FROM RESEARCH TO INDUSTRY

www.cea.fr

ABINIT school 2019

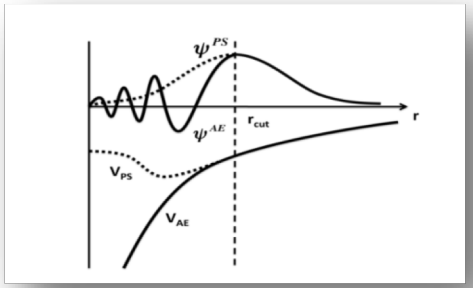
New-comer Oriented School to Ab initio Nanoscience Simulations

January 21–25 2019, Bruyères-le Châtel, France

ABINIT BASICS

François Jollet

CEA, DAM, DIF. Arpajon, France



OUTLINE

Historical context

Structure of the ABINIT code

Pseudopotentials and PAW atomic data

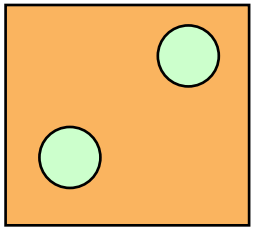
Validation of atomic data

HISTORICAL CONTEXT

HISTORICAL CONTEXT

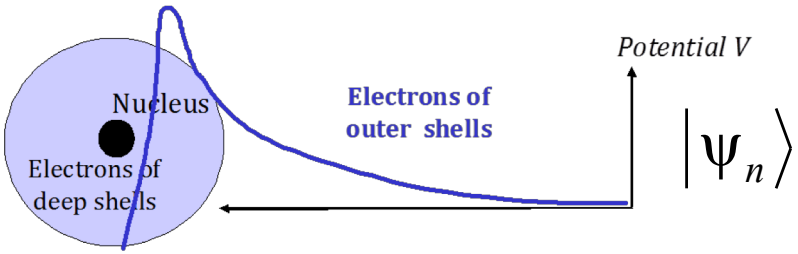
Wavefunctions are developped on a basis which is…

Localized



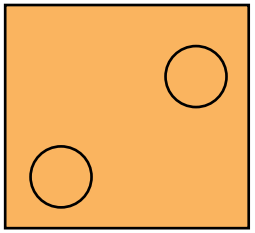
Spherical harmonics + special functions

All electrons are taken into account



Pb: - The atomic basis is moving with atoms

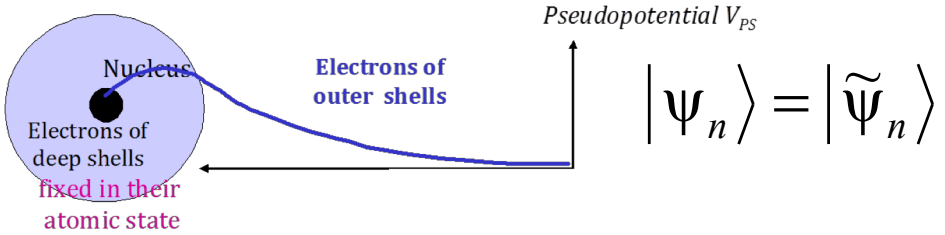
Delocalized



Plane waves

Only valence electrons are taken into account

Norm-conserving Pseudopotentials



Pb: - Use of pseudos wavefunctions
- Big size of the plane wave basis

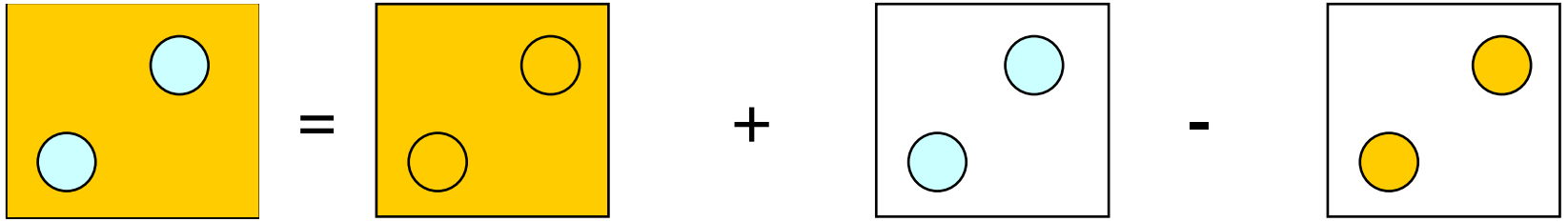
HISTORICAL CONTEXT

PAW

« *The Projector Augmented-Wave method is an extension of augmented wave methods and the pseudopotential approach, which combine their traditions into a unified electronic structure method* »

Peter Blöchl

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

Some atomic quantities are to be known to calculate $\tilde{H}, S, \tau$

PAW atomic data (pseudopotentiel)

STRUCTURE OF THE ABINIT CODE

STRUCTURE OF THE ABINIT CODE

The wavefunction basis

ABINIT is a code that only manipulates the auxiliairy function $\left|\tilde{\psi}_n\right\rangle$ for valence electrons

In ABINIT, $\left|\tilde{\psi}_n\right\rangle$ is developped either on a wavelet basis or on a plane wave basis.

In the following, we shall tackle only the case of a plane wave basis

On a plane wave basis: $\varphi_i(\mathbf{r}) = \sum_G \varphi_i(\mathbf{G}) e^{i\mathbf{G}.\mathbf{r}}$ with **G** a reciprocal space vector

and $\varphi(\mathbf{G})$ the Fourier transform of φ

The sum is truncated so that: $\frac{\hbar^2}{2m}|\mathbf{G}|^2 \leq E_{cut}$ where Ecut is the cutoff enregy : ***ecut*** variable in ABINIT

ABINIT solves the Schroedinger equation: $\tilde{H}\tilde{\psi}_n = \varepsilon_n S\tilde{\psi}_n$

STRUCTURE OF THE ABINIT CODE

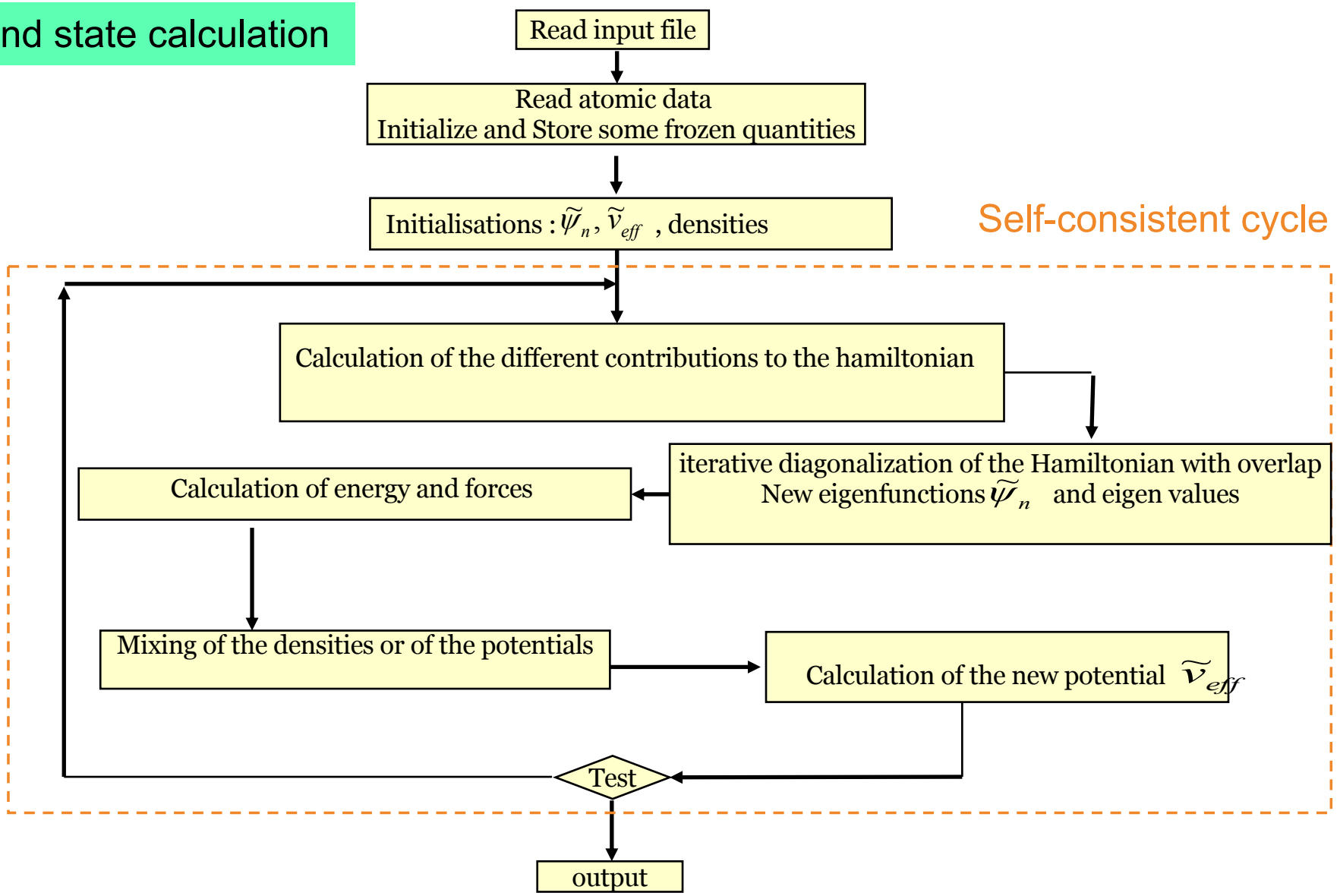
The electronic density:

$$\rho(\vec{r}) = \sum_{\substack{\sigma \\ spins}} \sum_{\substack{n \\ Bands}} \left[\int_{\substack{\vec{k} \\ Reciprocal \\ space}} \left(\left| \sum_{\substack{\vec{g} \\ Plane \\ waves}} \left(C_{n,k}(\vec{g}) \cdot e^{i \cdot (\vec{k}+\vec{g})\vec{r}} \right) \right|^2 \cdot d\vec{k} \right) \right] + \sum_{\substack{A \\ atoms}} \rho^{A}_{compensation}(\vec{r})$$

Parallelism over: *Spins* *States* *k vectors* *Plane waves* *Atoms*

STRUCURE OF THE ABINIT CODE

ground state calculation



INPUT VARIABLES: SOME DETAILS

Self-consistent cycle:

- maximal number of cycles: ***nstep***
- exit criterium: ***toldfe***, ***toldff***, ***tolwf***, ***tolvrs***

Iterative diagonalization of the Hamiltonian:

the convergence of the wavefunctions for a fixed potential is governed by ***nnsclo*** and ***nline***

Mixing: ***iscf*** available either on potentials for 2≤ ***iscf*** ≤ 7
or on densities for 12≤ ***iscf*** ≤ 17

Example, with a simple mixing: $n_{n+1}^{mix}(r) = n_n^{in}(r) + \alpha \cdot \underbrace{\left(n_n^{out}(r) - n_n^{in}(r)\right)^{PC}}_{resid_n^{PC}(r)}$

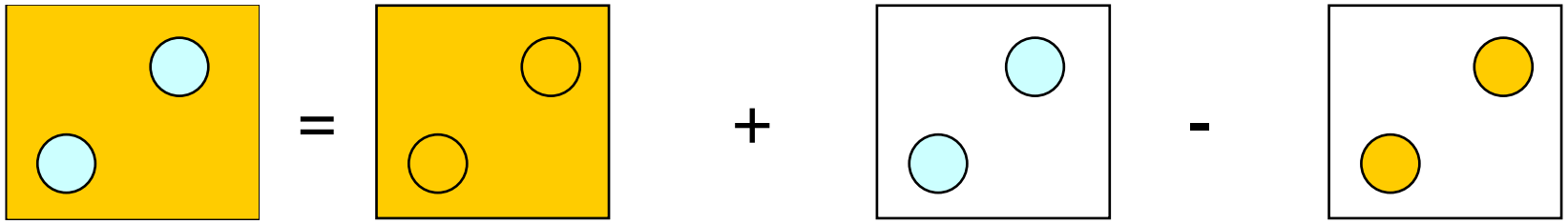
INPUT FILE: AN EXAMPLE

```
# LiH: rocksalt structure
#

# SYSTEM
natom 2
znucl     3 1
ntypat    2
typat     1 2

#CRISTALLOGRAPHY
acell  3*7.60
rprim  0.0 0.5 0.5
       0.5 0.0 0.5
       0.5 0.5 0.0
xred  0.00  0.00  0.00
      0.50  0.50  0.50
```

```
# K-POINTS
ngkpt 1 1 1  istwfk 1
kptopt 1
occopt 7
tsmear 0.005

# CONVERGENCY
nstep 100
toldfe 5.d-10
ecut      10.0
```

NORM-CONSERVING OR PAW CALCULATION ?

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



Advantages of the PAW method:

- 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 accurate 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.

Advantages of the Norm-conserving method:

- The development is easier → more features are available

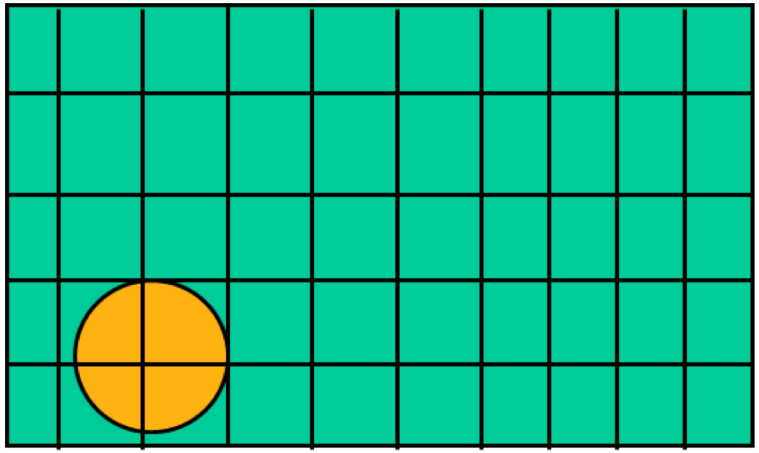
NORM-CONSERVING OR PAW CALCULATION ?

The choice is made by the atomic data file you choose in the *files* file:

- If a norm-conserving file is chosen → OK
- If a PAW file is chosen → set the ***pawecutdg*** variable

Calculations of the wavefunctions are done on a coarse grid defined by ecut
Some quantities are required both on the coarse grid and inside the spheres.

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



pawecutdg defines a fine grid

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

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

NORM-CONSERVING PSEUDOPOTENTIALS

NORM-CONSERVING PSEUDOPOTENTIALS

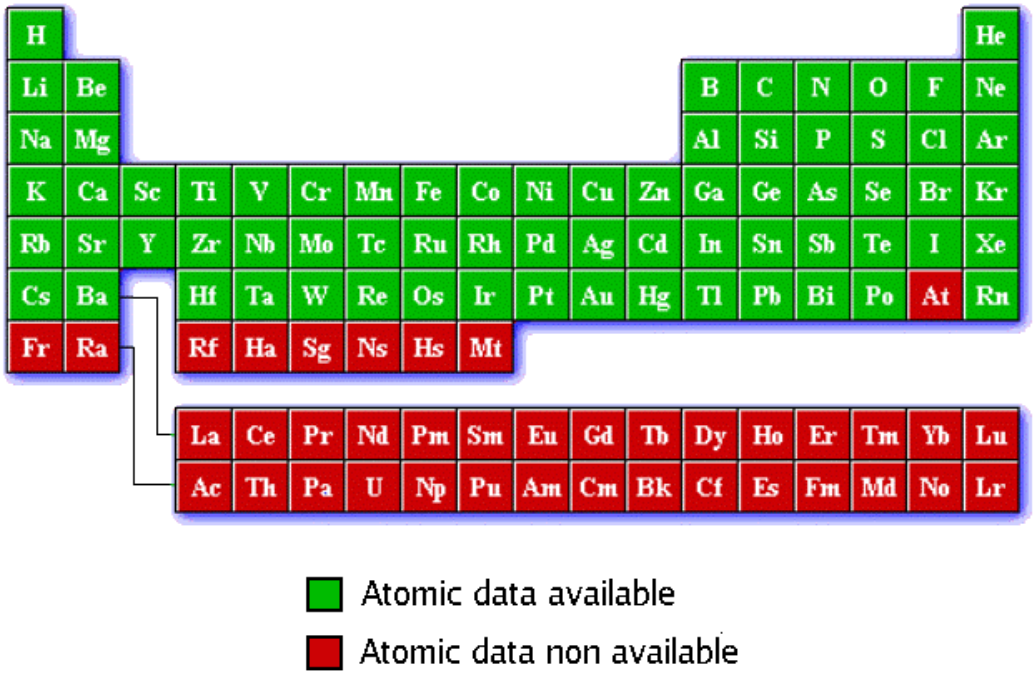
The norm-conserving approximation: $\left(-\frac{1}{2}\Delta + V_H + V_{xc} + V_{PS}\right)\tilde{\Psi}_n = \varepsilon_n \tilde{\Psi}_n$

$$V_{PS}(\mathbf{r},\mathbf{r}') = V_{loc}^{l_{loc}}(\mathbf{r})\cdot\delta(\mathbf{r}-\mathbf{r}') + \sum_{l\neq l_{loc},n,m} \frac{\langle \mathbf{r}|\tilde{\varphi}_{lmn}\rangle\langle\tilde{\varphi}_{lmn}|\mathbf{r}'\rangle}{\langle\tilde{\varphi}_{lmn}|V_{nl}-V_{loc}^{l_{loc}}|\tilde{\varphi}_{lmn}\rangle}$$

Inside circles: atomic data needed

Atomic files for each element

ONCVPSP table



www.abinit.org/downloads/pseudodojo/pseudodojo

THE PAW DATASETS

THE PAW ATOMIC DATASETS

The PAW framework: $\left(-\frac{1}{2}\Delta+\tilde{v}_{eff}+\sum_{i,j}|\tilde{p}_i\rangle D_{ij}\langle\tilde{p}_j|\right)\tilde{\Psi}_n=\varepsilon_n S\tilde{\Psi}_n$

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

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

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

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

Inside circles: atomic data needed

In order to perform a PAW calculation, following atomic data are needed: *For each atomic element*

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

- $\{\phi_i^R\}$: *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 nucleus and core electrons (local pot.)
- n_c: Core density
- $\tilde{n}_c$: Pseudized core density

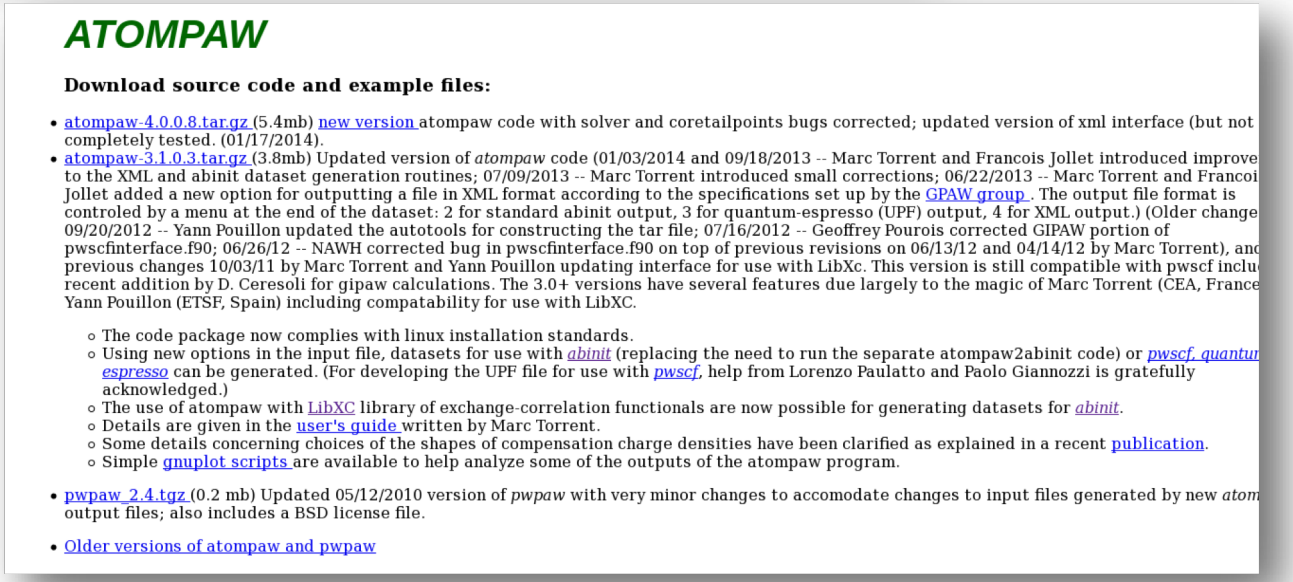
THE PAW ATOMIC DATASETS

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, quantur 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://users.wfu.edu/natalie/papers/pwpaw/man.html

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

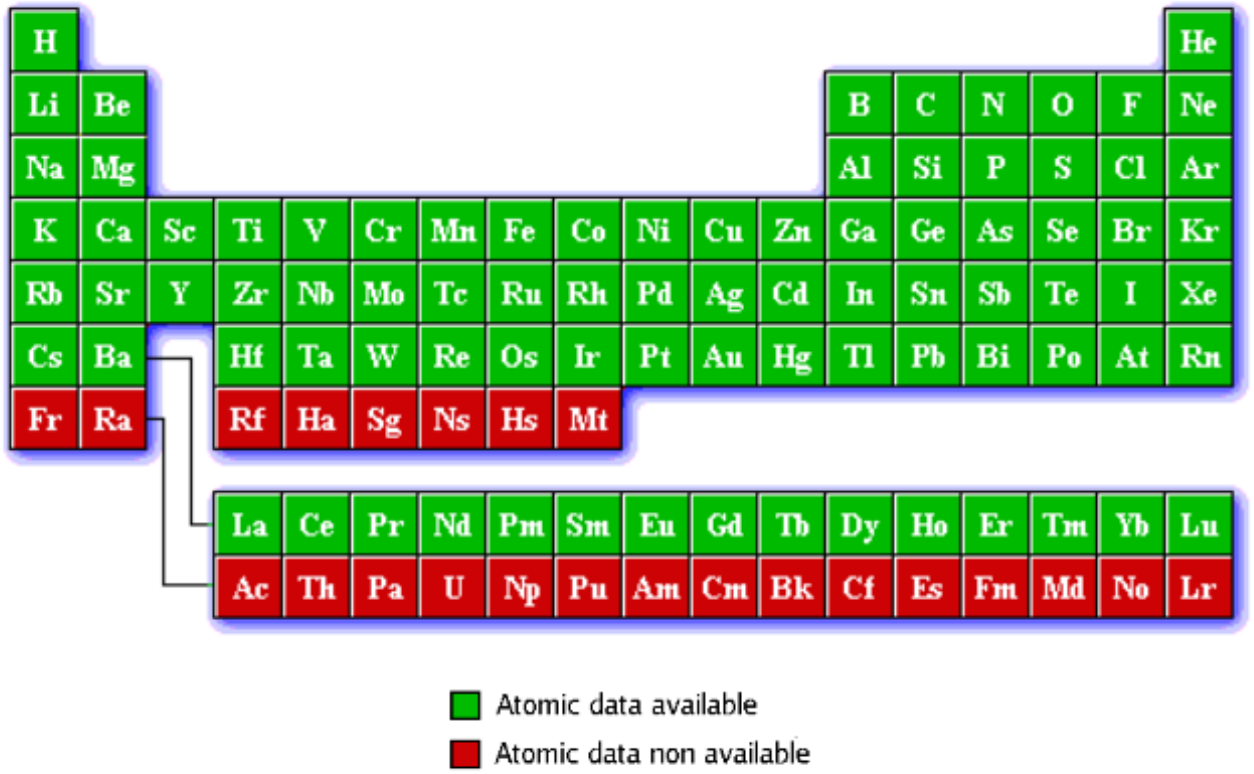
Efficiency can be controlled

- 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

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

THE PAW DATASETS

JTH table : from ABINIT website – http://www.abinit.org/downloads/PAW2



F. Jollet, M. Torrent and N. Holzwarth, Computer Physics Communications, **185** (2014) 1246-1254

VALIDATION OF ATOMIC DATA

Error estimation: the delta factor

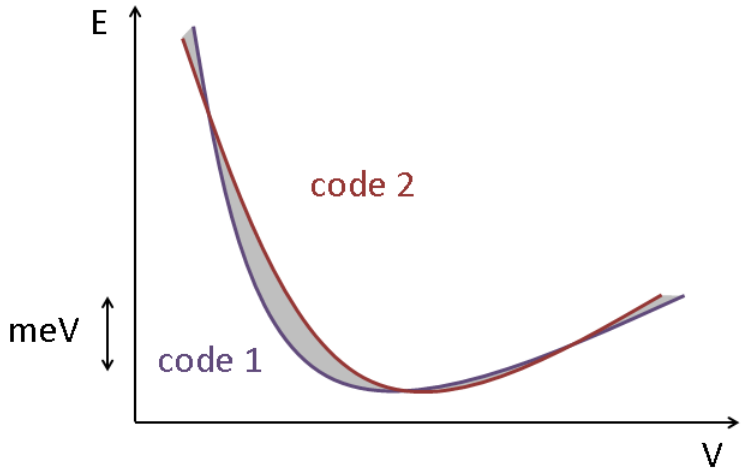
« Error estimates for solid-state density-functional theory predictions: an overview by means of the ground-state elemental crystals »,

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

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

The Delta parameter:

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



With the delta calculation package, CIF files for 71 elements are available.

- 71 input files 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 the two codes

Error estimation: the delta factor

Reference point: WIEN2k 13.1 with basis LAPW/APW+lo and potential all-electron

Code: ABINIT 7.8.2 with basis plane waves and potential PAW JTH v1.0

Maximum at Pt. Minimum at He

All values are in meV.

H 0.25																	He 0.01
Li 0.01	Be 0.09											B 0.24	C 0.15	N 0.49	O 0.24	F 0.22	Ne 0.01
Na 0.50	Mg 0.26											Al 0.10	Si 0.31	P 0.49	S 0.30	Cl 0.06	Ar 0.02
K 0.07	Ca 0.11	Sc 0.02	Ti 1.25	V 1.69	Cr 0.72	Mn 0.89	Fe 0.56	Co 1.07	Ni 1.46	Cu 0.65	Zn 0.28	Ga 0.14	Ge 0.56	As 0.49	Se 0.24	Br 0.11	Kr 0.02
Rb 0.29	Sr 0.76	Y 0.33	Zr 0.25	Nb 0.19	Mo 1.63	Tc 1.03	Ru 0.34	Rh 0.94	Pd 1.16	Ag 0.21	Cd 0.02	In 0.21	Sn 0.11	Sb 0.30	Te 0.07	I 0.73	Xe 0.01
Cs 0.12	Ba 0.74		Hf 0.19	Ta 0.43	W 1.35	Re 0.89	Os 0.48	Ir 0.51	Pt 2.10	Au 1.11	Hg 0.14	Tl 0.06	Pb 0.29	Bi 0.11	Po 0.19	At	Rn 0.02
Fr	Ra																
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu 0.21	
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

Error estimation: the delta factor

SCIENCE sciencemag.org 25 MARCH 2016 • VOL 351 ISSUE 6280

RESEARCH ARTICLE

DFT METHODS

Reproducibility in density functional theory calculations of solids

Kurt Lejaeghere,[1*] Gustav Bihlmayer,[2] Torbjörn Björkman,[3,4] Peter Blaha,[5] Stefan Blügel,[2] Volker Blum,[6] Damien Caliste,[7,8] Ivano E. Castelli,[9] Stewart J. Clark,[10] Andrea Dal Corso,[11] Stefano de Gironcoli,[11] Thierry Deutsch,[7,8] John Kay Dewhurst,[12] Igor Di Marco,[13] Claudia Draxl,[14,15] Marcin Dułak,[16] Olle Eriksson,[13] José A. Flores-Livas,[12] Kevin F. Garrity,[17] Luigi Genovese,[7,8] Paolo Giannozzi,[18] Matteo Giantomassi,[19] Stefan Goedecker,[20] Xavier Gonze,[19] Oscar Grånäs,[13,21] E. K. U. Gross,[12] Andris Gulans,[14,15] François Gygi,[22] D. R. Hamann,[23,24] Phil J. Hasnip,[25] N. A. W. Holzwarth,[26] Diana Iuşan,[13] Dominik B. Jochym,[27] François Jollet,[28] Daniel Jones,[29] Georg Kresse,[30] Klaus Koepernik,[31,32] Emine Küçükbenli,[9,11] Yaroslav O. Kvashnin,[13] Inka L. M. Locht,[13,33] Sven Lubeck,[14] Martijn Marsman,[30] Nicola Marzari,[9] Ulrike Nitzsche,[31] Lars Nordström,[13] Taisuke Ozaki,[34] Lorenzo Paulatto,[35] Chris J. Pickard,[36] Ward Poelmans,[1,37] Matt I. J. Probert,[25] Keith Refson,[38,39] Manuel Richter,[31,32] Gian-Marco Rignanese,[19] Santanu Saha,[20] Matthias Scheffler,[15,40] Martin Schlipf,[22] Karlheinz Schwarz,[5] Sangeeta Sharma,[12] Francesca Tavazza,[17] Patrik Thunström,[41] Alexandre Tkatchenko,[15,42] Marc Torrent,[28] David Vanderbilt,[23] Michiel J. van Setten,[19] Veronique Van Speybroeck,[1] John M. Wills,[43] Jonathan R. Yates,[29] Guo-Xu Zhang,[44] Stefaan Cottenier[1,45*]

		average <Δ>	AE: Elk	exciting	FHI-aims/tier2	FLEUR	FPLO/T+F+s	RSPt	WIEN2k/acc
AE	Elk	0.6		0.3	0.3	0.6	1.0	0.9	0.3
	exciting	0.5	0.3		0.1	0.5	0.9	0.8	0.2
	FHI-aims/tier2	0.5	0.3	0.1		0.5	0.9	0.8	0.2
	FLEUR	0.6	0.6	0.5	0.5		0.8	0.6	0.4
	FPLO/T+F+s	0.9	1.0	0.9	0.9	0.8		0.9	0.9
	RSPt	0.8	0.9	0.8	0.8	0.6	0.9		0.8
	WIEN2k/acc	0.5	0.3	0.2	0.2	0.4	0.9	0.8	
PAW	GBRV12/ABINIT	0.9	0.9	0.8	0.8	0.9	1.3	1.1	0.8
	GPAW09/ABINIT	1.4	1.3	1.3	1.3	1.3	1.7	1.5	1.3
	GPAW09/GPAW	1.6	1.5	1.5	1.5	1.5	1.8	1.7	1.5
	JTH02/ABINIT	0.6	0.6	0.6	0.6	0.6	0.9	0.7	0.5
	PSlib100/QE	0.9	0.9	0.8	0.8	0.8	1.3	1.1	0.8
	VASPGW2015/VASP	0.6	0.4	0.4	0.4	0.6	1.0	0.8	0.3
USPP	GBRV14/CASTEP	1.1	1.1	1.1	1.0	1.0	1.4	1.3	1.0
	GBRV14/QE	1.1	1.0	1.0	0.9	1.0	1.4	1.3	1.0
	OTFG9/CASTEP	0.7	0.4	0.5	0.5	0.7	1.0	1.0	0.5
	SSSP/QE	0.5	0.4	0.3	0.3	0.5	0.9	0.8	0.3
	Vdb2/DACAPO	6.3	6.3	6.3	6.3	6.3	6.4	6.5	6.2
NCPP	FHI98pp/ABINIT	13.3	13.5	13.4	13.4	13.2	13.0	13.2	13.4
	HGH/ABINIT	2.2	2.2	2.2	2.2	2.0	2.3	2.2	2.1
	HGH-NLCC/BigDFT	1.1	1.1	1.1	1.1	1.0	1.2	1.1	1.0
	MBK2013/OpenMX	2.0	2.1	2.1	2.1	1.9	1.8	1.8	2.0
	ONCVPSP(PD0.1)/ABINIT	0.7	0.7	0.7	0.7	0.6	1.0	0.8	0.6
	ONCVPSP(SG15)1/QE	1.4	1.4	1.3	1.3	1.3	1.6	1.5	1.3
	ONCVPSP(SG15)2/CASTEP	1.4	1.4	1.4	1.4	1.3	1.6	1.5	1.4

Error estimation: the delta factor

Center for Molecular Modeling

HOME | THESIS SUBJECTS 2016-17 | PUBLICATIONS | STAFF | RESEARCH | NEWS & VACANCIES | EDUCATION | THESES | SOFTWARE | MEDIA | LOGIN

https://molmod.ugent.be/deltacodesdft

Comparing Solid State DFT Codes, Basis Sets and Potentials

Code	Version	Basis	Electron treatment	Δ-value	Authors
WIEN2k	13.1	LAPW/APW+lo	all-electron	0 meV/atom	S. Cottenier [16]
FHI-aims	081213	tier2 numerical orbitals	all-electron (relativistic atomic_zora scalar)	0.2 meV/atom	ASE [2,16]
Exciting	development version	LAPW+xlo	all-electron	0.2 meV/atom	Exciting [10,16]
VASP	5.2.12	plane waves	PAW 2015 GW-ready (5.4)	0.3 meV/atom	K. Lejaeghere [16]
FHI-aims	081213	tier2 numerical orbitals	all-electron (relativistic zora scalar 1e-12)	0.3 meV/atom	ASE [2]
Quantum ESPRESSO	5.1	plane waves	SSSP Accuracy (mixed NC/US/PAW potential library)	0.3 meV/atom	QuantumESPRESSO [12,16]
Elk	3.1.5	APW+lo	all-electron	0.3 meV/atom	Elk [14,16]
ABINIT	7.8.2	plane waves	PAW JTH v1.0	0.4 meV/atom	F. Jollet and M. Torrent
FLEUR	0.26	LAPW (+lo)	all-electron	0.4 meV/atom	FLEUR [9,16]
Quantum ESPRESSO	5.1	plane waves	SSSP Efficiency (mixed NC/US/PAW potential library)	0.4 meV/atom	QuantumESPRESSO [12]
CASTEP	9.0	plane waves	OTFG CASTEP 9.0	0.5 meV/atom	CASTEP [7,16]
ABINIT	7.7.3	plane waves	PAW JTH v0.2	0.5 meV/atom	F. Jollet and M. Torrent [16]
FHI-aims	081213	tight numerical orbitals	all-electron (relativistic atomic_zora scalar)	0.5 meV/atom	ASE [2,16]

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:

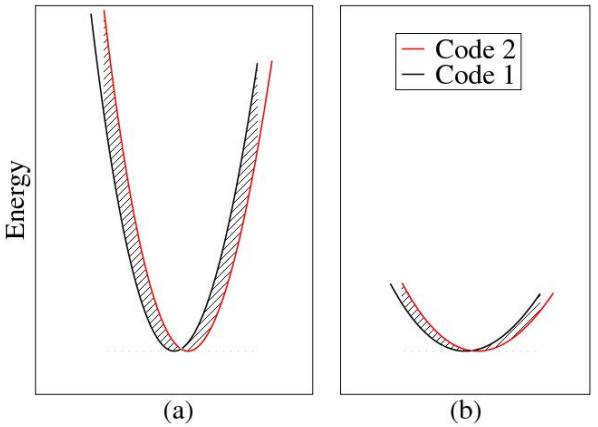
-For Cs: ΔV_0=0.76% leads to Δ_{Cs}=0.39 meV
-For Os: ΔV_0=0.76% leads to Δ_{Os}=9.14 meV

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

For all elements:

B_{ref} is set to 100 GPa
V_{ref} is set to 30 Bohr^3



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

F. Jollet, M. Torrent and N. Holzwarth, Computer Physics Communications, **185** (2014) 1246-1254

The GBRV suite

K. F. Garrity, J. W. Bennett, K.M. Rabe and D. Vanderbilt, *Comput. Mater. Sci.* **81**, 446 (2014)

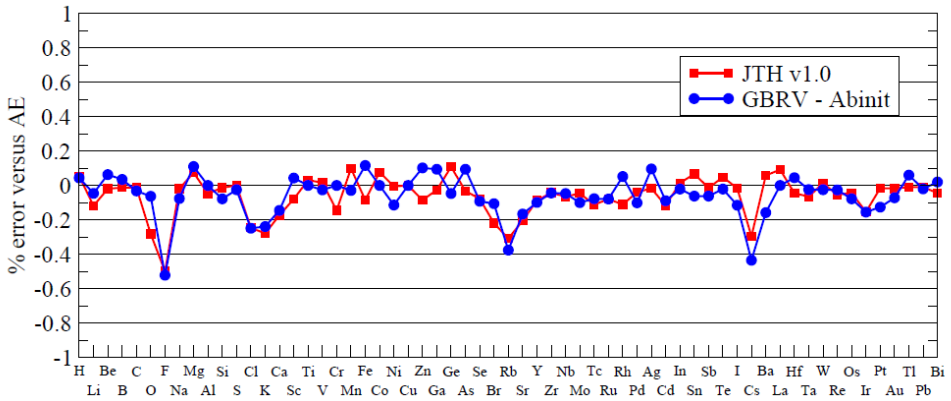


Figure 1: Percent difference in AE versus PAW data calculations for fcc lattice constant

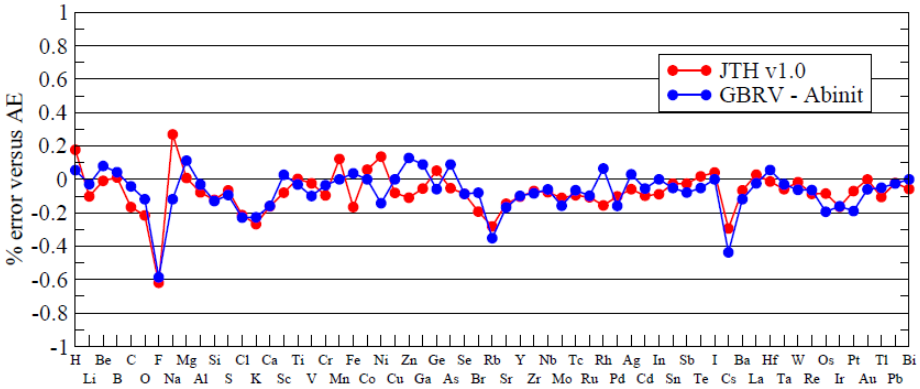


Figure 2: Percent difference in AE versus PAW data calculations for bcc lattice constant

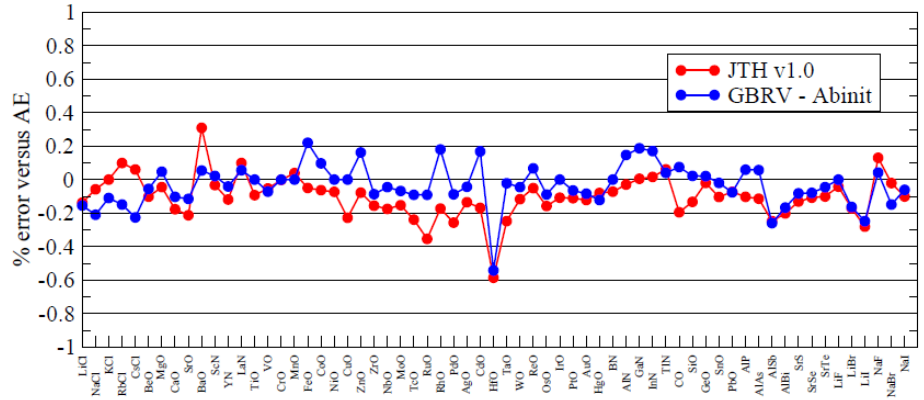


Figure 3: Percent difference in AE versus PAW data calculations for rocksalt lattice constant

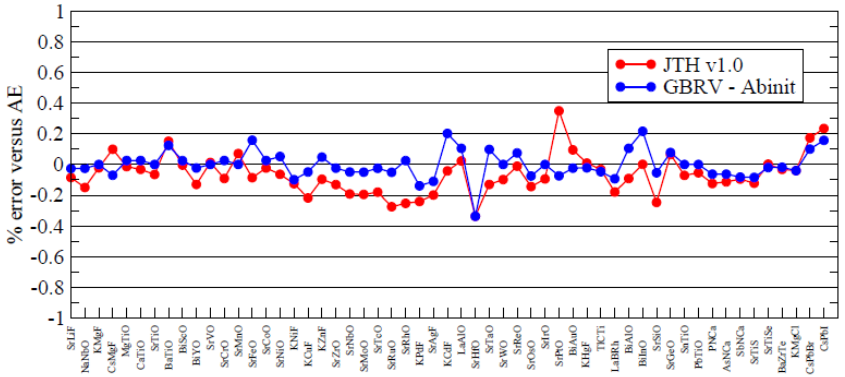


Figure 4: Percent difference in AE versus PAW data calculations for perovskite lattice constant

The GBRV suite

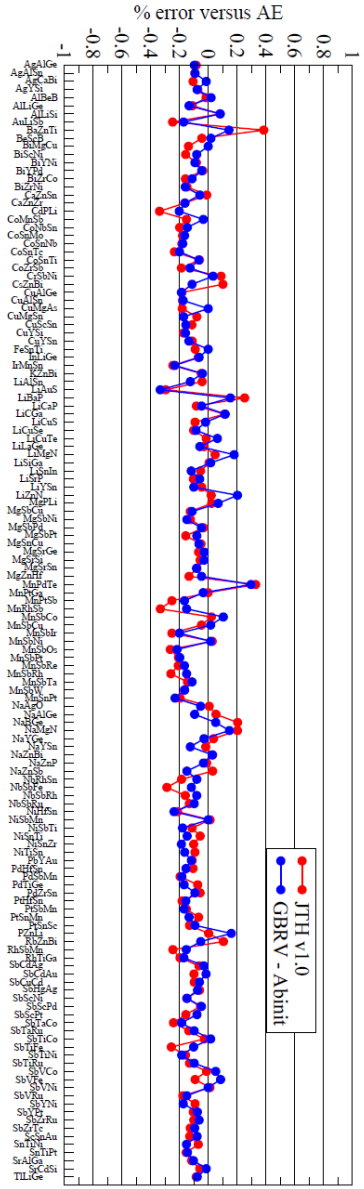


Figure 5: Percent difference in AE versus PAW data calculations for half-heusler lattice constant

Compound	μ_{AE}	$\mu_{GBRV-Abinit}$	$\mu_{JTHv1.0-Abinit}$
VO	1.32	1.27	1.24
CrO	2.99	3.04	3.05
MnO	3.85	3.84	3.86
FeO	3.83	3.84	3.86
CoO	2.42	2.53	2.56
NiO	1.68	1.47	1.36
MoO	0.54	0.53	0.49
TcO	1.92	1.90	1.95
RuO	1.64	1.63	1.67
OsO	1.56	1.50	1.50
IrO	0.62	0.62	0.75

Table II: Magnetic moments of transition metal oxides

Test	GBRV-Abinit	JTHv1.0-Abinit
fcc latt. const. (%)	0.13	0.13
bcc latt. const. (%)	0.15	0.14
rocksalt latt. const. (%)	0.13	0.16
perovskite latt. const. (%)	0.09	0.14
half-heusler latt. const. (%)	0.13	0.15
zinc-blend Δ (meV/atom)	1.2	0.95
zinc-blend $\Delta 1$ (meV/atom)	2.1	1.7

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.

Goto : ABINIT home Page | Suggested acknowledgments | List of input variables | Tutorial home page | Bibliography

Help files : New user guide | Abinit (main) | Abinit (respfn) | Mrgddb | Anaddb | AIM (Bader) | Cut3D | Optic | Mrgscr

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

Etablissement public à caractère industriel | RCS Paris B 775 685 019