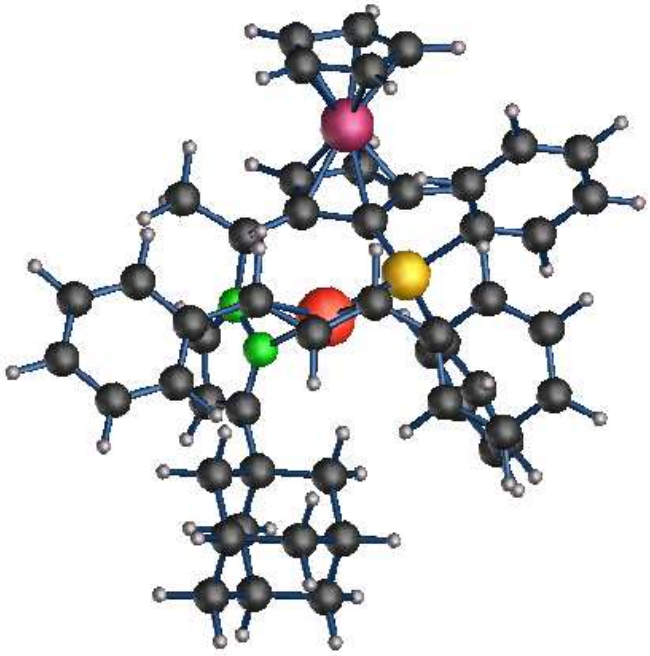
History Report for the Projector Augmented Wave Method

Version 2.0



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(December 4, 2007)

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

Contents

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 `!STUCTURE!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 Γ-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 ldaplusu 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 siumulation 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 occurances in text strings.)

1.13 May 1, 2007

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

1.14 May 1, 2007

Tesselation 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 explicitely. 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 forcefied UFF was now explicitely 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 acess directly. Makefile.in is used to create Makefile and Makefile_parallel in the Object directries 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 fore 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 tha 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 explicitely. 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 explicitely 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_mpelib.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^ℓ 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-

rameter 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 ldaplusu 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 stilll needed. I went back to the original Parrinllo-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 withg "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 Ultility libraries for Pathscale etc.

1.48 November, 2007

Bugfix in paw_ldaplusu.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)

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.