Good How to generate ^ PAW Atomic Datasets*

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How to generate ^ PAW Atomic Datasets

- Challenges
- Tricks
- Opportunities for collaboration
- Importance of having several independent codes (both for atomic dataset generation and for materials simulations)
- Advantages of developing a common format for atomic datasets

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How to generate ^ PAW Atomic Datasets

- **Challenges**

  Experience of a long time generatrice –
  very personal opinions:
  - Large number of **great** generation schemes have been developed
  - There appears to be no perfect scheme (yet)
  - It is important to continue to test, refine, and compare

From *ABINIT*: "Users must carefully test … [datasets] adequately before using them in their applications."

From *Quantum Espresso*: "Remember: always test the PPs on simple test systems before proceeding to serious calculations."

From *GBRV (USPS datasets from Rutgers)*: "Despite our relatively thorough testing, we cannot guarantee that these potentials will be appropriate for every application…"

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How to generate ^ PAW Atomic Datasets

- **Challenges**
  - Goal: for any physical approximation scheme, the dataset should provide numerically well-controlled results that match the all-electron results as well as possible
  - Large number of pseudofunctions to develop

Basis functions: $\tilde{\varphi}_{n_i l_i}(r)$ Matching radii: $r_{c;n_i l_i}$

Projector functions: $\tilde{p}_{n_i l_i}(r)$ Matching radius: r_c

Compensation charge shape function: $\hat{n}(r)$ Augmentation radius: $\hat{r}_c$

Unscreened local potential: $V^{PS}(r)$ Pseudopotential radius: r_c^{PS}

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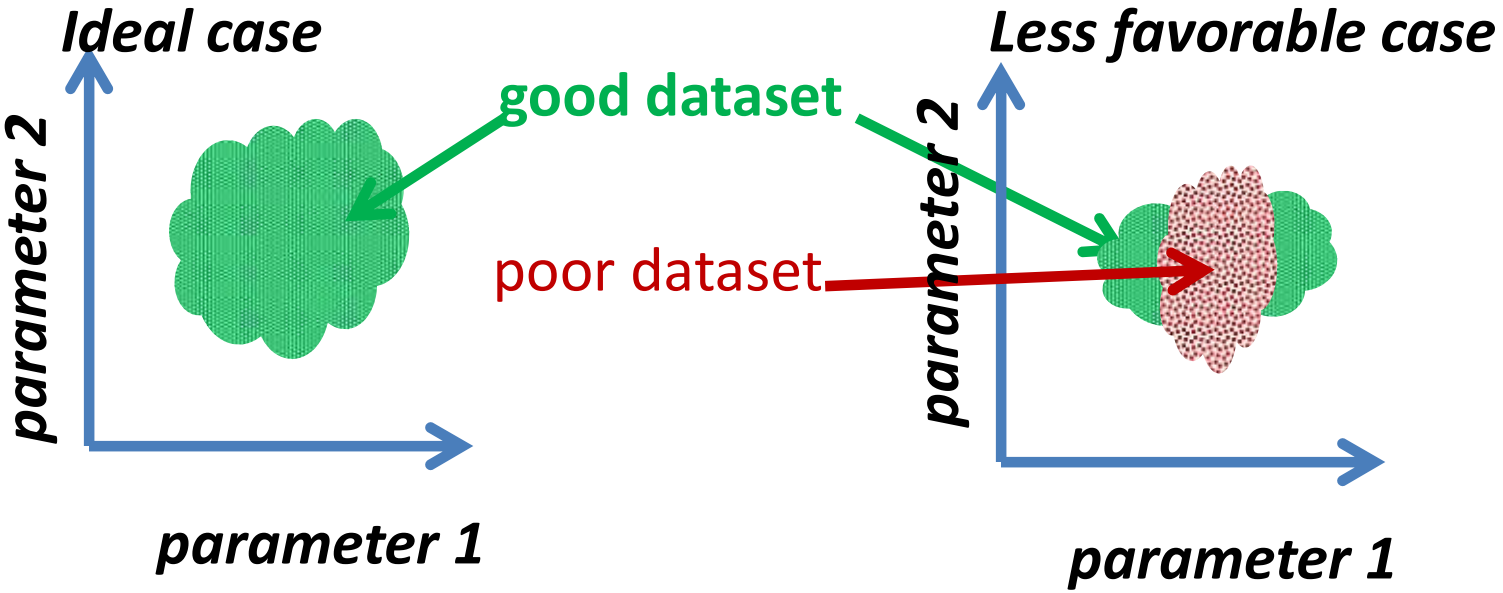
- **Tricks**



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- **Tricks**

Scheme for systematic exploration of pseudo parameters, recently implemented in ATOMPAW code version 4.x series, based on machine optimization approach. (Original idea from Alan Wright (Sandia National Laboratory), Alan Tackett, Greg Walker, and Rachael Hansel (Vanderbilt University). Further inspiration from Qi Li (WFU).)

ATOMPAW scheme:

New keyword “explore” allows you to run up to 9999 sets of input parameters, keeping track of the best overall success value for each *l* channel.

Example input file for Na
For dataset generation

```
Na 11
LDA-PW   loggrid    2001
3 2 0 0 0 0
3 0 1
0 0 0
c
v
v
v
1
1.7   1.5   1.7    1.7
n
y
4.6
n
MODRRKJ VANDERBILTORTHO  Besselshape
2 0   MTROULLIER
1.5
1.7
1.5
1.7
ABINITOUT
default
PWSCFOUT
UPFDX  0.0125d0   UPFXMIN   -7.d0     UPFZMESH 11.d0
END
```

Atomic configuration

Pseudo parameters

Output datasets

Example input file for Na with explore mode

```
Na 11
LDA-PW   loggrid   2001
3 2 0 0 0 0
3 0 1
0 0 0
c
v
v
v
1
1.7   1.5   1.7   1.7
n
y
4.6
n
MODRRKJ VANDERBILTORTHO  Besselshape
2 0   MTROULLIER
1.5
1.7
1.5
1.7
EXPLORE
2000
```

Fixed atomic configuration

Initial pseudo parameters

New keyword for “exploration”

# of pseudo parameter variations

2000 pseudo parameter sets

Merit criterion based on logderivative accuracy

$$L_\ell^{AE}(E) \equiv \left. \frac{d\Psi_{\ell E}^{AE} / dr}{\Psi_{\ell E}^{AE}} \right|_{r_c} \qquad L_\ell^{PAW}(E) \equiv \left. \frac{d\Psi_{\ell E}^{PAW} / dr}{\Psi_{\ell E}^{PAW}} \right|_{r_c}$$

Figure of merit for p^{th} pseudo parameter set for each ℓ :

$$M^{\ell}{}_{p} = \sum_{E} \left| \arctan\left(L_\ell^{AE}(E)\right) - \arctan\left(L_\ell^{PAW}(E)\right) \right|$$

(idea attributed to Alan Tackett)

➔For each *l* channel, choose set with smallest M^{l}_{p}

http://pwpaw.wfu.edu/newperiodictable

Periodic Table of the Elements for PAW Functions (>2013)

New datasets

The bulk of the development and testing of the new datasets was accomplished during the summer of 2013 by a team of students using the **MODKKRJ** and **EXPLORE** capabilities of version 4.0+ of ATOMPAW. We divide the database into two parts labeled "small core" and "large core" sets. In general the "small core" sets include more bound states in the basis and are more accurate for highly ionic materials, while the "large core" sets include only the states which are chemically valence states in the basis and therefore result in less costly calculations. User feedback and contributions are welcome.

Motivation

It has been approximately 5 years since we last made a concerted attempt to update our database of PAW functionals. In collaboration with several other groups, a number of improvements have been made to the atompaw code and dataset generation process. Our previous philosophy was that every new materials project should start with the generation and testing of the necessary atomic dataset generation. However, it is clear that the availablily of libraries of tested atomic datasets can expedit the first steps of a new materials project. We stress that **it is always necessary to test the atomic datasets** for each new materials study, even those obtained from a dataset library.

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"Small Core" Datasets for PAW Functions

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra																
			57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
			89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

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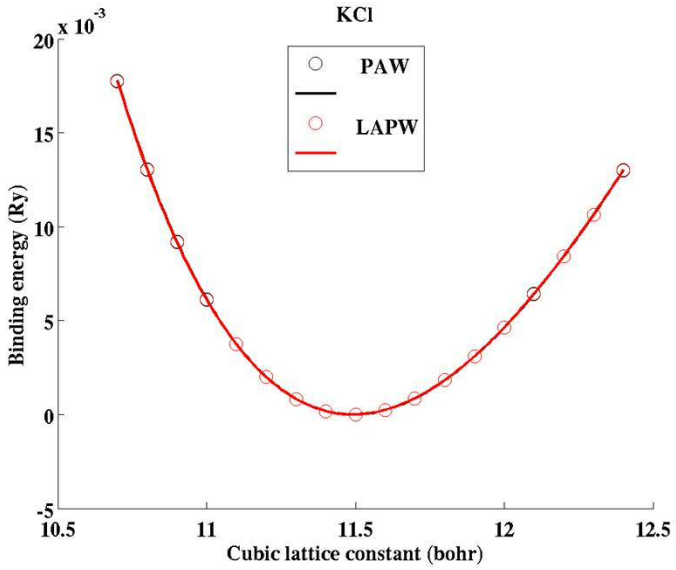
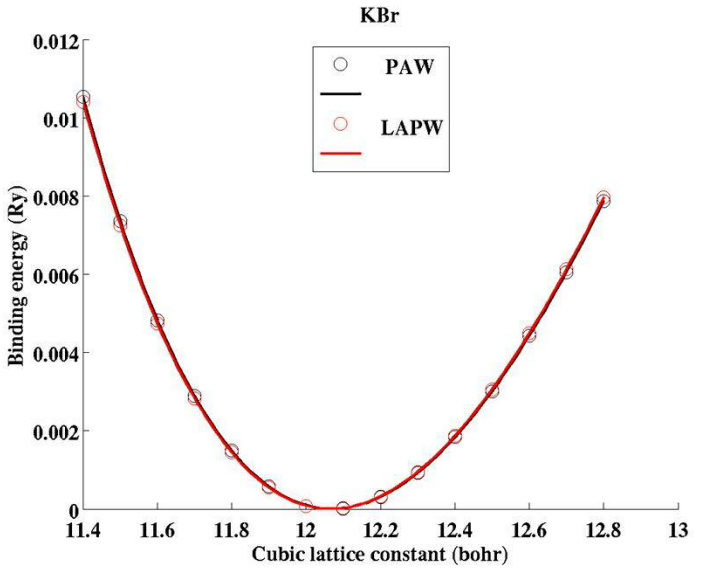
K

Atompaw input	Atompaw output	Comments	Datasets
K.in	K	Author: Cameron Kates	K.LDA-PW-paw.xml.gz K.LDA-PW-paw.abinit.gz K.LDA-PW-paw.UPF.gz K.atomicdata.gz

Tests

Material	Structure	Atomic datasets	Binding plot	Binding data
KCl	NaCl structure Fm -3m (#225)	Small core K Large core Cl	KCl plot	KCl data
KBr	NaCl structure Fm -3m (#225)	Small core K Large core Br	KBr plot	KBr data





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- **Opportunities for collaboration**
  Many database projects

GBRV at Rutgers University
GPAW from CAMP and the Technical University of Denmark
PSLibrary from THEOS @EPFL in Switzerland
abinit Francois Jollet's JTH dataset
quantum espresso

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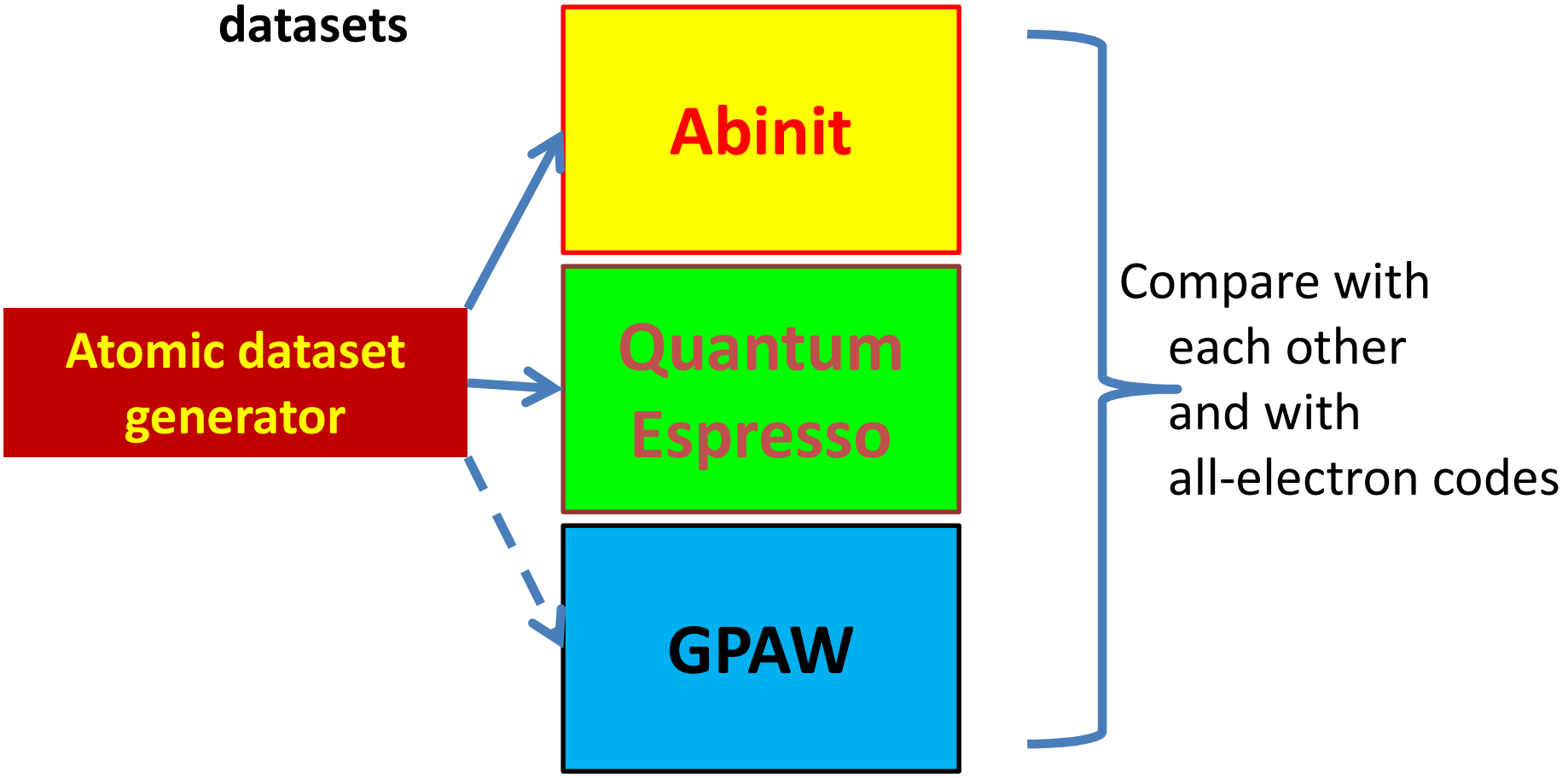

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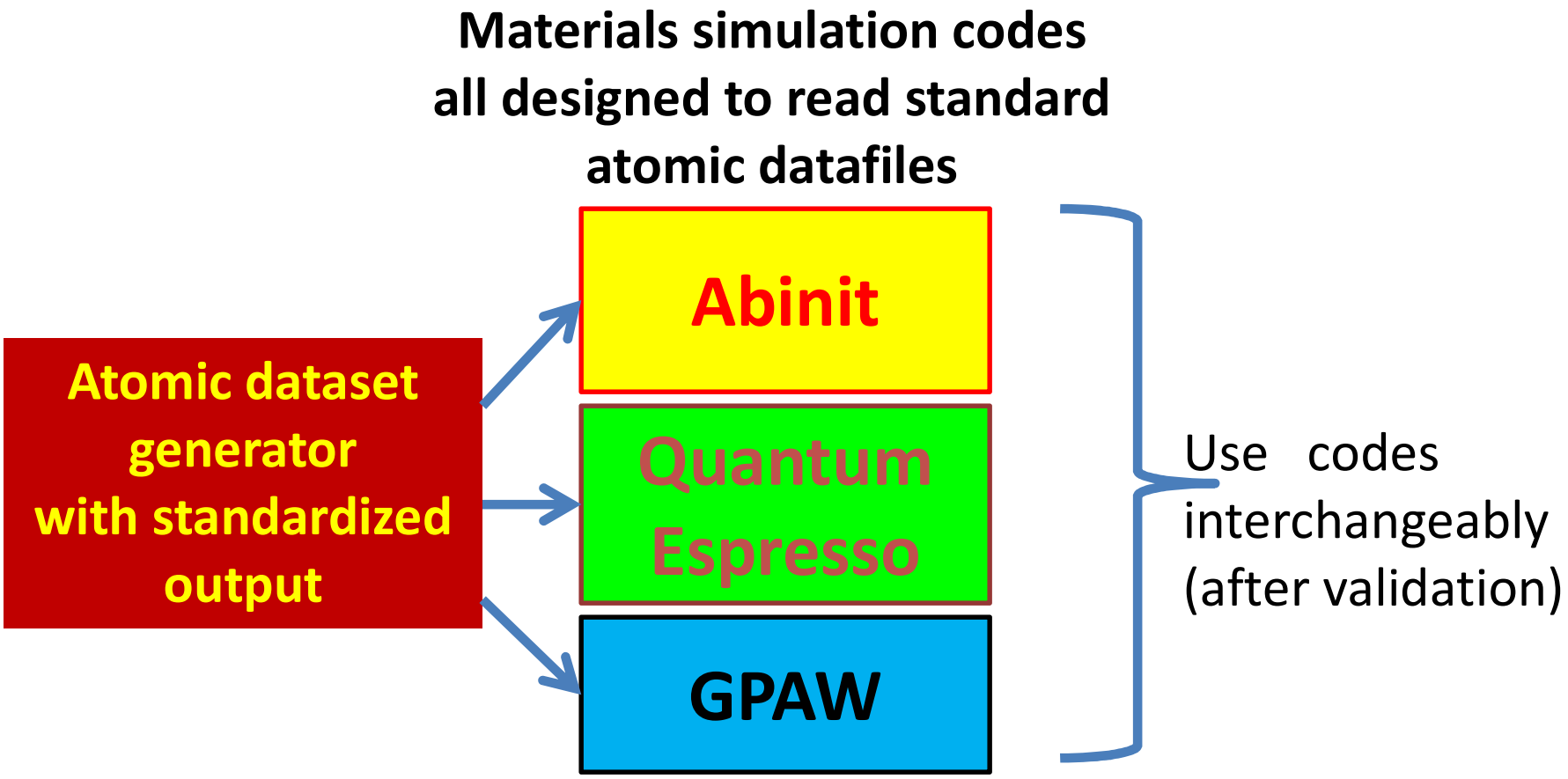
Ideal collaboration



Summary

- In order to develop an efficient collaboration both between alternative atomic dataset generator codes and materials simulation codes it would be ideal to develop a common comprehensive and accepted dataset format
- Also important is to develop a convenient and reliable all-electron "standard" for validating the atomic datasets and the materials simulation codes