FROM RESEARCH TO INDUSTRY

International school

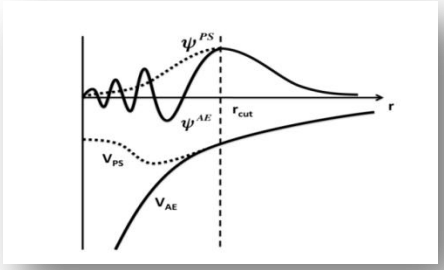
Lattice Dynamics of Solids with ABINIT

May 12-17, 2014 - Lyon, France

« PROJECTOR AUGMENTED-WAVE » METHOD: GENERATION OF ATOMIC DATASETS

François Jollet, Marc Torrent

CEA, DAM, DIF. Arpajon, France



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OUTLINE

The PAW data set

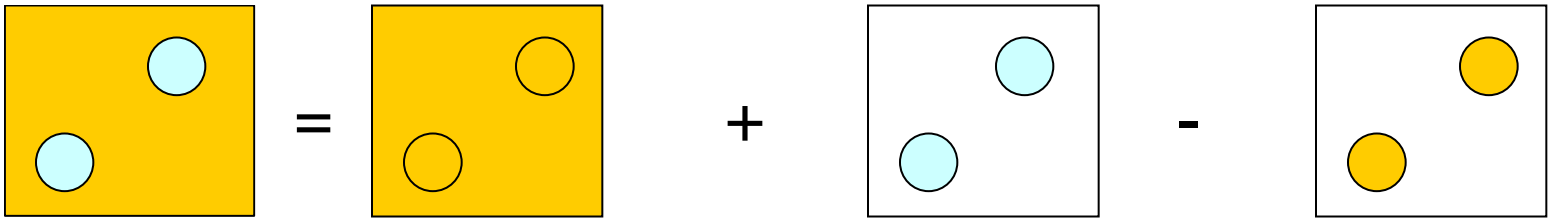
Generation of PAW atomic data

Validation of PAW atomic data

THE PAW DATASET

ATOMIC DATA: WHAT DO WE NEED?

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



Hamiltonian: $$\tilde{H}\tilde{\psi}_n = \varepsilon_n S \tilde{\psi}_n \qquad S = 1 + \sum_{R,ij} |\tilde{p}_i^R\rangle\left(\langle \phi_i^R | \phi_j^R\rangle - \langle \tilde{\phi}_i^R | \tilde{\phi}_j^R\rangle\right)\langle \tilde{p}_j^R|$$

$$D_{ij} = \sum_L \int \tilde{v}_{eff}(\mathbf{r}) Q_{ij}^L(\mathbf{r}) d\mathbf{r}$$

$$+\langle \phi_i | -\frac{\Delta}{2} + v_H\left[n^1 + n_{Zc}\right] + v_{xc}\left[n^1 + n_c\right]\phi_j\rangle$$

$$-\langle \tilde{\phi}_i | -\frac{\Delta}{2} + v_H\left[\tilde{n}^1 + \hat{n} + \tilde{n}_{Zc}\right] + v_{xc}\left[\tilde{n}^1 + \hat{n} + \tilde{n}_c\right]\tilde{\phi}_j\rangle - \sum_L \int \tilde{v}_{eff}^1(\mathbf{r}) \hat{Q}_{ij}^L(\mathbf{r}) d\mathbf{r}$$

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

Inside circles: atomic data needed

THE PAW ATOMIC DATASETS

In order to perform a PAW calculation, following atomic data are needed:

For each atomic specie

$\{\phi_i^R\}$, $\{\tilde{\phi}_i^R\}$, $\{\tilde{p}_i^R\}$, $V_H[\tilde{n}_{Zc}]$, n_c, $\tilde{n}_c$, D_{ij}^0

- $\{\phi_i^R\}$: *All electron* partial waves
- $\{\tilde{\phi}_i^R\}$: Pseudized soft partial waves
- $\{\tilde{p}_i^R\}$: Projectors (dual of $\tilde{\phi}_i^R$)
- $V_H[\tilde{n}_{Zc}]$: *Hartree* potential due to nuclueus and core electrons (local pot.)
- n_c: Core density
- $\tilde{n}_c$: Pseudized core density
- D_{ij}^0: Frozen part of D_{ij} term

Definitions of radial grids are also needed

Constraints:

- Precision of the calculation
- Speed of convergence (number of plane waves)

➢ Have to generate an adapted basis

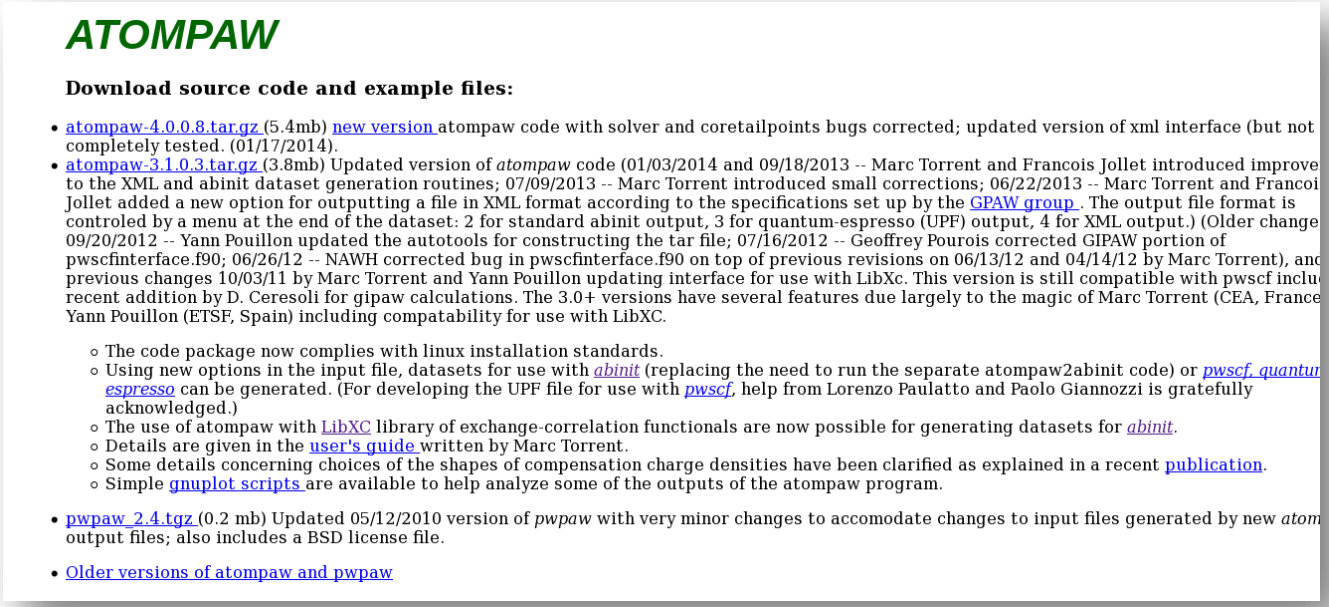
THE « PAW DATASETS »

Generation process

1- Solve "exactly" the atomic problem (for the given LDA/GGA functional)

2- Transform some quantities into smooth ones ("pseudization")

3- Build the partial wave basis and projectors



ATOMPAW

Download source code and example files:

- atompaw-4.0.0.8.tar.gz (5.4mb) new version atompaw code with solver and coretailpoints bugs corrected; updated version of xml interface (but not completely tested. (01/17/2014).
- atompaw-3.1.0.3.tar.gz (3.8mb) Updated version of *atompaw* code (01/03/2014 and 09/18/2013 -- Marc Torrent and Francois Jollet introduced improve to the XML and abinit dataset generation routines; 07/09/2013 -- Marc Torrent introduced small corrections; 06/22/2013 -- Marc Torrent and Francoi Jollet added a new option for outputting a file in XML format according to the specifications set up by the GPAW group . The output file format is controled by a menu at the end of the dataset: 2 for standard abinit output, 3 for quantum-espresso (UPF) output, 4 for XML output.) (Older change 09/20/2012 -- Yann Pouillon updated the autotools for constructing the tar file; 07/16/2012 -- Geoffrey Pourois corrected GIPAW portion of pwscfinterface.f90; 06/26/12 -- NAWH corrected bug in pwscfinterface.f90 on top of previous revisions on 06/13/12 and 04/14/12 by Marc Torrent), and previous changes 10/03/11 by Marc Torrent and Yann Pouillon updating interface for use with LibXc. This version is still compatible with pwscf inclu recent addition by D. Ceresoli for gipaw calculations. The 3.0+ versions have several features due largely to the magic of Marc Torrent (CEA, France Yann Pouillon (ETSF, Spain) including compatability for use with LibXC.
  - The code package now complies with linux installation standards.
  - Using new options in the input file, datasets for use with *abinit* (replacing the need to run the separate atompaw2abinit code) or *pwscf, quantu espresso* can be generated. (For developing the UPF file for use with *pwscf*, help from Lorenzo Paulatto and Paolo Giannozzi is gratefully acknowledged.)
  - The use of atompaw with LibXC library of exchange-correlation functionals are now possible for generating datasets for *abinit*.
  - Details are given in the user's guide written by Marc Torrent.
  - Some details concerning choices of the shapes of compensation charge densities have been clarified as explained in a recent publication.
  - Simple gnuplot scripts are available to help analyze some of the outputs of the atompaw program.
- pwpaw_2.4.tgz (0.2 mb) Updated 05/12/2010 version of *pwpaw* with very minor changes to accomodate changes to input files generated by new *atom* output files; also includes a BSD license file.
- Older versions of atompaw and pwpaw

Independent of ABINIT (initiated by N. Holzwarth from Wake Forest University)

Automatically download and installed by ABINIT build system

http://pwpaw.wfu.edu

GENERATION OF PAW ATOMIC DATA

BUILDING PAW ATOMIC DATA

Step 1

All electrons atomic calculation (with ATOMPAW for instance)

$$\left[T + V_{AE}(r)\right]\phi_i = \varepsilon_i \phi_i$$

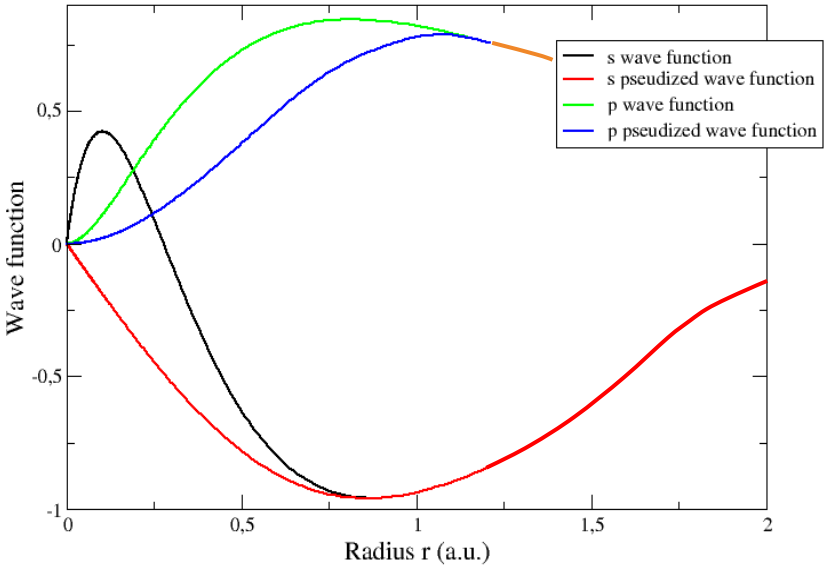
- ✓ Choose an electronic valence configuration $O : 1s^2 2s^2 2p^4$
- ✓ Solve atomic Schrödinger equation Get $n_c(r), V_{ae}(r)$
- ✓ Choose an energy set $\{\varepsilon_i\}$ an radii $\{r_i\}$
- ✓ and invert the Schrödinger equation Get $\{\phi_i(r)\}$

Step 2

Pseudo functions

- ✓ Apply a soft pseudization scheme

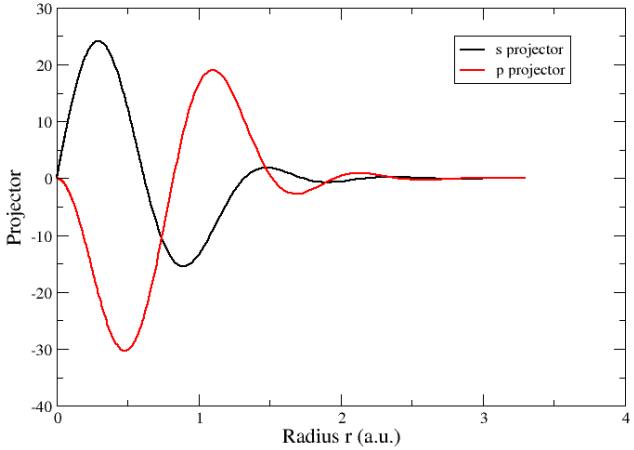
$$\tilde{\phi}_i \quad \text{and} \quad \phi_i \quad \text{join at} \quad r_i$$
$$\tilde{n}_c \quad \text{and} \quad n_c \quad \text{join at} \quad r_{core}$$
$$V_{loc} \quad \text{and} \quad V_{ae} \quad \text{join at} \quad r_{loc}$$



BUILDING PAW ATOMIC DATA

Step 3 Projectors

✓ Apply a scheme (Vanderbilt or Bloechl) to calculate (optimized) $\{\tilde{p}_i(r)\}$



Step 4 Local potential

✓ Compute $v_H(\tilde{n}_{Zc})$ from V_{loc}

Step 5 Additional data

$$D_{ij}^0 = \langle \phi_i | -\frac{\Delta}{2} + v_H[n_{Zc}] | \phi_j \rangle - \langle \tilde{\phi}_i | -\frac{\Delta}{2} + v_H[\tilde{n}_{Zc}] | \tilde{\phi}_j \rangle - \sum_{lm} \int_R v_H[\tilde{n}_{Zc}] \hat{Q}_{ij}^{lm} d\mathbf{r}$$

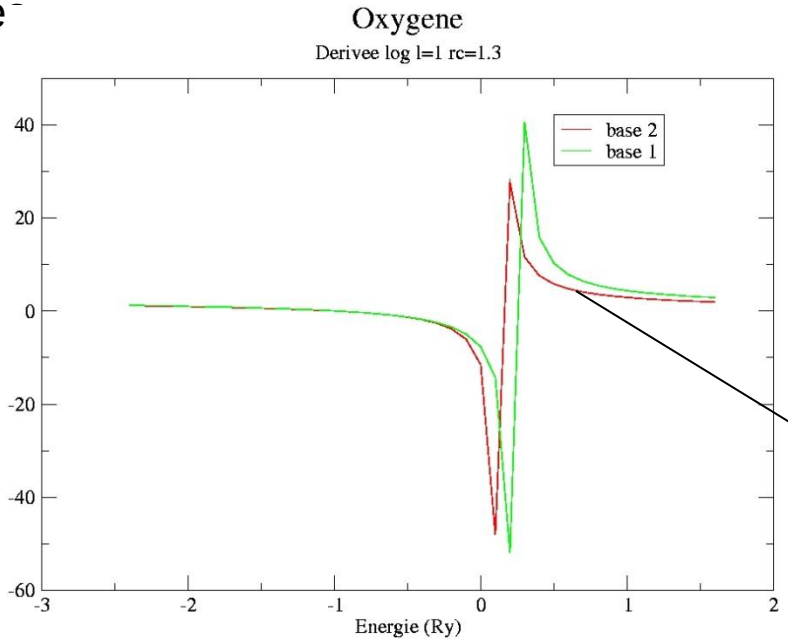
VALIDATION AT THE ATOMIC LEVEL

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

- ✓ The logarithmic derivatives of wavefunctions must be equal to the ones of a reference calculation (good diffusion properties)

$$\left[-\Delta + V_l(r)\right]\phi_l(\varepsilon, r) = \varepsilon\phi_l(\varepsilon, r) \quad \Rightarrow \quad \left[\phi_l^2(\varepsilon, r)\frac{d}{d\varepsilon}\frac{d}{dr}\ln\phi_l(\varepsilon, r)\right]_R = -\int_0^R \phi_l^2(\varepsilon, r)dr$$

- ✓ The energies of excited configurations must be equal to the *all electron* one



AE log derivatives and "base 2" log derivatives are superimposed

⌦ *Transferability*

ATOMIC DATA EFFICIENCY

The plane wave basis must be as small as possible

- ✓ Radius of augmentation regions (spheres).
  Spheres are in principle not allowed to overlap
  In practice a little overlap is allowed
- ✓ Number of partial waves per atom
- ✓ Pseudization scheme
- ✓ Size of radial grids
- ✓ Softness of V_{loc}

⌦ Good atomic data are always a compromise between accuracy and efficiency

THE PAW ATOMIC DATASETS

With *PAW datasets*…

Approximations can be controlled

- Frozen-core approximation: adding more *semicore* states
- Size of PW basis: choosing the radius of spheres, the *pseudization* scheme
- Size of partial waves basis: adding more basis elements

Efficiency can be controlled

- Plane wave basis:
  Adjusting the radius of spheres, choosing a « soft » *pseudization* scheme
- Partial waves basis:
  Reducing the number of basis elements by choosing them judiciously

ATOMIC DATASETS : XML TRANSFERABLE FORMAT

In addition to its proprietary format, ABINIT is able to read atomic datasets in an XML specification shared by several PAW codes

```
<?xml  version="1.0"?>
<paw_setup version="0.5">
<atom symbol="Fe" Z="26.00" core="10.00" valence="16.00"/>
<xc_functional type="GGA" name="PBE"/>
<generator type="scalar-relativistic" name="atompaw">
</generator>)
<!-- Atompaw 3.1.0.2
 Contact info:Natalie Holzwarth
     email: natalie@wfu.edu   web: pwpaw.wfu.edu
 Energy units=Hartree, length units=bohr
 PAW functions generated on 09/26/2013, 10:29:07.032
 by F. Jollet and M.Torrent
 Atompaw -->
<ae_energy kinetic="  1.28767947549867108E+03" xc=" -5.57396
  electrostatic=" -2.50441869925487845E+03" total=" -1.27247
<core_energy kinetic="  1.14775669337194381E+03"/>
<PAW_radius rpaw=" 2.1153157434"/>
<valence_states>
  <state n=" 3" l="0" f=" 2.0000000E+00" rc=" 2.0126126692"
  <state n=" 4" l="0" f=" 1.0000000E+00" rc=" 2.0126126692"
  <state n=" 3" l="1" f=" 6.0000000E+00" rc=" 1.8068708301"
  <state n="20" l="1" f=" 0.0000000E+00" rc=" 1.8068708301"
  <state n=" 3" l="2" f=" 7.0000000E+00" rc=" 2.0126126692"
  <state n="20" l="2" f=" 0.0000000E+00" rc=" 2.0126126692"
</valence_states>
<radial_grid eq="r=a*(exp(d*i)-1)" a="3.1899154755203081E-04
<radial_grid eq="r=a*(exp(d*i)-1)" a="3.1899154755203081E-04
<radial_grid eq="r=a*(exp(d*i)-1)" a="3.1899154755203081E-04
<radial_grid eq="r=a*(exp(d*i)-1)" a="3.1899154755203081E-04
<shape_function type="sinc" rc=" 1.8068708301055161"/>
<ae_core_density grid="log1">
  6.2456540783871445E+04  6.0299957939601460E+04  5.87834630
  5.7907056089984064E+04  5.7288238393672291E+04  5.62483968
  5.5829380385990808E+04  5.5517928447627492E+04  5.52281732
  5.4975824157697360E+04  5.4749499469137903E+04  5.45436337
  5.4354874830453264E+04  5.4180398325253991E+04  5.40180347887197O6E+04
```

XML specification for atomic PAW setups

Introduction

This page contains information about the PAW-XML data format for the atomic setups necessary for doing projector-augmented wave calculati pseudopotential method.

An example XML file for nitrogen PAW setup using LDA can be seen here: N.LDA.

Note: Hartree atomic units are used in the XML file ($\hbar = m = e = 1$).

What defines a setup?

The following quantities defines a minimum PAW setup (the notation from Ref. [1] is used here):

Quantity	Description
Z	atomic number
$E_{\mathrm{XC}}[n]$	exchange-correlation functional
E_c^{kin}	kinetic energy of the core electrons
$g_{\ell m}(\mathbf{r})$	shape function for compensation charge
$n_c(r)$	all-electron core density
$\tilde{n}_c(r)$	pseudo electron core density
$\tilde{n}_v(r)$	pseudo electron valence density
$\bar{v}(r)$	zero potential
$\phi_i(\mathbf{r})$	all-electron partial waves
$\tilde{\phi}_i(\mathbf{r})$	pseudo partial waves
$\tilde{p}_i(\mathbf{r})$	projector functions
$\Delta E_{ij}^{\mathrm{kin}}$	kinetic energy differences

Contents of a PAW setup (in order of appearance).

Specification of the elements

An element looks like this:

```
<name> ... </name>
```

or for an empty element:

```
<name/>
```

Tip: An XML-tutorial can be found here

The header

The first two lines should look like this:

```
<?xml version="1.0"?>
<paw_setup version="0.6">
```

The first line must be present in all XML files. Everything else is put inside an element with name `paw_setup`, and this element has an attribute called v

Reading XML PAW atomic data in ABINIT

We follow the XML specification for atomic PAW setups (http://wiki.fysik.dtu.dk/gpaw/setups/pawxml.html)

```
<?xml version="1.0"?>
<paw_setup version="0.6">
  <!-- Aluminium setup for the Projector Augmented Wave method. -->
  <!-- Units: Hartree and Bohr radii.                           -->
  <atom symbol="Al" Z="13" core="10.0" valence="3"/>
  <xc_functional type="LDA" name="PW"/>
  <generator type="scalar-relativistic" name="gpaw-0.4.2039">
    Frozen core: [Ne]  </generator>
 <valence_states>
    <state n="3" l="0" f="2"  rc="2.050" e="-0.28773" id="Al-3s"/>
    <state n="3" l="1" f="1"  rc="2.050" e="-0.10229" id="Al-3p"/>
    <state       l="0"       rc="2.050" e=" 0.71227" id="Al-s1"/>
    <state       l="1"       rc="2.050" e=" 0.89771" id="Al-p1"/>
    <state       l="2"       rc="2.050" e=" 0.00000" id="Al-d1"/>
  </valence_states>
  <radial_grid eq="r=a*i/(n-i)" a="0.400000" n="450" istart="0" iend="449"
id="g1"/>
  <shape_function type="gauss" rc="6.482669203345e-01"/>
  <ae_core_density grid="g1">
     4.997112961473e+03 4.997112961473e+03 4.857659435098e+03
4.730193936643e+03
     3.078708573034e+03 3.000624028901e+03 ...
  </ae_core_density>
  <pseudo_core_density grid="g1">
     1.783527380470e-01 1.783526543607e-01 1.783524018058e-01
1.783519781162e-01
     1.783472111919e-01 1.783457113822e-01 1.783440237043e-01 ...
  </pseudo_core_density>
  <pseudo_valence_density grid="g1">
     7.836203580181e-02 7.836203580181e-02 7.836211517332e-02
     7.836421778452e-02 7.836474816881e-02 ...
  </pseudo_valence_density>
  <zero_potential grid="g1">
     1.154109661258e+01 1.154108143790e+01 1.154103564273e+01
     1.153982255831e+01 1.153951657690e+01 ...
  </zero_potential>
```

```
<ae_partial_wave state="Al-3s" grid="g1">
     6.333026304612e+00 6.245234361727e+00 6.157050490525e+00
     5.624207462754e+00 5.552447960346e+00 ...
</ae_partial_wave>
  <pseudo_partial_wave state="Al-3s" grid="g1">
     3.726835050749e-01 3.726836067287e-01 3.726837088363e-01
     3.726864137237e-01 3.726870960264e-01 ...
  </pseudo_partial_wave>
  <projector_function state="Al-3s" grid="g1">
     2.936351924351e+00 2.936360229566e+00 2.936368571858e+00
     2.937019519487e+00 2.937114112636e+00 ...
  </projector_function>
...
...
...
  <kinetic_energy_differences>
     9.548475423963e-01 0.000000000000e+00 -6.270780268138e-01
0.000000000000e+00
     0.000000000000e+00 3.991846008068e-01 0.000000000000e+00 -1.404411364367e-
01
     -6.270780268138e-01 0.000000000000e+00 -1.206059432108e-01
0.000000000000e+00
     0.000000000000e+00 -1.404411364367e-01 0.000000000000e+00 6.321237281771e-
02
     0.000000000000e+00 0.000000000000e+00 0.000000000000e+00
0.000000000000e+00
  </kinetic_energy_differences>
</paw_setup>
```

AVAILABLE PAW ATOMIC DATASETS FOR ABINIT

abinit.org

PAW atomic data JTH table

You can find on this page pre-built data files containing PAW atomic data for ABINIT (*v7.4.x+*)
Current version of the table : **JTH-0.1**

All these PAW datasets of this *JTH* table have been generated by F. Jollet, M. Torrent and N. Holzwarth with ATOMPAW 3.1.0.2 .

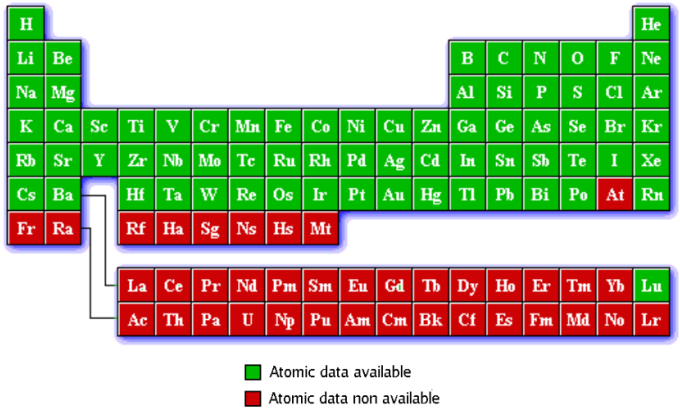
They have been validated in **ABINIT** against *all-electron* calculations using the delta package.

The results are published *here*.
The Δ-factor (resp. Δ_1-factor) factors have been calculated for each element.

Curent average values of these indicators:
Δ=0.4 meV
Δ_1=0.9 meV

*Right now, only **GGA-PBE** datasets are provided; LDA datasets coming soon...*
All the datasets are in XML format according to specifications making them readable by several codes.

Clicking on a highlighted element in the periodic table will bring you into a directory corresponding to the selected chemical element.
Browse down the sub-directories and start a download procedure that will transfer a text file containing PAW atomic data.



The PAW atomic data present on this page are provided without any guarantee.
Users must carefully test them adequately before using them in their applications.

Note : The size of the file may vary between 100 kB and 500 kB.

Last modification : september 26, 2013

AVAILABLE PAW ATOMIC DATASETS FOR ABINIT

- J-T-H table : from ABINIT website – http://www.abinit.org/PAW2/JTH-TABLE
  CEA France + Wake-Forest University
- G-B-R-V table : http://physics.rutgers.edu/gbrv
  Rutgers University
- ATOMPAW table : http://pwpaw.wfu.edu
  Wake-Forest University
- GPAW table : http://wiki.fysik.dtu.dk/gpaw/setups/setups.html
  DTU Denmark

And more to come…

VALIDATION OF PAW ATOMIC DATA

THE DELTA FACTOR

« Error estimates for solid-state density-functional theory predictions: an overview by means of the ground-state elemental crystals »,

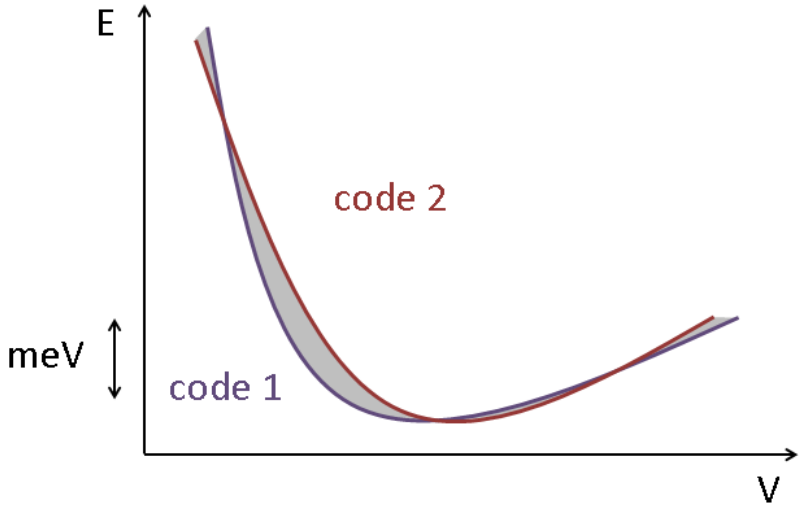
by K. Lejaeghere, V. Van Speybroeck, G. Van Oost and S. Cottenier

*Critical Reviews in Solid State and Materials Sciences,**39**,1, 1-24 (2014)*

available on arXiv: 1204.2733v3

The Delta parameter:

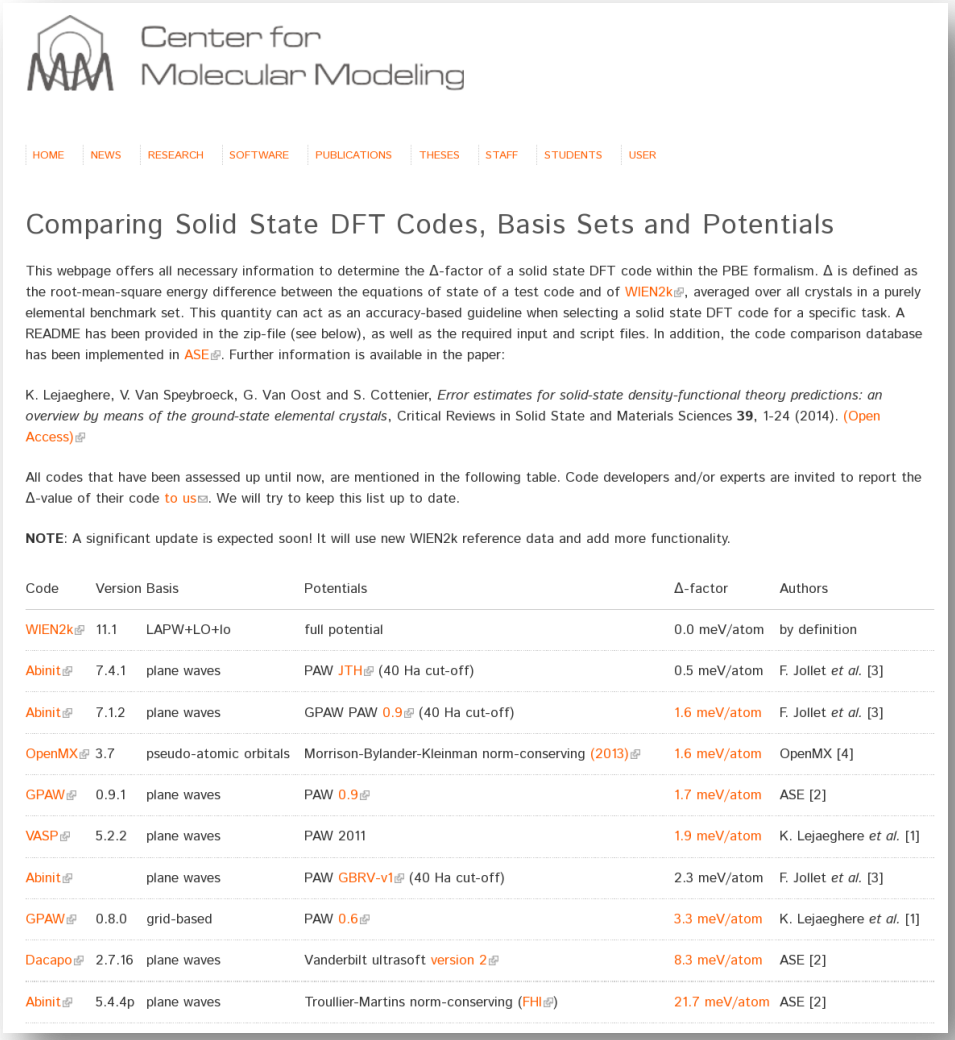
$$\Delta = \left\langle \sqrt{\frac{\int \Delta E^2(V)\,\mathrm{d}V}{\Delta V}} \right\rangle$$



Tested on 71 elements (from H to Rn)

THE DELTA FACTOR

Atomic datasets validation against all electron calculations



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Comparing Solid State DFT Codes, Basis Sets and Potentials

This webpage offers all necessary information to determine the Δ-factor of a solid state DFT code within the PBE formalism. Δ is defined as the root-mean-square energy difference between the equations of state of a test code and of WIEN2k, averaged over all crystals in a purely elemental benchmark set. This quantity can act as an accuracy-based guideline when selecting a solid state DFT code for a specific task. A README has been provided in the zip-file (see below), as well as the required input and script files. In addition, the code comparison database has been implemented in ASE. Further information is available in the paper:

K. Lejaeghere, V. Van Speybroeck, G. Van Oost and S. Cottenier, *Error estimates for solid-state density-functional theory predictions: an overview by means of the ground-state elemental crystals*, Critical Reviews in Solid State and Materials Sciences **39**, 1-24 (2014). (Open Access)

All codes that have been assessed up until now, are mentioned in the following table. Code developers and/or experts are invited to report the Δ-value of their code to us. We will try to keep this list up to date.

NOTE: A significant update is expected soon! It will use new WIEN2k reference data and add more functionality.

Code	Version	Basis	Potentials	Δ-factor	Authors
WIEN2k	11.1	LAPW+LO+lo	full potential	0.0 meV/atom	by definition
Abinit	7.4.1	plane waves	PAW JTH (40 Ha cut-off)	0.5 meV/atom	F. Jollet *et al.* [3]
Abinit	7.1.2	plane waves	GPAW PAW 0.9 (40 Ha cut-off)	1.6 meV/atom	F. Jollet *et al.* [3]
OpenMX	3.7	pseudo-atomic orbitals	Morrison-Bylander-Kleinman norm-conserving (2013)	1.6 meV/atom	OpenMX [4]
GPAW	0.9.1	plane waves	PAW 0.9	1.7 meV/atom	ASE [2]
VASP	5.2.2	plane waves	PAW 2011	1.9 meV/atom	K. Lejaeghere *et al.* [1]
Abinit		plane waves	PAW GBRV-v1 (40 Ha cut-off)	2.3 meV/atom	F. Jollet *et al.* [3]
GPAW	0.8.0	grid-based	PAW 0.6	3.3 meV/atom	K. Lejaeghere *et al.* [1]
Dacapo	2.7.16	plane waves	Vanderbilt ultrasoft version 2	8.3 meV/atom	ASE [2]
Abinit	5.4.4p	plane waves	Troullier-Martins norm-conserving (FHI)	21.7 meV/atom	ASE [2]

The delta factor

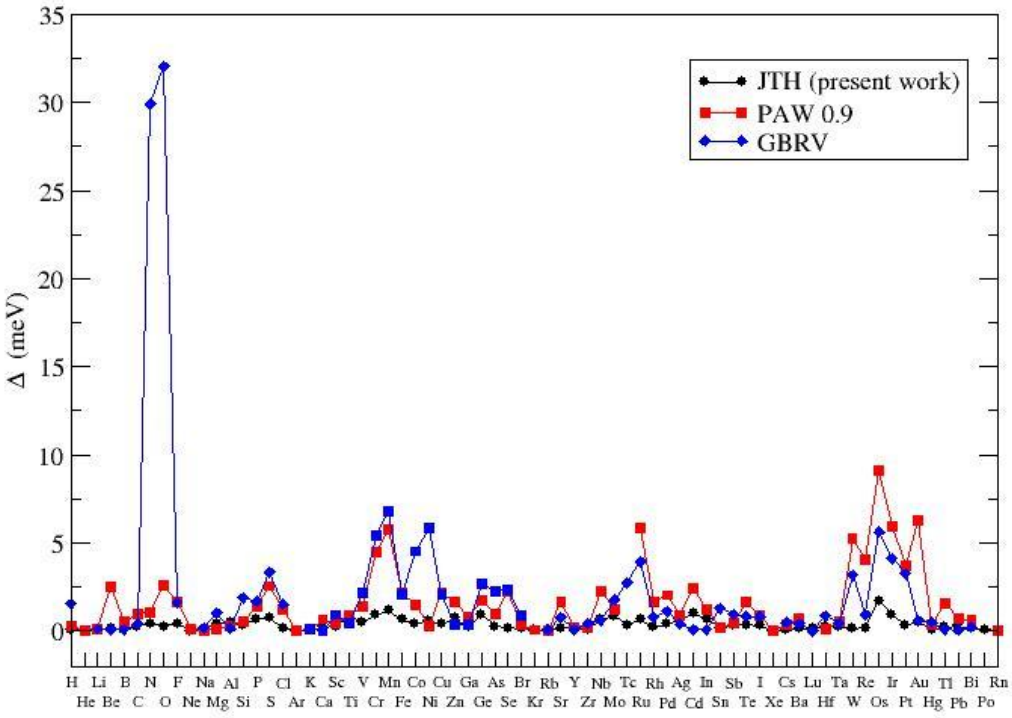
With the delta calculation package (v1.1), CIF files for 71 elements are available.

- 71 input files for ABINIT are generated (python script)
- 6750/N kpoints for a N atoms unit cell
- 7 calculations with volumes from 0.94 V_0^{ref} to 1.06 V_0^{ref}
- V_0, B_0, B'_0 are deduced from the E(V) curve
- The delta factor is calculated comparing with the Wien2k results

Results in ABINIT

JTH table : 71 elements

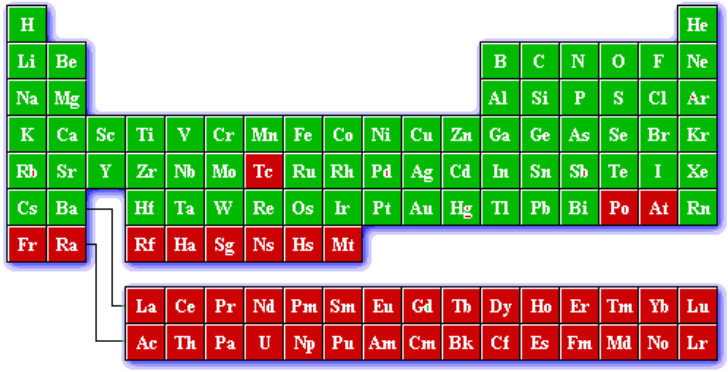
Δ (meV)	12 Ha	15 Ha	20 Ha	40 Ha
PAW 0.9 68 elements	4.845	2.289	1.559	1.552
GBRV 63 elements	4.486	2.617	2.420	2.345
JTH 71 elements	2.461	0.817	0.363	0.453



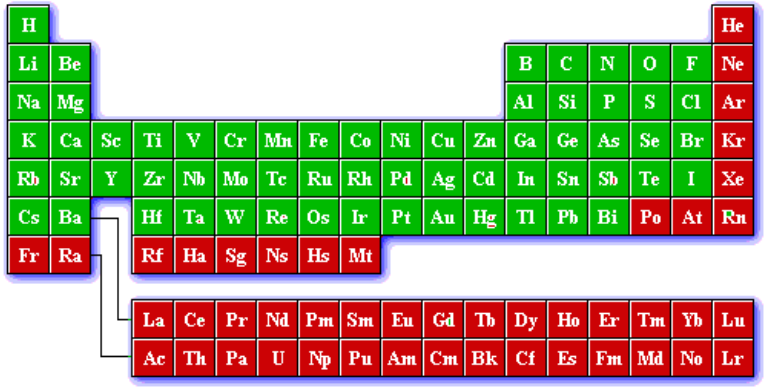
GBRV-v1.01: Δ=1.606 m eV

Results about ABINIT efficiency ecut=20 Ha

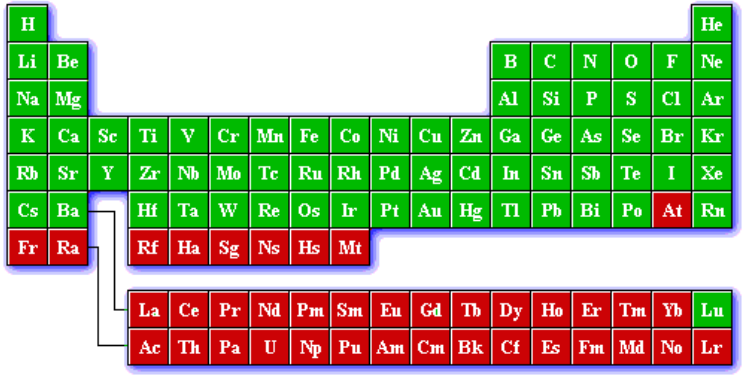
GPAW 0.9 Δ=1.6 meV



GBRV Δ = 1.606 meV



JTH Δ=0.4 meV



Comments about the Δ factor

The Δ factor is a good tool to benchmark codes and pseudopotentials

However, it supposes:

- The reference all-electron calculation is well done
- References are calculated for lanthanides and actinides
- Some compounds are added (oxydes,…)
- It is given together with a cut-off energy (for plane waves)

The Δ factor is very sensitive to the values of V_0, B and B' for some elements and not for others.

For instance:

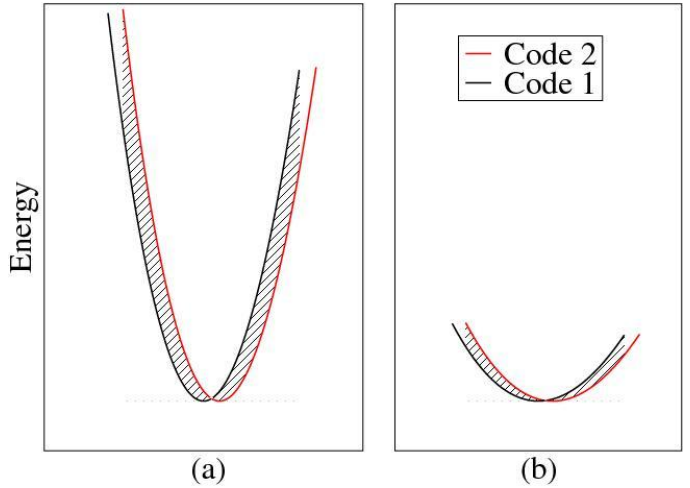
-For Cs: ΔV_0=0.76% leads to Δ_{Cs}=0.39 meV

-For Os: ΔV_0=0.76% leads to Δ_{Os}=9.14 meV

Towards a modified Δ factor?

The Δ_1 factor

(a) High B element
(b) Low B element



0.57 GPa (Ar) < B < 401 GPa (Os)
7.2 Bohr^3(B) <V< 117.7 Bohr^3(Cs)

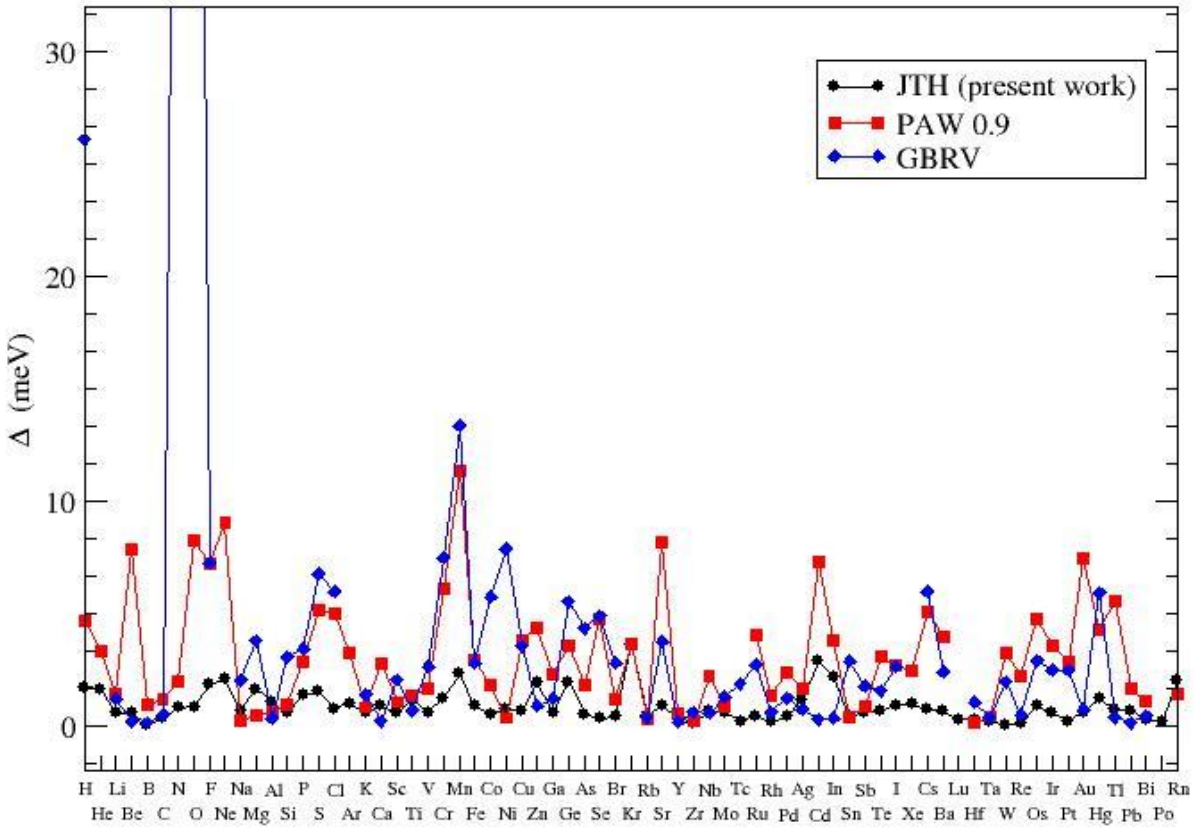
Δ_1 factor ➡ renormalized Δ factor

$$\Delta_1 = \frac{V_{ref} B_{ref}}{V_{AE} B_{AE}} \Delta$$

For all elements:
B_{ref} is set to 100 GPa
V_{ref} is set to 30 Bohr^3

Δ_1 (meV)	12 Ha	15 Ha	20 Ha	40 Ha
PAW 0.9 68 elements	12.117	5.267	3.092	2.828
GBRV 63 elements	8.243	5.698	5.363	5.155
JTH 71 elements	7.671	2.187	0.888	0.970

The Δ_1 factor



F. Jollet, M. Torrent, N. Holzwarth, *Generation of Projector Augmented-Wave atomic data: A 71 element validated table in the XML format* , Comp. Physics Comm., **185** (2014) 1246-1254

HOW TO GENERATE ATOMIC DATASETS

Follow the tutorial!

Delivered with ABINIT package

ABINIT, lesson PAW2:

Projector augmented-wave technique : the generation of atomic data files

This lesson aims at showing how to compute atomic data files for the projector-augmented-wave method.

You will learn how to generate the atomic data and what the main variables are to govern their softness and transferability.
It is supposed you already know how to use ***ABINIT*** in the PAW case

This lesson should take about 1h30.

Contents of lesson PAW2 :

1. The PAW atomic dataset - introduction

The PAW method is based on the definition of atomic spheres (augmentation regions) of radius r_{PAW} around the atoms of the system in which a base of atomic partial waves φ_i, of "pseudized" partial waves $\tilde{\varphi}_i$, and of projectors $\tilde{p}_i$ (dual to $\tilde{\varphi}_i$) have to be defined. This set of partial-waves and projectors functions plus some additional atomic data are stored in a so-called *PAW dataset*. A PAW dataset has to be generated for each atomic species in order to reproduce atomic behavior as accurate as possible while requiring minimal CPU and memory resources in executing ABINIT for the crystal simulations. These two constraints are conflicting.
The PAW dataset generation is the purpose of this tutorial.
It is done according the following procedure (*all parameters that define a PAW dataset are in **bold***):

1. Choose and **define the concerned chemical species** (name and atomic number).
2. Solve the atomic all-electrons problem in a given atomic configuration. The atomic problem is solved within the DFT formalism, using an **exchange-correlation functional** and either a Schrödinger (default) or **scalar-relativistic approximation**. It is a spherical problem and it is solved on a **radial grid**. The atomic problem is solved for a given **electronic configuration** that can be an ionized/excited one.
3. Choose a set of electrons that will be considered as frozen around the nucleus (**core electrons**). The others electrons are valence ones and will be used in the PAW basis. The **core density** is then deduced from the core electrons wave functions. A **smooth core density** equal to the core density outside a given r_{core} **matching radius** is computed.

Commissariat à l’énergie atomique et aux énergies alternatives

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