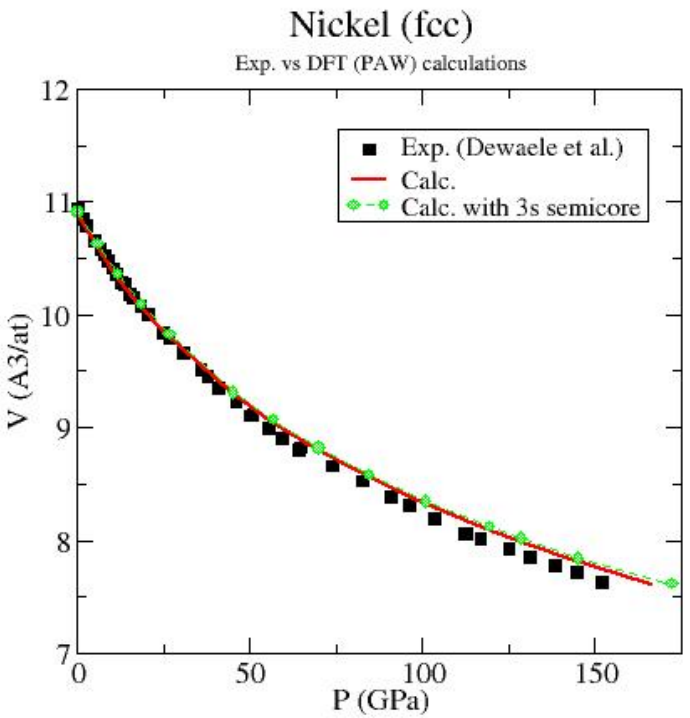
The plane wave basis must be as minimal as possible

Good atomic data are always a compromise between accuracy and efficiency

Building atomic data for PAW

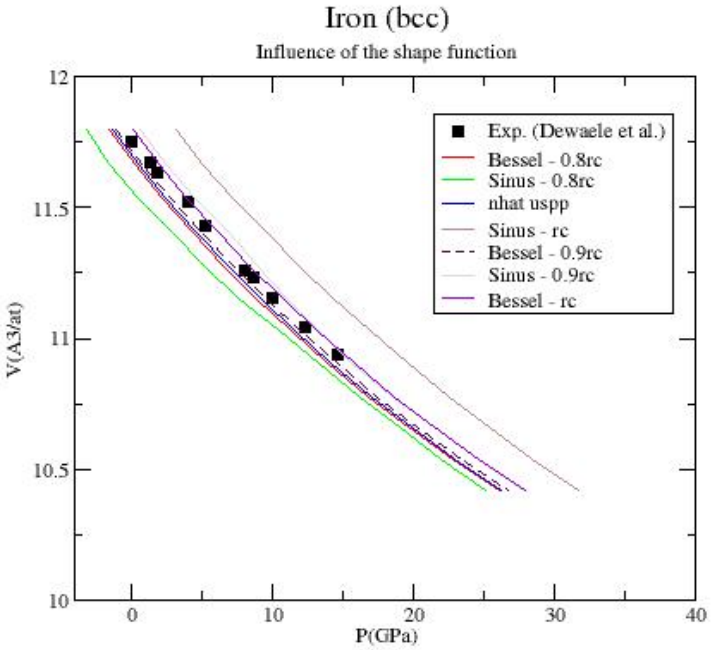
```
Nickel 28.
GGA-PBE loggrid 1500 scalarrelativistic pointnucleus
4 4 3 0 0          ! Up to 4s, 4p and 3d
3 2 9.0! Electronic configuration 3d⁹ 4s¹ 4p⁰
4 0 1.0
4 1 0.0
0 0 0
c                  ! 1s
c                  ! 2s
c                  ! 3s
v                  ! 4s valence
c                  ! 2p
c                  ! 3p
v                  ! 4p valence
v                  ! 3d valence
2                  ! Basis contains s, p and d partial-waves
2.3 2.3 1.1 2.2    ! rpaw=2.3, rshape=2.3, rveff=1.1, rcore=2.2
y                  ! Additional s partial-wave
4.                 ! at Eref=4.0 Ha
n
y                  ! Additional p partial-wave
4.                 ! at Eref=4.0 Ha
n
y                  ! Additional d partial-wave
2.5                ! at Eref=2.5 Ha
n
custom rrkj grahamschmidtortho sinc  ! RRKJ PW + sinc shape func.
Bessel             ! Simple Bessel Vloc
2.3                ! Matching radius for Phi1 (l=0)
2.3                ! Matching radius for Phi2 (l=0)
2.3                ! Matching radius for Phi3 (l=1)
2.3                ! Matching radius for Phi4 (l=1)
2.3                ! Matching radius for Phi5 (l=2)
2.3                ! Matching radius for Phi6 (l=2)
0                  ! END
```

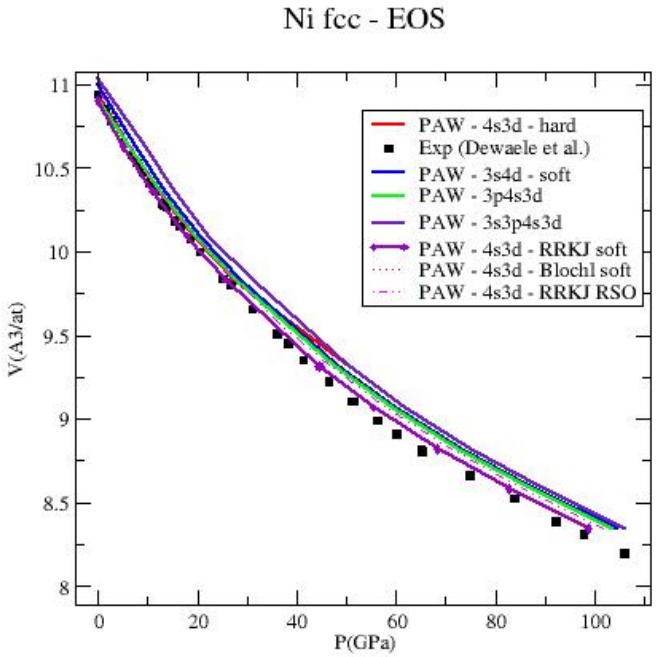
Input file for ATOMPAW



Building atomic data for PAW

Parameters adjustment…





…can be tedious

Conclusion

PAW atomic data generation needs a **trial-error** type of adjustment

Each set of data must be **tested** in the context of each

- Two types of atomic data now available
- Abinit's user can download/generate atomic data
- Fully documented on Abinit's web site

To be continued…

- Evaluate accuracy and performance for elements of the periodic table
- XML "universal" format for PAW atomic data
- Spin orbit ?