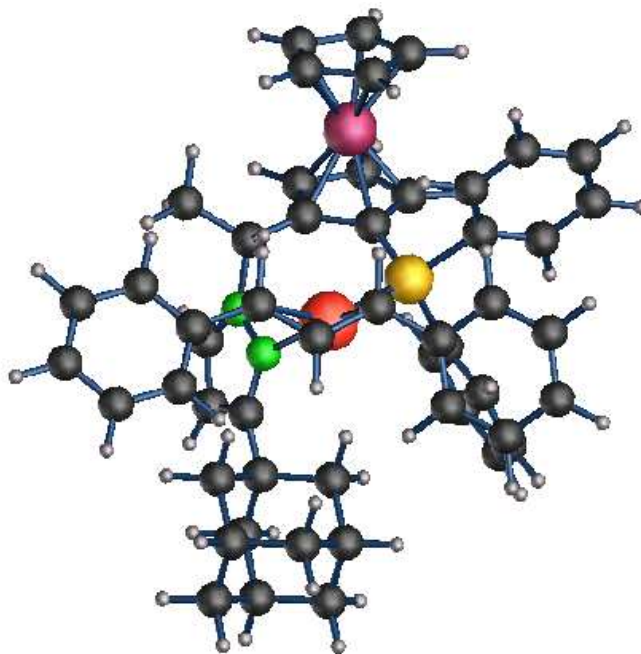


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# History Report for the Projector Augmented Wave Method

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Version 2.0



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(December 14, 2008)

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<sup>1</sup>The title picture shows the a chiral Pd complex with P,N ligands, a highly enantio-selective catalyst for allylic amination [1].

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# 1 Changes

## 1.1 28.Dec.06

The Brillouin zone integration has been reworked substantially.

The k-point grid can now be determined by a real space cutoff specified with `!STRUCTURE!KPOINT:R`. This value specifies how fine the k-point grid is chosen. The k-point grid corresponds to a supercell chosen so large that real space points related by translational symmetry are separated at least by the real space cutoff.

Using the option `STRUCTURE!KPOINTS:SHIFT`, the Monkhorst-Pack k-point grid can now be shifted away from the  $\Gamma$ -point. Apparently this shift improves the k-point convergence substantially. A shift of (1,1,1) is recommended for crystals. The option may also improve the convergence with cell-size for isolated molecules. However that needs to be tested.

In the block `!CONTROL!MERMIN` the option of quasi-adiabatic treatment of the occupations is provided. A new set of energy levels is introduced that approaches the Kohn Sham levels in a retarded fashion. The occupations are optimized in each time step for this set of occupations. This option is recommended for static calculations. It does not lead to an energy conserving dynamics, because it is not a true adiabatic implementation.

As one of the quasi-adiabatic options the improved tetrahedron method[2] has been included. Unlike the Mermin functional[3], this method does not require finite temperatures. It is the recommended method for static calculations of metals.

In the printout the occupations are compared with those obtained from the current energy eigenvalues. An estimate for the error in the energy is given together with the maximum deviation of the occupations.

## 1.2 Jan. 11, 2007

LDA+U option of Christian Walther implemented into main code. Some changes have been made in this course. therefore testing will be required.

## 1.3 Jan. 30, 2007

COSMO can write an input file for COSMOTHERM.

## **1.4 Feb. 25, 2007**

Rewrite of the linear algebra routines in paw\_library.f90. Test routines have been included for the new routines. They are called by “call lib\$test()” Library specific driver routines are used, which distangles different libraries. Has not been tested for ESSL library. Version has been checked into devel\_blo/devel version 562.

## **1.5 Feb 25.2007**

change in linkedlist\$existd. If a the nth data are searched true was only returned, if nth was the total number NUM of data in the list. It has been changed so, that the number NUM of elements in the list must be equal or larger than nth.

## **1.6 Apr 12. 2007**

The approximate hybrid functional has been included into the ldaplu object.

## **1.7 Apr 14. 2007**

Bugfix for plotting electrostatic potential. Symptom: The potential oscillated strongly. Cause: POTSHIFT, an additive shift for the potential was added to all Fourier components of the potential instead of its real space values.

## **1.8 Apr 14. 2007**

Bugfix in paw\_library.f90. plans for fftw calls are now specified as integer(8). (integer(4), and integer did not work and produced a “Speicherzugriffsfehler” in the three dimensional fourier transform.)

## **1.9 Apr 14. 2007**

Included tool paw\_1davpot.x located in src/Tools/Wave. It uses the .wv file produced by the !control!analyse!potential option and produces the one-dimensional potential averaged over lattice planes. This tool can be used to determine work functions and band offsets.

### **1.10 Apr 14. 2007**

Change of input parameters:

Removed the parameter `!control!dft!lda+u`. Now the program decides based only on the presence of a corresponding block in `!structure!species`.

### **1.11 Apr 16. 2007**

Included tool `paw_cmcwave.x`, that converts a wave function output file of the simulation code into a `cmcv` format for `crymolcad`. It is located in `src/Tools/Wave`.

### **1.12 Apr 24. 2007**

Linkedlist allows for tabs in the input files. Tabs are replaced by spaces. (includes also occurrences in text strings.)

### **1.13 May 1, 2007**

Bugfix in `paw_ldaplu`. For non-collinear calculations, the hybrid functional and LDA+U did not apply the correction to the potential. Problem has been fixed in `paw_ldaplu` in routine `ldaplu_spindenmat`.

### **1.14 May 1, 2007**

Tessellation files `tess_32`, `tess_122`, `tess_482`, `tess_1922` for COSMO calculations have been included in the directory "parameters".

### **1.15 May 3, 2007**

Bugfix in `paw_linkedlist.f90`: With the `ifc91` compiler `buffer$read` did not read all strings properly. The origin was that an substring character array with assumed shape and assumed len parameter has been passed to `linkedlist$set`. The problem may be a compiler problem or a violation of the fortran standard. New routines `linkedlist_setchr1withlength` and `linkedlist_getchr1withlength` have been created, that pass the length of the array explicitly. This may also solve the problems we had with the `xlf` compiler, for which a workaround has been implemented. It needs to be checked if the present fix also makes the `xlf`-workaround superfluous.

## 1.16 May 5, 2007

configure scripts changed. `configure.in` has been replaced by `configure.ac`, the default input for `autoconf`. `Makefile.in` has been changed a little. The changes affect the parameters in `parmfiles`. The old `parmfiles` have been placed temporarily in the directory `oldparmfiles`.

the new configure process also creates a version (`paw_prof.x`) for profiling. Create it with “`make prof`”.

## 1.17 May 5, 2007

The `preopt` tool did not work after the amber forcefield had been implemented as optional force field in addition to the UFF force field. The forced UFF was now explicitly set in the `preopt` tool and introduced as default for the classical object.

## 1.18 May 13, 2007

Change of configuration procedure.

- `configure.ac` has been simplified. Obsolete `autoconf` features removed.
- `configure` must be used with `-with-parmfile=`. No other variables are allowed.
- `Makefile.in` has been split into `Makefile_targets.in` and `Makefile.in`. `Configure` uses `Makefile_targets.in` to create `Makefile` in the PAW root directory. This `Makefile` contains all targets the user can access directly. `Makefile.in` is used to create `Makefile` and `Makefile_parallel` in the Object directories `bin/$ARCH/none`, `bin/$ARCH/fast`, `bin/$ARCH/dbg`, `bin/$ARCH/prof`.
- instead of `mpif.h`, now the `mpif.f90` is used. (the latter creates a module “MPI”, that is used by the other routines.)
- parallel compilation allowed for `none`, `fast`, `dbg`, `prof`.
- processed fortran files remain in the object directories.
- there is a function “`make clean`” which removes the files in `bin/$ARCH/none`, `bin/$ARCH/fast`, `bin/$ARCH/dbg`, `bin/$ARCH/prof`. In addition it removes all files from the `doc` directory except the `tex` files.



- there are new parameters for the parmfiles and other ones have been removed.

### **1.19 May 14, 2007**

change in paw\_linkedlist.f90: xlf workaround commented out. (special fix for xlf compiler is probably not needed any more).

### **1.20 May 14, 2007**

Bugfix in paw\_occupations.f90: The variable sigma was not defined at one place. Affects behavior of Mermin with adiabatic=false for spin-polarized calculations.

### **1.21 May 20, 2007**

PDoS tool also writes the spin for collinear calculations.

### **1.22 May 25, 2007**

Included FFTW3 interface routines in paw\_library. They are not tested and still blocked from usage.

### **1.23 May 28, 2007**

Bugfix in paw\_graphics.f90. it was not possible to write the density in a parallel environment.

### **1.24 May 28, 2007**

paw\_trace.f90 also writes into files trace\_i. where  $i$  is the task-id in a parallel environment. This avoids that the trace information is incomplete after a crash, because the information is not written in time to standard output.

### **1.25 May 28, 2007**

A routine to extract the dependencies from the fortran codes has been written. (src/F90PP/findependencies.f90, src/F90PP/finddep). The dependencies have been

included in the Makefiles. This makes the targets `..._new` unnecessary. Dependencies for the documentation have been included to avoid frequent recompiling.

### **1.26 May 28, 2007**

Change of configuration procedure.

The names of the variables in the `parmfile` have been changed to be compatible with common standards.

### **1.27 May 29, 2007**

The source files for the documentation have been copied into `src/Docs`. During installation the files are copied into the `doc` directory, where they are compiled. The `doc` directory has been removed from the repository. It will be recreated each time!

### **1.28 May 30, 2007**

reworked `paw_trace.f`. Trace files are written only if trace is switched on explicitly. The object can be set temporarily silent. It obtained a function to return if a trace file is attached, which allows to write arbitrary information into the trace files. It obtained functions to report numbers into the trace information, only if the trace object is on.

### **1.29 May 30, 2007**

the target `"docs"` has been removed from the targets `"all"`, `"all_new"` and `"small"`.

### **1.30 May 31, 2007**

Bugfix. Noncollinear calculations with general k-point do not allow to reduce the number of k-points using time inversion symmetry. The program uses now automatically all k-points in connection with non-collinear calculations.

### **1.31 June 2, 2007**

The position trajectory has been extended to include also the integrated valence density and spin density for each `"ASA"` sphere.

### **1.32 June 17, 2007**

The MPI module specified by CP-PAW has been renamed to avoid conflicts with the MPI module of the MPI library itself. In future the user has to include the mpi module mpi.mod explicitly in the compiler call or use mpif90, best with the -choicemod option. If an mpi module is not supplied with the distribution, the module mpi\_mine in paw\_mplib.f90 can be modified to include the mpif90.h file as before.

### **1.33 June 27, 2007**

Bugfix in paw\_waves2.f90 in waves\_read, line 3146. The code messed up the color table for the k-parallelization. The loop is now executed on all nodes and the code-snippets for the first and the kgroup nodes are selected individually. I did not follow up what exactly caused the bug, but the change solved the problem.

### **1.34 July 13, 2007**

Change of functionality for the rotation constraint. See “!STRUCTURE!CONSTRAINTS!ROTATION”. The documentation has been updated. The angular momentum constraint did not separate out the motion of the center of gravity. An earlier attempt was buggy and had been switched off. The rotation constraint enforced the angular momentum to be constant and not equal to zero, as it is now.

### **1.35 August 15, 2007**

Changed pawldaplusu, so that the J parameter are calculated correctly. Now it is also possible to enforce  $F^4/F^2$  and  $F^6/F^2$ . Where  $F^\ell$  are the Slater integrals of the main shell.

### **1.36 August 22, 2007**

Dependencies during installation corrected. The make file did not work efficient for some compilers such as ifc7, because the compiler produces uppercase module file names with lowercase extension, while the make file assumed all lowercase module file names as used by the g95 compiler. The configure.ac has been modified so that it can accept a new parameter “TUPPERCASEMOD” from the pa-

parameter file. If its value is true, the make file assumes ifc7-like module file names. otherwise lowercase module file names are assumed.

### **1.37 August 22, 2007**

In Idaplusu the double counting term still used some old, l-dependent definitions for the u and j-parameter. Now the general definition has been included.

### **1.38 August 22, 2007**

There was an inconsistency in the manual for the confining potential !structure!confine. The manual asked correctly for a parameter "POT" while the code was looking for "V0". Now the code has been changed to "POT" as well.

### **1.39 August 31, 2007**

The make file construction did not treat the upper/lowercase module names properly. The configure.ac has been modified. It is necessary to use the new configure script of to run autoconf with the new configure.ac.

### **1.40 August 31, 2007**

minor Bugfix: The variable "kread" in subroutine waves\_read in file paw\_waves2.f90 has not been fully initialized, which resulted in unpredictable crashes.

### **1.41 August 31, 2007**

Minor Bugfix: I changed the position of trace\$push in routine qmmm\$propagate.

### **1.42 September 12, 2007**

Fixed the Parrinello-Rahman option. Further testing is still needed. I went back to the original Parrinello-Rahman implementation. Only constant pressure and no constant stress calculations are possible. The formulation has been changed so that the wave functions are not scaled with the unit cell. This scaling will be done by the orthogonalization.

### **1.43 September 19, 2007**

The routine `waves_readpsi` has been rewritten to fix the startip problem. The option to switch between k-point sets and between different spin treatments (unpolarized, collinear and non-collinear) has been removed.

It is possible to change the plane wave cutoff, the number of states, and it is possible to switch from a non-spin polarized to a spin polarized calculation.

### **1.44 September 24, 2007**

Included deterministic option for choosing random wave functions. Even starting with “random” numbers the initial wave functions are the same irrespective of the number of tasks in the parallelization.

### **1.45 September 25, 2007**

Fixed a subtle bug writing an output file for cosmo. (the bug only occurred with ifc.) it only resulted in crashes.

### **1.46 September 25, 2007**

The change for the random wave function from sept. 24, 2007 resulted in spherical initial wave functions. The symmetry made the convergence much worse. Now I implemented that the initial wave functions also have a random angular dependence.

### **1.47 November, 2007**

Interfaces for the Fourier transforms of ACML included. Interfaces for Utility libraries for Pathscale etc.

### **1.48 November, 2007**

Bugfix in `paw_ldaplu.f90`. A loop for transformation matrix to local orbitals started with  $l=1$  instead of  $l=0$ .

### **1.49 November 25, 2007**

After reading the wave function the logical variable `tsuper_` is redefined, so that insignificant bits are properly set. Apparently, the insignificant bits are written differently from compiler to compiler. Some logical operations such as `.eqv.` and `.neqv.` are, depending on the compiler, sensitive to all bits or only the significant one. This resulted in errors.

### **1.50 December 4, 2007**

Included new installation instructions in Docs. (still in German)

### **1.51 December 9, 2007**

Included a constraints for the variable cell shape dynamics. It is now possible to restrict the cell dynamics to isotropic expansions or reductions or to remove shear components of the dynamics.

The installation description has been partly translated.

### **1.52 January 4, 2008**

The interface for the 3d-fft using the acml ffts was not implemented. It has been done now.

### **1.53 January 5, 2008**

Bugfix. The tetrahedron method did not work if the total spin was fixed. It was a problem with dimensions in `paw_occupations.f90` around line 1910.

## References

- [1] P.E. Blöchl and A. Togni. First-principles investigation of enantioselective catalysis: Asymmetric allylic amination with pd-complexes bearing p,n-ligands. *Organometallics*, 15:4125, 1996.
- [2] P.E. Blöchl, O. Jepsen, and O.K. Andersen. Improved tetrahedron method for brillouin-zone integrations. *Phys. Rev. B*, 49:16223, 1994.
- [3] N.D. Mermin. Thermal properties of the inhomogeneous electron gas. *Physical Review*, 1965.