Comparison of first-principles methods / codes

Benchmarks run by

Jörg Behler (DMol),
Jutta Rogal (APW+lo),
Mira Todorova (LAPW),
Cathy Stampfl (FHI98md and sFHIngx)

... and Peter Blaha and Peter Blöchl will hopefully comment during (or after) my talk.

Comparison of First-Principles Methods/Codes

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In this talk I will discuss the properties of 5 different total-energy DFT codes, namely DMol, LAPW, APW+lo, and pseudopotential plane waves (the FHI89md and sFHIngx codes). I will explain their inherent approximations and accuracy by using benchmark calculations for selected, topical systems that are expected to bring forth the strengths and
weaknesses.

Some noticeable differences exist between these codes. Though one code may need less CPU time for some system, another code performs better for another one. Altogether there is no clear "super star", implying that the best code is that, one understands best: Only
good understanding of the underlying methodology guarantees best CPU performance with the desired and needed accuracy.

For modern problems, that go beyond what has been published already, a simple black-box code does not exist. Code improvement and development is still a very important challenge, and some modern tasks will be mentioned as well.

(*) in collaboration with Jörg Behler (DMol), Jutta Rogal (APW+lo), Mira Todorova (LAPW), and Cathy Stampfl (FHI89md and sFHIngx)

How to choose the code ?

most important: The best code is the code that YOU understand:

- What are the approximations (in addition to xc)? For example: frozen core, pseudopotentials [or linearization of phaseshifts, $\delta_l(\varepsilon)$]
- basis set, k-points
- approach to solve Poisson equation
- approach to solve the Kohn-Sham equation
- approach to optimize the atomic structure

also interesting is the computer requirement:

- CPU time
- memory

Some differences between codes

FHI98md and sFHIngx employ pseudopotentials:

1. Frozen core approx. (this can be problematic for magnetic systems, or for strong electrostatic fields)
2. Pseudoization (linearization of scattering properties): "making it soft" is a noticeable approximation and can result in errors of about 0.1 eV in the Kohn-Sham eigenvalues and total energies, and several percent in the lattice constant.
3. Linearization of core-valence xc; can be corrected (approximately), but must be checked.

DMol, LAPW, and APW+lo do not suffer from problems #1 and #3, and only little from #2.

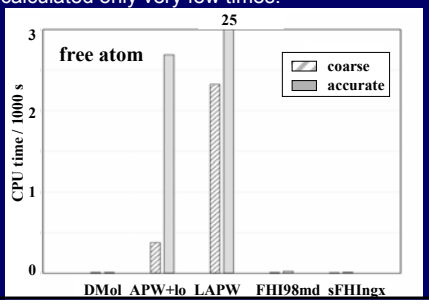
Our benchmark systems

We compare the FHI98md, sFHIngx, DMol, LAPW and APW+lo codes for systems that are expected to bring up strengths and weaknesses of the different methodologies and approximations. And these systems are topical and modern:

- Al bulk
- Al(111) surface
- O adsorbed on Al(111) in (1x1) and (2x2) structures

Aluminum: Free atom and bulk

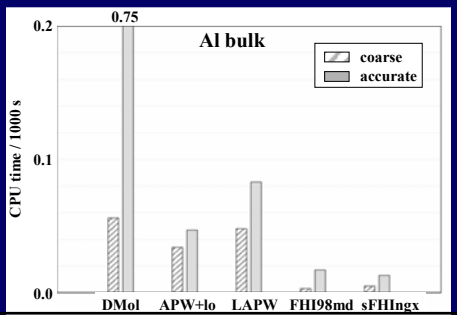
Sometimes we need results for the free atom with the same basis set as that used in the condensed phase. For this the CPU time is not so important, because it will be calculated only very few times.



memory:
< 250 MB

Aluminum bulk

Typically we need results with coarse and accurate basis sets; "coarse" should be "quick but not very dirty", and will be applied often. "Accurate" will be applied only a few times.

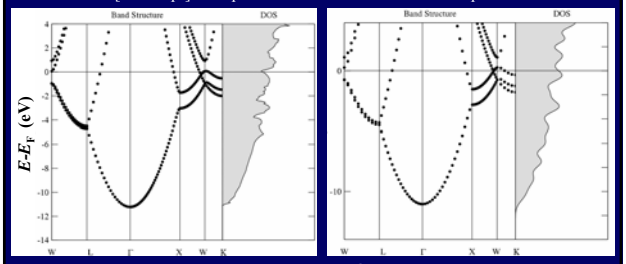


memory: < 125 MB

Aluminum: Bulk

all-electron calculation
$[1s^2 2s^2 2p^6]\ 3s^2\ 3p^1$

PPW calculation
$3s^2\ 3p^1$

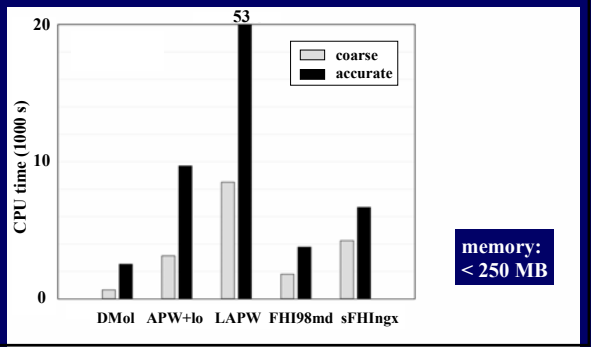


All codes give the same results for the bandstructure, E^{coh}, a_0, and B_0. (The DOS difference is only due to the smearing used in the PPW calculations.)

Bigger calculations: Oxygen adlayers with (1x1) and (2x2) structures

The (2x2) surface cell and a 7-layer slab has 28 Al atoms plus 2 O atoms per cell. This is demanding, because oxygen is difficult to handle. There are 28*3+2*6 = 96 valence electrons.

(1x1) Oxygen adlayer on a 7-layer slab of aluminum



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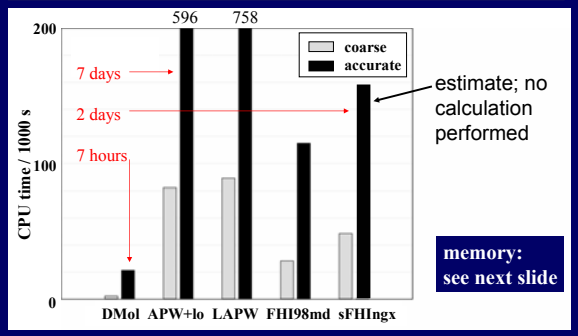
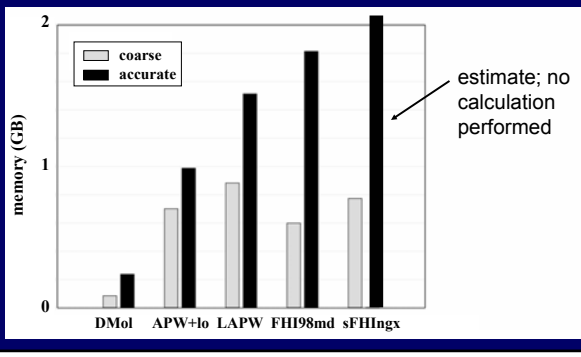
(2x2) Oxygen adlayer on a 7-layer slab of Aluminum



estimate; no calculation performed

memory: see next slide

(2x2) Oxygen adlayer on a 7-layer slab of Aluminum



estimate; no calculation performed

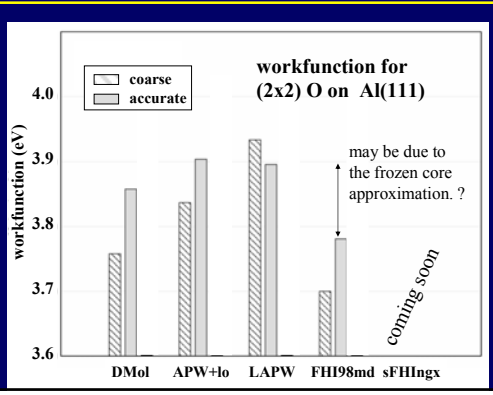
Remarks

LAPW and APW+lo exploit the inversion symmetry of the benchmark systems. This implies that the wavefunctions are real, which reduces the CPU time. If inversion symmetry would not exist (or would not be exploited) the CPU time would increase by a factor of 4.

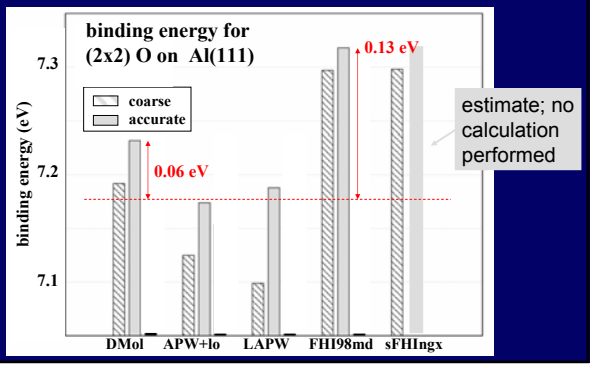
DMol, FHI98md, and sFHIngx do not exploit inversion symmetry. Thus a symmetric slab and an antisymmetric slab require the same CPU time.

Also vacuum costs (for PPW and ..APW..): Reducing the vacuum from 15 to 9.4 Å reduces the CPU time to about 70% and the memory to about 80%. -- No change for DMol.

Comparison of results:



Comparison of results:



Conclusions

PPW codes are most efficient for Al, Si, GaAs and alike. Don't forget that the pseudopotential approach is an approximation (largely due to the frozen-core approximation and the linearization of the core-valence xc). PPW codes are simpler than other codes.

For systems with nuclei lighter than Fe (or close to it), DMol is apparently the best, fastest, and lowest memory code. Many things that are missing right now may come in about 2 years or so. ***A big problem***: This is a commercial code, i.e., it is expensive and you don't get the source (we have it).

The most accurate code with most add-ons is APW+lo (the WIEN2k code). There is also a nice, active community. However, this code is slow – in particular for OH-systems.

Some words about the future

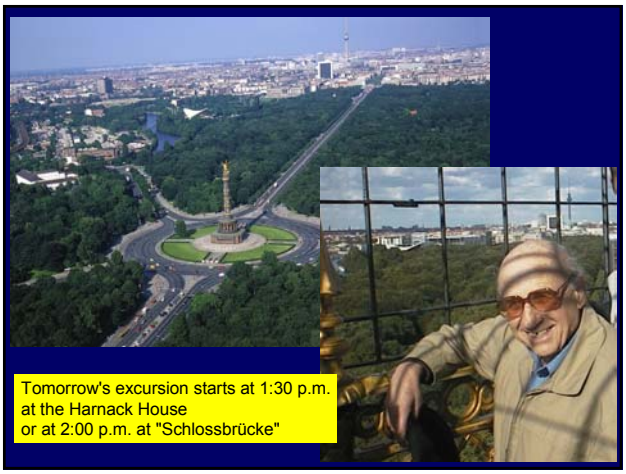
The planned improvements for sFHIngx were described by Sixten Boeck: e.g. PAW, GW, etc.

We plan to incorporate scalar relativity into DMol (necessary to use it for the 4*d* and 5*d* metals).

We are developing a GW add-on to APW+lo (Ricardo Gomez Abal (here), Claudia Ambrosch-Draxl (Graz), et al.)

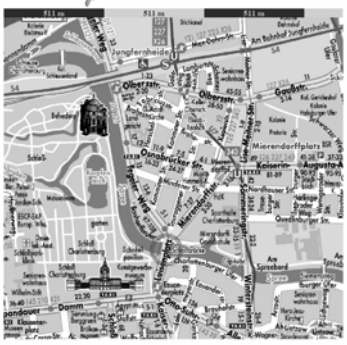
We are about to finish a massive parallel version for APW+lo (together with colleagues at the MPG-Garching-Computer-Center and Peter Blaha).

We are also working on alternative (non DFT) methods, e.g., Quantum Monte Carlo.... (not for this workshop).



Tomorrow's excursion starts at 1:30 p.m.
at the Harnack House
or at 2:00 p.m. at "Schlossbrücke"

Excursion on Saturday, July 26, 2003



1:30 p.m	Departure at Harnack House (we rented a bus, but this is only for participants and lecturers).
	It is recommended that you had lunch before. You may also decide to go earlier and meet us at
2:00 p.m.	"Schlossbrücke" close to the Schloss Charlottenburg (see map). Note, that we leave from there by boat (company: Reederei Winkler) , and **the boat will cast off at 2:20 p.m.**
	Boat tour on the river Spree, going, e.g., to Berlin Mitte (government district, museum island, etc.) to Oberbaumbrücke and back to Friedrichstraße.
	10 min. walk to the museum island to visit the
ca. 5:00 p.m.	Pergamon museum.
	Then a 15 min. walk to the
ca. 6:30 p.m.	Reichstag,
	Then a 20 min. walk through the "Tiergarten" (Berlin's central park) to the
7:00 p.m.	Siegessäule.
	Going to the top of the Siegessäule,
	and then continuing the walk through the Tiergarten (another 15 min.) to the
ca. 8:00 p.m.	"Cafe am Neuen See",
	a nice Biergarten, where we take a Bavarian style dinner.
11:30 p.m. sharp !!!	our rented bus departs from corner Stülerstr./Rauchstr., going back to the Harnack House.
	... you should feel free to miss the bus and to explore the Berlin night life.

If you get lost, you may call the "emergency phone" of Matthias Scheffler: 0170 78 59 591