PAW for Abinit

M. Torrent , F. Jollet, G. Zerah, F. Bottin

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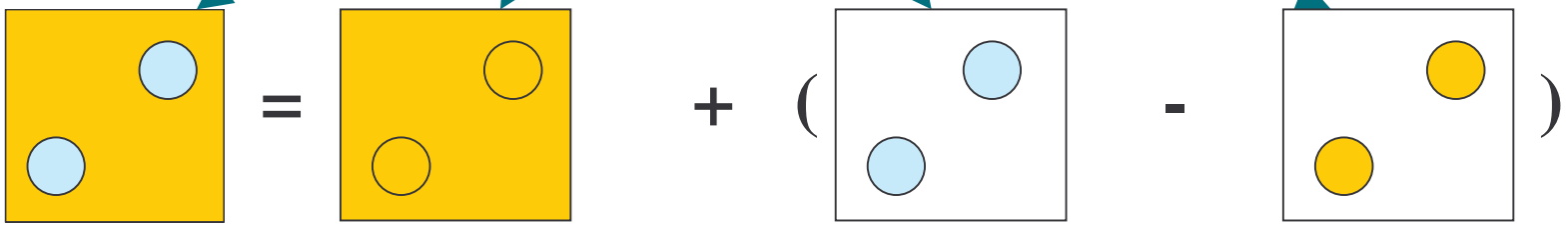
Introduction

PAW atomic data generation

Implementation of PAW formalism:
present, future and perspectives

PAW – Framework

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



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

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

~ → Plane-waves development in the whole FFT box

1 → Development over spherical partial waves of AE quantities

~1 → Development over spherical partial waves of PSEUDIZED quantities

PAW – Framework

$$H\tilde{\Psi}_n = \varepsilon_n S\tilde{\Psi}_n$$

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

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

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

$$\tilde{v}_{eff} = v_H\left[\tilde{n}_{Z+C} + \tilde{n} + \hat{n}\right] + v_{xc}\left[\tilde{n}_C + \tilde{n} + \hat{n}\right]$$

$$\hat{Q}_{ij}^L(r) = q_{ij}^L g_l(r) Y_L(r)$$

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

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

PAW atomic data generation for Abinit

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- What do we need for a PAW calculation in Abinit ?
- Two PAW Atomic data generators for Abinit
- Performances and accuracy
- Practical example

Motivations…

PAW in Abinit:
Need to produce specific "PSP" files
(pspcod=7)

- Simplicity and accessibility for user
- Availability on web site
- Abinit needs specific PAW tools (models, format)

- Work of the last 6 months (2003/04)
- PAW in Abinit was improved (perf, accuracy)
- Need for PAW "input" data became clearer

PAW – Framework

$$H\tilde{\Psi}_n = \varepsilon_n S\tilde{\Psi}_n$$

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

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

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

$$\tilde{v}_{eff} = v_H\left[\tilde{n}_{Z+C} + \tilde{n} + \hat{n}\right] + v_{xc}\left[\tilde{n}_C + \tilde{n} + \hat{n}\right]$$

$$\hat{Q}_{ij}^L(r) = q_{ij}^L g_l(r) Y_L(r)$$

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

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

PAW – What is frozen during e⁻ iterations

$$H\tilde{\Psi}_n = \varepsilon_n S\tilde{\Psi}_n$$

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

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

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

$$\tilde{v}_{eff} = v_H\left[\tilde{n}_{Z+C} + \tilde{n} + \hat{n}\right] + v_{xc}\left[\tilde{n}_C + \tilde{n} + \hat{n}\right]$$

V_{loc}

$n_c(r)$

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

$$\hat{Q}_{ij}^L(r) = q_{ij}^L g_l(r) Y_L(r)$$

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

Starting value

PAW in Abinit – Atomic data needed…

- Definition of spheres: r_c, radial grids definitions
- Partial waves: $\varphi_i(r)$
- Pseudized partial waves: $\tilde{\varphi}_i(r)$ $\quad i = l,m,n$
- Nonlocal Projectors : $\tilde{p}_i(r)$
- Core density: $n_c(r)$
- Pseudized core density: $\tilde{n}_c(r)$
- Compensation *"shape"* functions: $g_l(r)$
- Frozen part of D_{ij}: D_{ij}^0
- Starting value for ρ_{ij}: ρ_{ij}^0
- Local potential $v_H(\tilde{n}_{Z+C})$: $V_{loc}(r)$

Building PAW atomic data…

1 All-electrons atomic calculation

Get $\{\varepsilon_n^{at}\}, \{\varphi_n^{at}\}, \{f_n\}, V^{AE}(r), n_c(r)$

2 Chose $\{\varepsilon_i\}$ $i = l, m, n$ $\varepsilon_i = \varepsilon_n^{at}$ possible

Choose $\{r_c\}$

and reverse Sch. Equation to get $\{\varphi_i\}$

3 Pseudize $\{\varphi_i\}$ and $n_c(r)$

Get $\{\tilde{\varphi}_i\}$ $\tilde{n}_c(r)$

4 Get $\{\tilde{p}_i\}$ dual of $\{\tilde{\varphi}_i\}$

5 Compute $V_{loc}(r)$

Pseudize and unscreen $V^{AE}(r)$

Choose $g_l(r)$

6 Compute additional data

D_{ij}^0 ρ_{ij}^0

Atomic data "generators" for Abinit

- *Use of "existing" all-electrons and pseudized data*
- *Ultrasoft pseudization scheme*

- Use of "existing" ultrasoft generators
- Write "converters"

  - to compute additional PAW atomic data

  - to put data into Abinit's format

- Ultrasoft generators used

AtomPAW

PAW atomic data generator for "PWPAW"

Written by Natalie Holzwarth and coworkers

Dept. of Physics, Wake Forest University

USPP

Ultrasoft pseudopotential generator

Written by David Vanderbilt

Department of Physics and Astronomy

Rutgers, The State University of New Jersey

PAW atomic data – Generators and "converters"

From existing atomic data generator

- Definition of spheres: r_c, radial grids definitions
- Partial waves: $\varphi_i(r)$
- Pseudized partial waves: $\tilde{\varphi}_i(r)$ $i = l,m,n$
- Nonlocal Projectors : $\tilde{p}_i(r)$
- Core density: $n_c(r)$
- Pseudized core density: $\tilde{n}_c(r)$

In "converter"

- Compensation *"shape"* functions: $g_l(r)$
- Frozen part of D_{ij}: D_{ij}^0
- Starting value for ρ_{ij}: ρ_{ij}^0
- Local potential $v_H(\tilde{n}_{Z+C})$: $V_{loc}(r)$

PAW atomic data – Generators and "converters"

AtomPAW

Launch AtomPAW and a converter separately…

Only one input file

AtomPAW produces 3 files:
Atomic data, densities, potentials

3 files used by *AtomPAW2Abinit*

Downloadable on abinit.org

USPP

Add a "plugin" into USPP…

Extract "add-on" into USPP's directory and compile…

USPP's behaviour is not changed

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

PAW atomic data – Generators and "converters"

AtomPAW

AtomPAW

- Impose $\varepsilon_i = \varepsilon_n^{at}$
- Regular radial grid
- Shape function: sin or exp
- LDA or GGA
- No control on pseudiz. scheme

AtomPAW2Abinit

- Possibility to transfer some data onto a log. radial grid
- Possibility to optimize nonlocal projectors with King-Smith et al. Scheme
- Compute V_{loc} (Kresse's formulation)

USPP

USPP

- No constraint on ε_i
- Logarithmic radial grid
- LDA or GGA, multiple func.
- Efficient pseudiz. scheme
- Control on pseudiz. scheme

USpp2Abinit

- Possibility to optimize nonlocal projectors with King-Smith et al. Scheme
- Compute V_{loc} (Kresse's formulation)

Validating PAW atomic data…

Accuracy

- *Atomic level*

  Number of partial waves per atom ?

  Choice of reference energies for partial waves

  [Test] Logarithmic derivatives of the wave functions

$$\left[\phi_l^2(\varepsilon,r)\frac{d}{d\varepsilon}\frac{d}{dr}\ln\phi_l(\varepsilon,r)\right]$$

  [Test] Excited states

- *Solid level*

  Test of transferability on some physical properties

Performances

- Radius of augmentation regions (no overlap allowed)
- Number of partial waves per atom
- Pseudization scheme
- Size of radial grids
- $\tilde{p}_i(g)$ behaviour's for large g

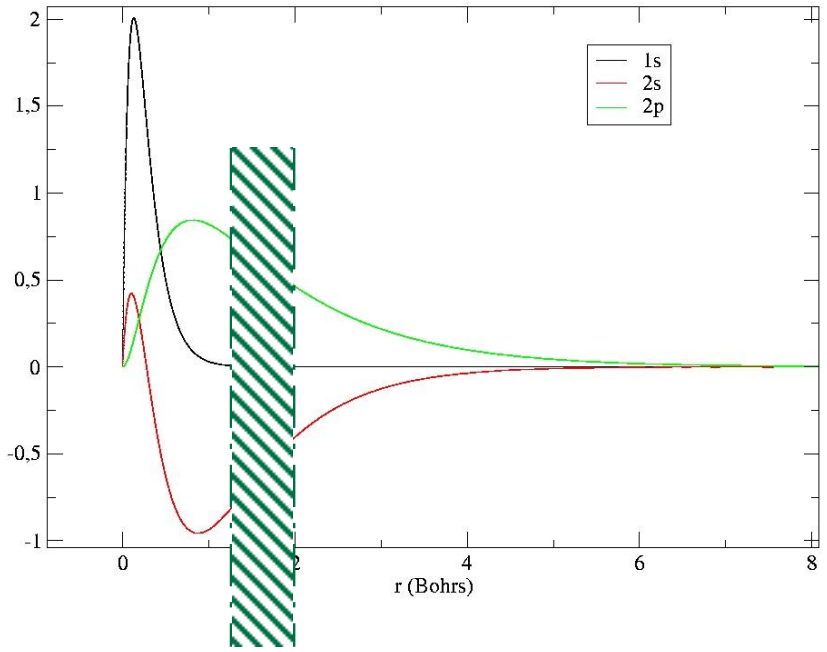
  King-Smith optimization
- Softness of $V_{loc}(r)$

Example: oxygen…

O : $1s^2 2s^2 2p^4$

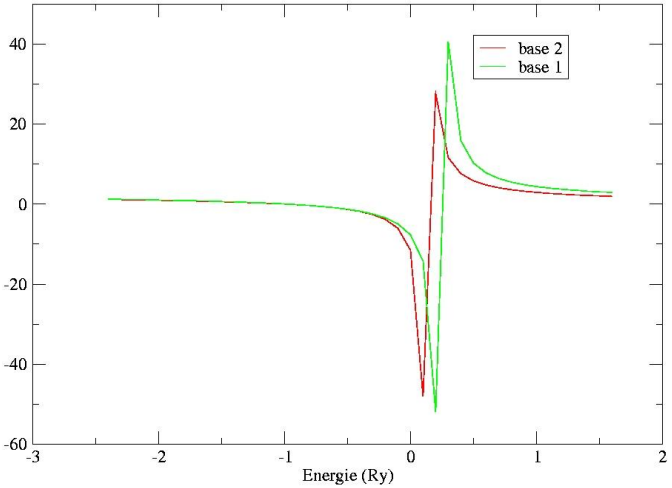
E(1s)=-37.51685 Ry
E(2s)=-1.74236 Ry
E(2p)=-0.6766 Ry

All-electrons wave functions



r_c

Log. Derivative (p-p) – r_c=1.3 au



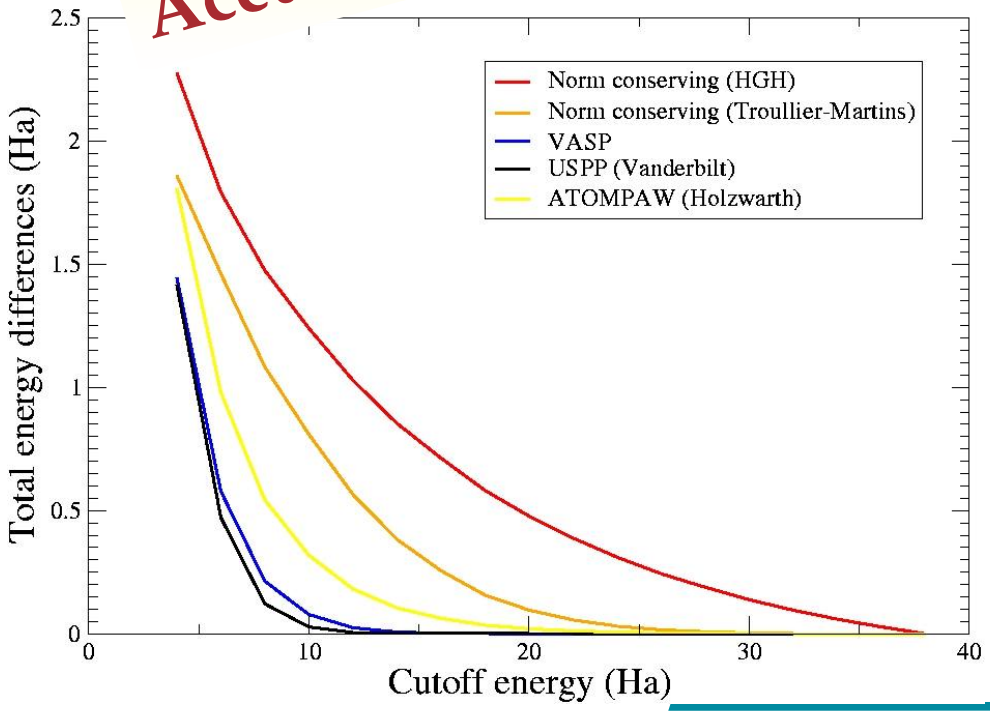
Choice of partial waves basis:
2 partial waves per angular momentum

Example: oxygen…

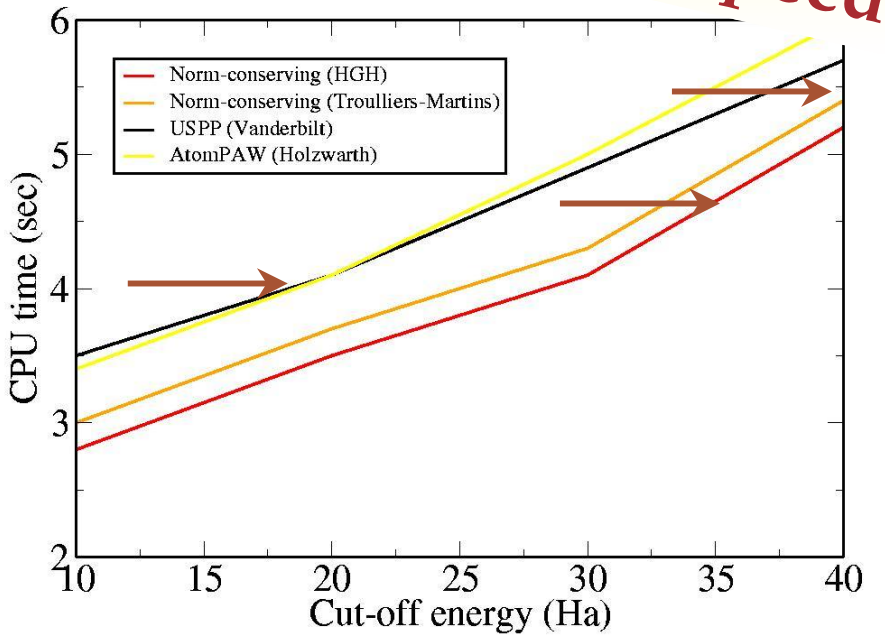
Model system: oxygen fcc

	NC HGH	NC TM	PAW Vasp	PAW AtomPAW	PAW USPP
Cut-off ΔE=1 mHa	50	35	20	26	22
a (Å)	3.11	3.10	3.09	3.07	3.06
B (GPa)	182		194	194	
E_{coh} (eV)	2.60		2.81	2.89	

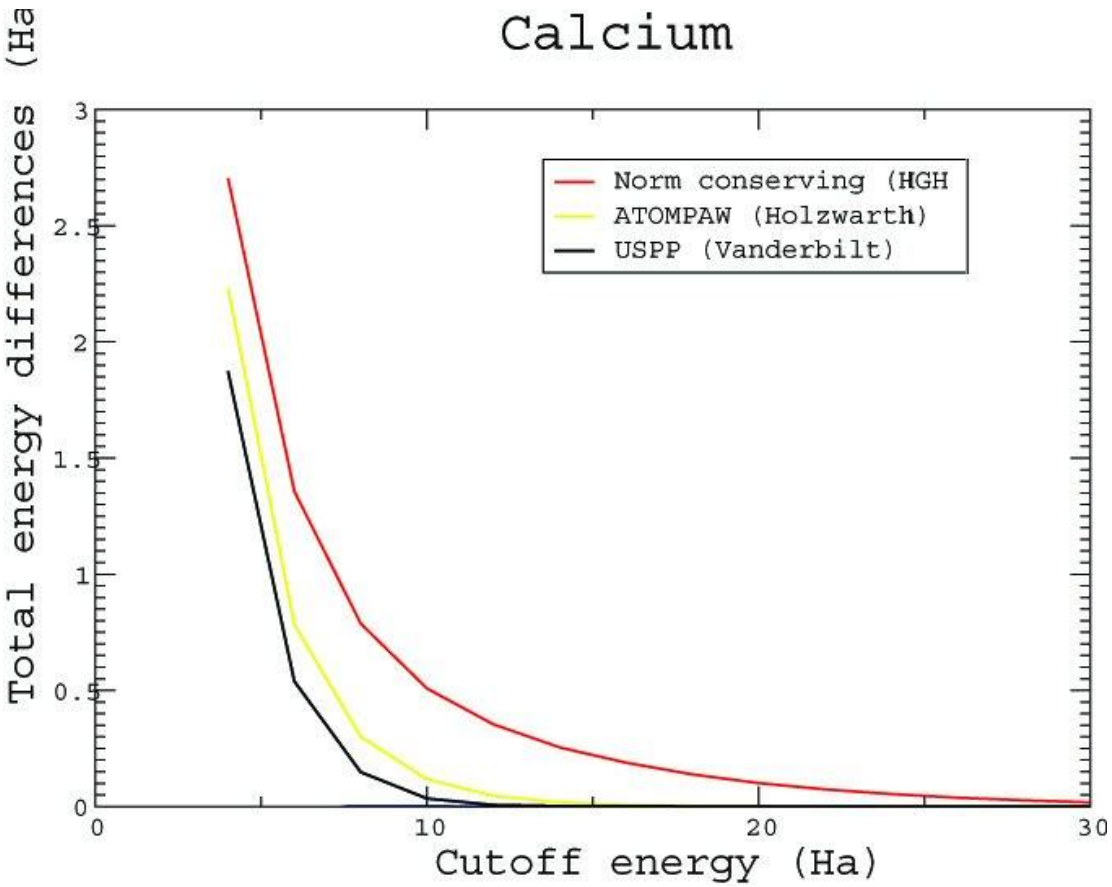
Accuracy



Speed



Convergence - example…



O.input

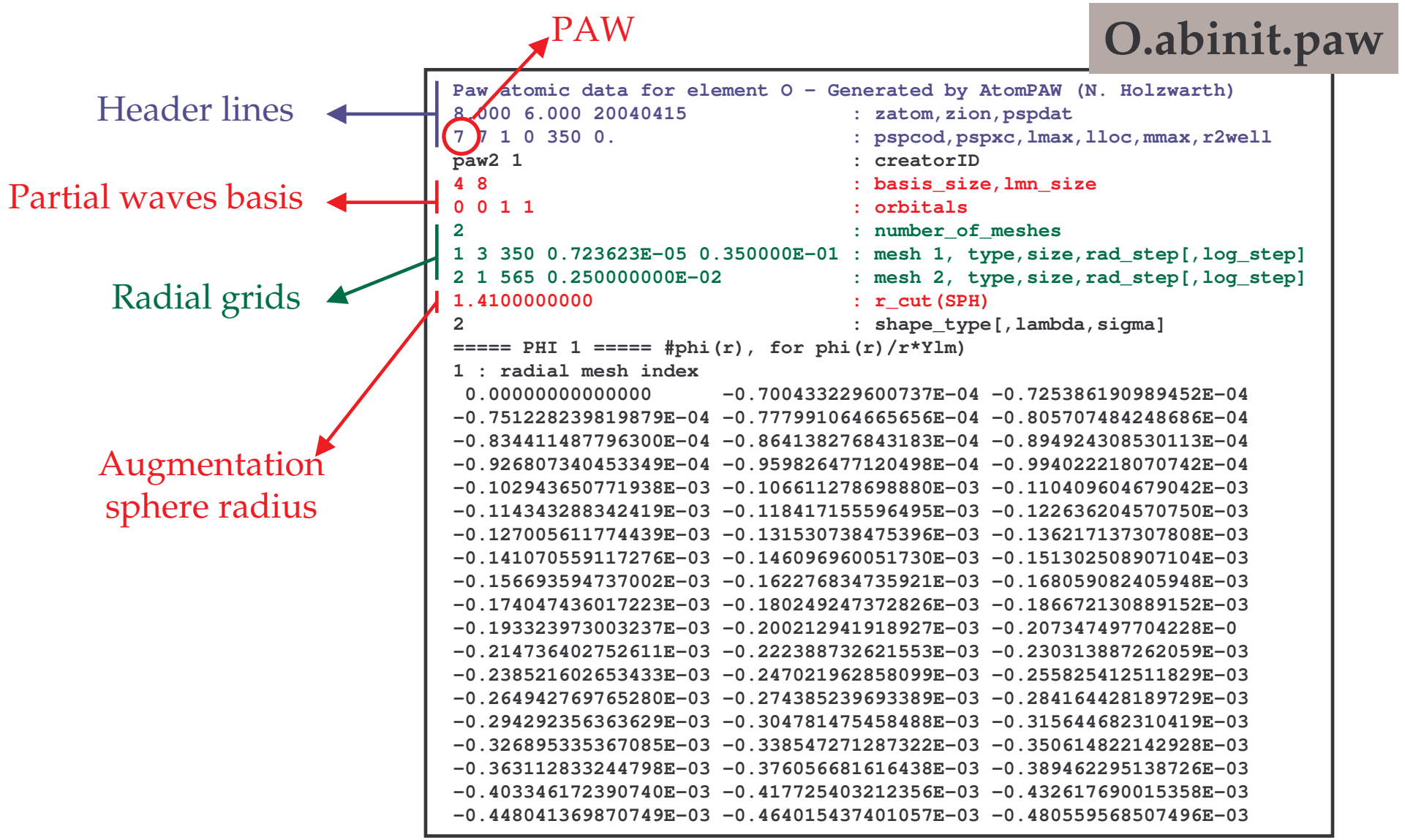
```
O                   Atom summary file name
'LDA-PW'    Z       exchange-correlation keyword
2 2 0 0 0           maximum n for s, p, d, f, g shells
2 1 4               correction to maximum occupancy (n l occ)
0 0 0               end corrections
c                   core state
v                   valence state
v                   valence state
vloc0               allow for Vloc contribution
2.3987351           Vloc amplitude
ipass               use default parameters
1                   lmax
1.4                 rc
y                   add new l=0 basis function
7                   energy of new l=0 basis function
n                   end of l=0 basis functions
y                   add new l=1 basis function
7                   energy of new l=1 basis function
n                   end of l=1 basis functions
O                   Atom symbole
```

AtomPAW + AtomPAW2Abinit

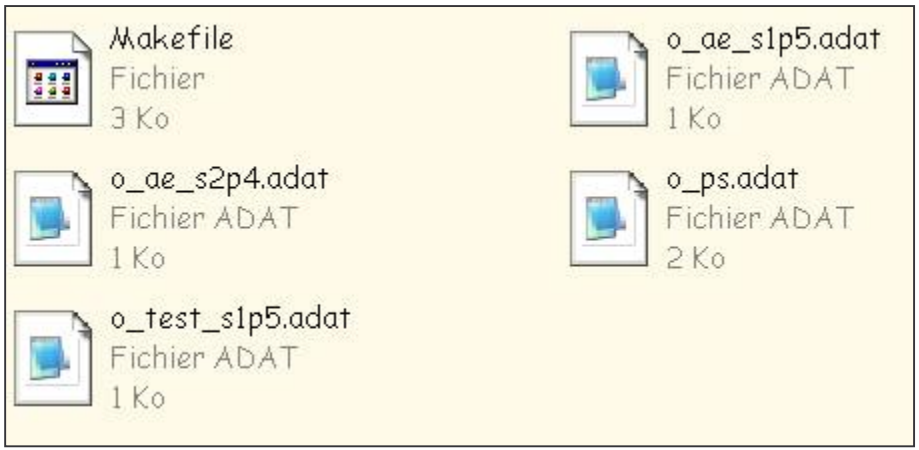
```
============================================================
==   atompaw2abinit - v1.4.0:                             ==
============================================================
Input atomicdata file name (from atompaw) [atomicdata] ?
Input densities file name (from atompaw) [density] ?
Input potentials file name (from atompaw) [potential] ?
Output psp file name (for Abinit) [abinit.pawps] ?
Do you want to transfer atomic data from AtomPAWon a (reduced) logarithmic grid
(recommended) [y] ?
Logarithmic grid: Number of pts, logarithmic step [350, 0.035] ?
Do you want to improve non-local projectorby using "Real Space Optimization" (King-Smith
et al.) [y] ?
Real Space optim.: Ecut, Gamma/Gmax, Wl(error) [20.0, 2.0, .1E-02] ?

Info:
  Mesh size for Vloc=Vhtnzc(r) has been set to   565
  with Vh(tnzc(  565))= -Z/r+  4.255E-07
Info:
  Optimizing non-local projectors
  using Real Space Optimization...
  Parameters: Ecut (Hartree)=  25.00
              Gamma/Gmax    =  2.00
              Wl max (error)=  0.100E-02
  New radius R0 for nl projectors (Bohr)= 1.4125 (= 1.0018*Rc)
Info:
  All quantities (except nl projectors) are transfered
  into a logarithmic grid (r(i)=A*exp[B(i-2)])...
  Log. grid parameters: rad_step=0.7236E-05
                        log_step=0.3500E-01
                        Size       = 350
                        Size (Vloc)= 350
Program ended.
```

AtomPAW + AtomPAW2Abinit



USPP + USPP2Abinit




```
============================================================
==   uspp2abinit - v1.6.0:                                ==
==   Use D. Vanderbilt ultrasoft psp generator (uspp)     ==
==   to produce a PAW atomic data file readable           ==
==   by Abinit (v4.3.1+)                                  ==
============================================================
> USpp->Abinit translator: reading uspp2abinit.dat...
> USpp->Abinit translator INFO:
  At r_vloc=r( 737), VHartree(ntild(Zv+Zc))= -Zv/r + -0.3033E-08
  This quantity must be as small as possible.
> USpp->Abinit translator INFO:
   Optimizing non-local projectors
   using Real Space Optimization...
   Parameters: Ecut (Hartree)=  15.00
               Gamma/Gmax    =  2.00
               Wl max (error)=  0.100E-02
   New radius R0 for nl projectors (Bohr)= 2.1552 (= 1.6350*Rc)
   Warning:  Radius for nl projectors (R0) seems to be high !
> PAW atomic data file successfully created.
```

USPP + USPP2Abinit

O.abinit.paw

Header lines

Partial waves basis

Radial grids

Augmentation sphere radius

```
Paw atomic data extracted from US-psp (D.Vanderbilt): oxygen
   8.000   6.000 20040503           : zatom,zion,pspdat
  7  2  1 0   494 0.                 : pspcod,pspxc,lmax,lloc,mmax,r2well
 paw2  2                            : creatorID
  4  8                               : basis_size,lmn_size
 0 0 1 1                            : orbitals
 3                                  : number_of_meshes
 1 2  494 0.309844E-03 0.169492E-01 : mesh 1, type,size,rad_step[,log_step]
 2 2  523 0.309844E-03 0.169492E-01 : mesh 2, type,size,rad_step[,log_step]
 3 2  737 0.309844E-03 0.169492E-01 : mesh 3, type,size,rad_step[,log_step]
  1.3181847962                      : r_cut(SPH)
 2                                  : shape_type[,lambda,sigma]
===== PHI 1 ===== #phi(r), for phi(r)/r*Ylm)
 1  : radial mesh index
0.00000000000000       0.531829581672144E-04  0.107274881307508E-03
0.162291177240415E-03  0.218247509442237E-03  0.275159801439171E-03
0.333044240984221E-03  0.391917284300236E-03  0.451795660390204E-03
0.512696375415963E-03  0.574636717146483E-03  0.637634259476910E-03
0.701706867019563E-03  0.766872699768094E-03  0.833150217836044E-03
0.900558186271021E-03  0.969115679945753E-03  0.103884208852728E-02
0.110975712152553E-02  0.118188081342260E-02  0.125523352888392E-02
0.132983596805278E-02  0.140570917192918E-02  0.148287452783473E-02
0.156135377496443E-02  0.164116901002693E-02  0.172234269297445E-02
0.180489765282357E-02  0.188885709356826E-02  0.197424460018628E-02
0.206108414474034E-02  0.214940009257505E-02  0.223921720861105E-02
0.233056066373737E-02  0.242345604130327E-02  0.251792934371063E-02
0.261400699910806E-02  0.271171586818773E-02  0.281108325108612E-02
0.291213689438951E-02  0.301490499824541E-02  0.311941622358069E-02
0.322569969942747E-02  0.333378503035754E-02  0.344370230402624E-02
0.355548209882649E-02  0.366915549165380E-02  0.378475406578295E-02
```

Abinit.org

UCL Unité de Physico–Chimie et de Physique des Matériaux

ABINIT's Homepage

In brief | Available versions | Pseudopotentials | PAW | Atomic Densities | Mailing | Utilities | Infos | Links | FAQ

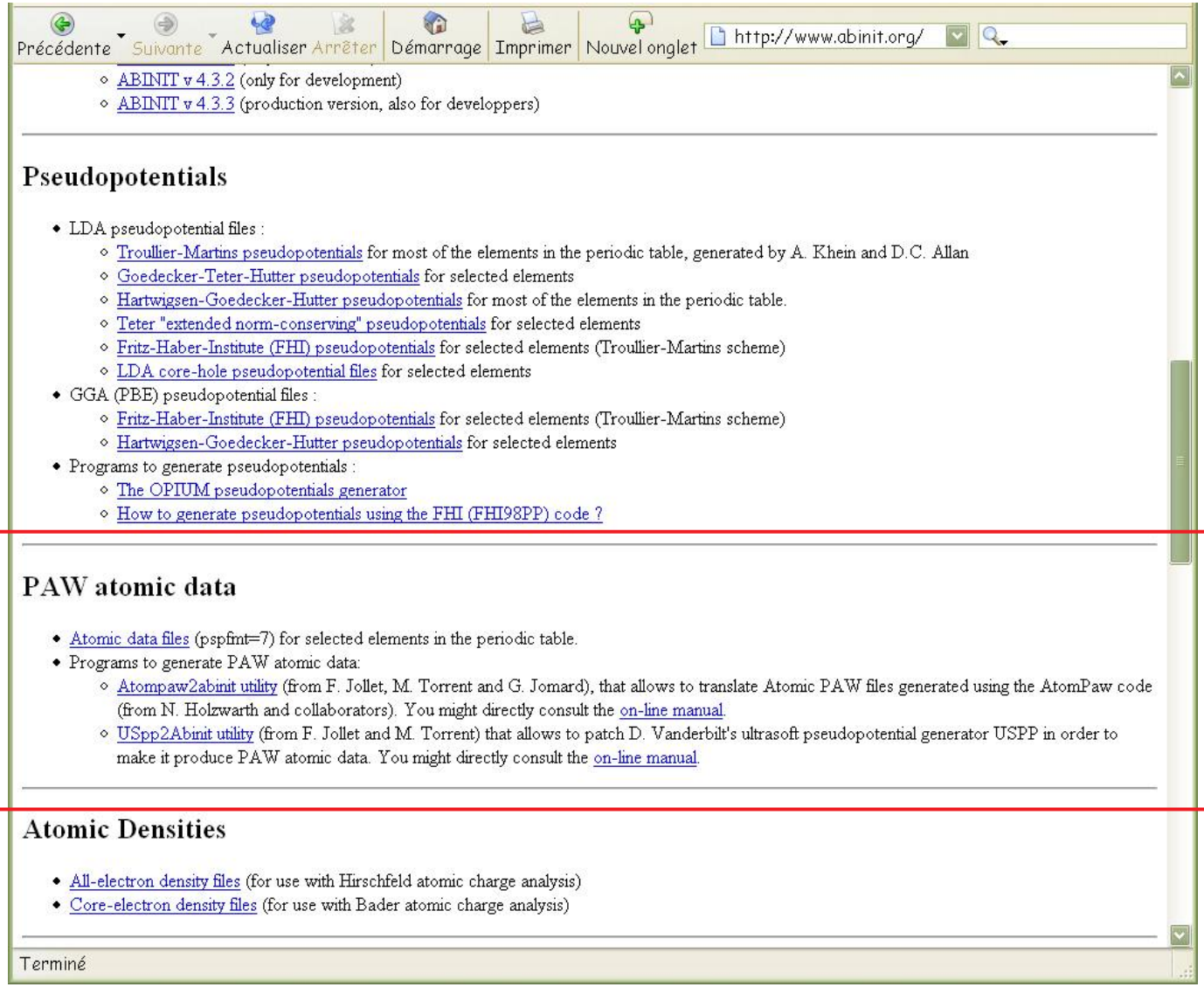
ABINIT is a package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a planewave basis. ABINIT also includes options to optimize the geometry according to the DFT forces and stresses, or to perform molecular dynamics simulation using these forces, or to generate dynamical matrices, Born effective charges, and dielectric tensors. Excited states can be computed within the Time-Dependent Density Functional Theory (for molecules), or within Many-Body Perturbation Theory (the GW approximation). In addition to the main ABINIT code, different utility programs are provided.

In brief

- Welcome to new users ! Please read the Readme and subscribe to the ABINIT users mailing list.
- ABINIT : a project that favours development and collaboration (short presentation of the ABINIT project - 10 pages in pdf).
- Starting from version 3, ABINIT is distributed under the GNU General Public Licence.
- If you plan to write a scientific article in which ABINIT was used, please read the acknowledgments suggestions. When your article is published, please register it in the ABINIT database.
- There are many ways to help the ABINIT project , including sponsoring.
- If you want to report a bug, please use the bug report information.

Available versions of the code (summary table):

- ABINIT v4.0 (installation notes, release notes, features, new user guide, abinis help, input variables, tutorial)
  - ABINIT v 4.0.5 (obsolete)
- ABINIT v4.1 (installation notes, release notes, features, new user guide, abinis help, input variables, tutorial)
  - ABINIT v 4.1.1 (only for reference)
  - ABINIT v 4.1.2 (only for reference)
  - ABINIT v 4.1.3 (only for reference)
  - ABINIT v 4.1.4 (only for reference)
  - ABINIT v 4.1.5 (production version, very robust, last of the 4.1 series)
- ABINIT v4.2 (installation notes, release notes, features, new user guide, abinis help, input variables, tutorial)
  - ABINIT v 4.2.1 (only for reference)
  - ABINIT v 4.2.2 (only for reference)
  - ABINIT v 4.2.3 (only for reference)
  - ABINIT v 4.2.4 (preferred production version, robust)
- ABINIT v4.3 (installation notes, release notes, features, new user guide, abinis help, input variables, tutorial)
  - ABINIT v 4.3.1 (only for reference)
  - ABINIT v 4.3.2 (only for development)
  - ABINIT v 4.3.3 (production version, also for developpers)


Précédente
Suivante
Actualiser
Arrêter
Démarrage
Imprimer
Nouvel onglet
http://www.abinit.org/
ABINIT v 4.3.2 (only for development)
ABINIT v 4.3.3 (production version, also for developpers)
Pseudopotentials
LDA pseudopotential files :
Troullier-Martins pseudopotentials for most of the elements in the periodic table, generated by A. Khein and D.C. Allan
Goedecker-Teter-Hutter pseudopotentials for selected elements
Hartwigsen-Goedecker-Hutter pseudopotentials for most of the elements in the periodic table.
Teter "extended norm-conserving" pseudopotentials for selected elements
Fritz-Haber-Institute (FHI) pseudopotentials for selected elements (Troullier-Martins scheme)
LDA core-hole pseudopotential files for selected elements
GGA (PBE) pseudopotential files :
Fritz-Haber-Institute (FHI) pseudopotentials for selected elements (Troullier-Martins scheme)
Hartwigsen-Goedecker-Hutter pseudopotentials for selected elements
Programs to generate pseudopotentials :
The OPIUM pseudopotentials generator
How to generate pseudopotentials using the FHI (FHI98PP) code ?
PAW atomic data
Atomic data files (pspfmt=7) for selected elements in the periodic table.
Programs to generate PAW atomic data:
Atompaw2abinit utility (from F. Jollet, M. Torrent and G. Jomard), that allows to translate Atomic PAW files generated using the AtomPaw code (from N. Holzwarth and collaborators). You might directly consult the on-line manual.
USpp2Abinit utility (from F. Jollet and M. Torrent) that allows to patch D. Vanderbilt's ultrasoft pseudopotential generator USPP in order to make it produce PAW atomic data. You might directly consult the on-line manual.
Atomic Densities
All-electron density files (for use with Hirschfeld atomic charge analysis)
Core-electron density files (for use with Bader atomic charge analysis)
Terminé

To be continued…

Work of the last year

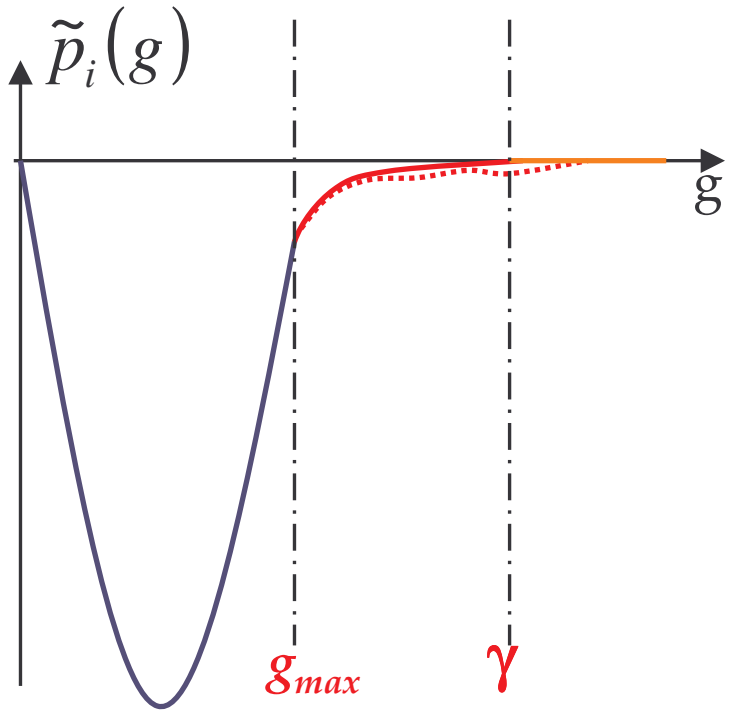
- Two types of atomic data now available
- Abinit's user can download/generate atomic data
- Fully documented on Abinit's web site

To be continued…

- … Final format ?
- Evaluate accuracy and performance for elements of the periodic table
- XML "universal" format for PAW atomic data ?
- An atomic data generator completely written for Abinit ?
- Spin orbit ?

Real Space Optimization

Essential for USPP's atomic data
Available for AtomPAW's atomic data



Real-space implementation of nonlocal pseudopotentials for 1st-principle total-energy calculations,

R.D. King-Smith, M.C. Payne, J.S. Lin, Phys. Rev. B 44, 13063 (1991)

- Impose error W_l
- Adjust g_{max} according to E_{cut}
- Choose $2g_{\max} \le \gamma \le 3g_{\max}$
- Deduce R_0

Choose reasonable R_0

$$\Delta\varepsilon_{n,k}^{nl}(l,m,n) \le W_{l,n} = \max_g \left[\int_{R_0}^{\infty} \tilde{p}_{l,n}(r) j_l(g) r^2 dr \right]$$

Return