dftatom: Routines for Radial Integration of Dirac, Schrödinger, and Poisson Equations

This library implements accurate and efficient radial Schrödinger and Dirac shooting-method solvers. They work with any grid and any numerical potential. In addition, it also implements a radial Poisson solver and density functional theory self-consistency cycle.

Accuracy

With the provided meshes, the solvers (both Schrödinger and Dirac) can converge to at least 1e-8 Ha accuracy (with double precision of approximately 16 significant digits) for all eigenvalues and total DFT energies for all atoms up to Uranium (Z=92).

The converged nonrelativistic and relativistic results agree with NIST benchmarks to the stated accuracy of those benchmarks (2e-6 Ha in eigenvalues and 1e-6 Ha in total energies).

http://physics.nist.gov/PhysRefData/DFTdata/Tables/ptable.html

License

This program is MIT licensed, see the LICENSE file for details.

Compilation

The main code is standard Fortran 95 with no extensions and so can be compiled with any standard f95 conforming compiler. The optional C interface requires Fortran 2003 `iso_c_binding` module. N.B.: Due to a bug in older versions of the Intel ifort compiler, ver. 12.0.191 or later is required.

We provide CMake and standard Makefiles. To use the standard Makefiles, do (from the top directory):

```
make -f Makefile.manual
```

The provided Makefile.manual uses the gfortran compiler to build the (slow, extensively checked) debug version of the library. Modify as desired for your preferred compiler/options (in particular, to build a faster release version; see comments in Makefile.manual). The optional C and Python interfaces are not built by default.

To use CMake, do (from the top directory):

```
cmake .
make
```

The first command generates the required Makefiles and the second command runs them. The default build uses your default Fortran compiler to make a debug version without C or Python interfaces (see below how to enable them or change other build options or the compiler).

Tests

It's important to check that the routines calculate correctly, before you use them for any serious calculation. To do that, execute (if you use CMake):

```
$ make test
[...]
100% tests passed, 0 tests failed out of 15
```

```
Total Test time (real) = 367.75 sec
```

or (if you use hand written Makefiles):

```
$ make -f Makefile.manual test
[...]
make[2]: Leaving directory `/home/ondrej/repos/dftatom/tests/atom_U'
make[1]: Leaving directory `/home/ondrej/repos/dftatom/tests'

All tests passed.
```

it will take around 6 minutes to run for release compilation (not debug), all tests should pass (in both cases you should see the summary above saying that all tests have passed). Here are examples of the output if there is any error for CMake:

```
$ make test
[...]
93% tests passed, 1 tests failed out of 15

Total Test time (real) =   9.36 sec

The following tests FAILED:
     13 - conv_lda (Failed)
Errors while running CTest
make: *** [test] Error 8
```

and manual Makefiles:

```
$ make -f Makefile.manual test
[...]
Test failed: error =   8.99E-04   >   5.00E-04 specified.
 Aborting...
STOP 1
make[2]: *** [test] Error 1
make[2]: Leaving directory `/home/ondrej/repos/dftatom/tests/lda'
make[1]: *** [test] Error 2
make[1]: Leaving directory `/home/ondrej/repos/dftatom/tests'
make: *** [test] Error 2
```

CMake Options (Python and C Bindings, Release Build, Lapack)

CMake has many standard options, see `man cmake`. For example you can set the compiler by doing (make sure you delete `CMakeCache.txt` if you ran CMake before):

```
FC=ifort cmake .
```

You can set whether to build `Debug` or `Release` builds by:

```
cmake -DCMAKE_BUILD_TYPE=Release .
cmake -DCMAKE_BUILD_TYPE=Debug .
```

The default compiler options that will be used for each build are specified for gfortran and ifort in `cmake/UserOverride.cmake` (for other compilers, the default CMake options will be used). You can set your own compiler options for each build by:

```
cmake -DCMAKE_Fortran_FLAGS_RELEASE="-O3" .
cmake -DCMAKE_Fortran_FLAGS_DEBUG="-g" .
```

Besides the standard options above, we provide several options specific for dftatom. By default, only Fortran code is compiled. To enable C and Python bindings, first install Cython and NumPy, for example in Ubuntu 12.04:

```
apt-get install cython python-numpy
```

and then you have to use CMake and set the `WITH_PYTHON` CMake variable to `yes`. You can either do:

```
cmake -DWITH_PYTHON=yes .
make
```

Alternatively you can also just edit the generated `CMakeCache.txt` file (this assumes that you have already run CMake before) and rerun `make` again.

To only enable the C interface (but not Python), set the variable `WITH_C_INTERFACE` to `yes`.

To run Python API tests (to make sure that things got compiled properly and that the Python module can be imported):

```
$ PYTHONPATH=. dftatom/test_runner
============================ test process starts ==============================
executable:   /home/ondrej/repos/qsnake/local/bin/python  (2.6.4-final-0)

tests/test_dftatom.py[4] ....                                               [OK]

================== tests finished: 4 passed in 1.90 seconds ===================
```

This will use the `dftatom` module from the current directory (that's why we need to add `.` to `PYTHONPATH` so that Python can find the module). To install the module into a different directory, do for example:

```
cmake -DWITH_PYTHON=yes -DCMAKE_INSTALL_PREFIX="$HOME/usr" -DPYTHON_INSTALL_PATH="$HOME/usr/lib/python2.7/site-packages" .
make
make install
```

This will install it into `~/usr`.

The `double_min` test depends on Lapack, so it is turned off by default. You can enable it by:

```
cmake -DWITH_LAPACK=yes
make
```

You need to have `lapack` and `blas` libraries. If non-standard linking is required, modify the link options in the file `tests/double_min/CMakeLists.txt` by hand.

Usage

Look into tests how to use the routines to get meaningful results. Run for example the Uranium LDA:

```
cd tests/atom_U
./F_atom_U
```

There are also a few Python examples in the examples/ directory, you can execute them for example using:

```
PYTHONPATH=. python examples/atom_U.py
```

Read "Structure Of The Program" section below for more information.

Development

The C bindings are defined in `c_dftatom.f90`. If you update this file, make sure you run:

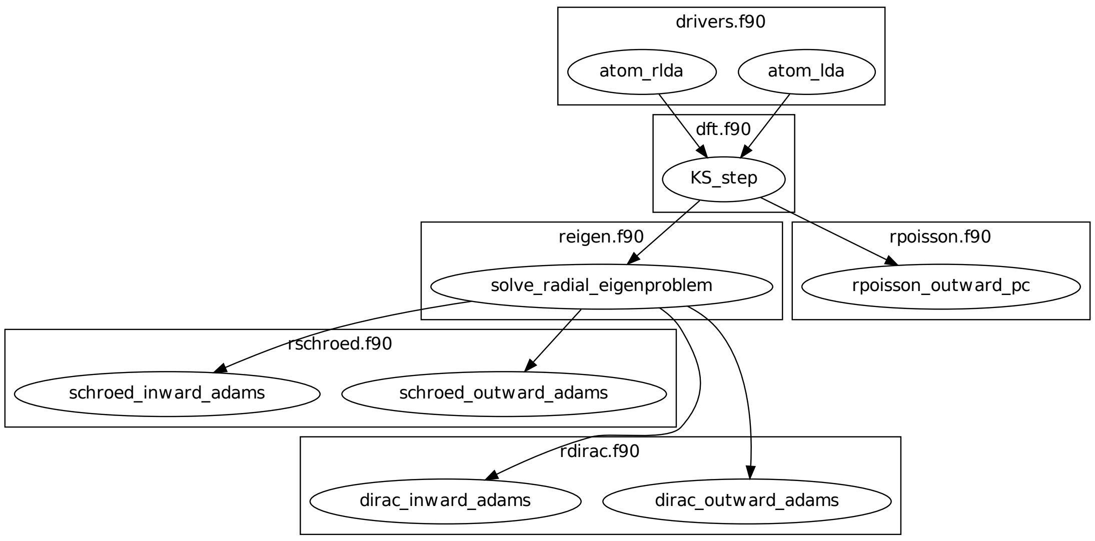
```
$ utils/generate
'src/c_dftatom.h' updated
'dftatom/lib/c_dftatom.pxd' updated
```

This will update the C `.h` file as well as Cython `.pxd` file. Then use it from C or Cython as usual, typically you probably want to export the new functionality to Python by updating the `.pyx` files and then just:

```
make
```

Structure Of The Program

The structure of the Fortran 95 modules is described here. The relations of the most important subroutines can be summarized in a dependency graph:



The `drivers` module contains higher level DFT subroutines `atom_lda` and `atom_rlda` that one can use to solve atoms. The atomic orbitals (radial wavefunctions) can be accessed in the argument `orbitals` of these functions. They are given on the radial mesh returned by the argument `R` and are normalized according to the equations (9) and (20) in the manuscript. These wavefunctions can then be used to construct interaction matrix elements. The radial density and Kohn-Sham energies are also returned as arguments `density` and `ks_energies`. Other parameters affecting the results that can be set are mesh parameters, atomic configuration, accuracy of the eigenproblem as well as selfconsistency iterations and whether or not to use the perturbation correction, see the definitions of the subroutines in `drivers.f90` for more details. As an example of usage, see for instance the program `tests/atom_U/F_atom_U.f90` which prints the orbitals and energies.

The `dft` module contains utilities to solve the Kohn-Sham equations.

The radial Schrödinger/Dirac integration is performed by the `reigen` module using the `solve_radial_eigenproblem` subroutine, which accepts the (external) potential as an argument `V` specified as an array of values on a mesh (argument `R`). There are several configuration options that can be supplied, see the documentation of the `solve_radial_eigenproblem` subroutine in `reigen.f90`. Examples of usage are given in the simple tests in `tests/pseudopotential/` or `tests/oscillator/`, where the potential and mesh is constructed in the main program.

Finally, the low level modules `rschroed`, `rdirac` and `rpoisson` handle the radial integration (they use the `ode1d` module that contains some common utilities for solving ordinary differential equations). Detailed documentation of these subroutines is given in the comments in the code.

A description of all modules follows:

rschroed.f90

Routines in this module solve the radial Schroedinger equation outward and inward using the implicit Adams method.

rdirac.f90

Routines in this module solve the radial Dirac equation outward and inward using the implicit Adams method.

rpoisson.f90

Routines in this module solve the radial Poisson equation outward using the predictor-corrector method (with Adams extrapolation/interpolation).

ode1d.f90

General utilities for solving 1D ODEs. the Adams and rk4 subroutines are used by Schroedinger, Dirac and Poisson solvers. The integrate function is used at other places in dftatom to calculate integrals of the radial density/orbitals.

reigen.f90

Solves the radial Schroedinger/Dirac eigenproblem

mixings.f90

This module contains SCF mixing algorithms.

mesh.f90

Contains mesh utilities (creating the exponential mesh and its derivatives).

dft.f90

Calculates the exchange and correlation potential, Hartree potential, and the full (single) Kohn-Sham iteration.

dft_data.f90

Contains the `dft_data_t` type used in the DFT routines. This data type stores mesh, potential, atomic configuration, orbitals and other parameters of the DFT problem.

states.f90

This module lists nonrelativistic and relativistic atomic configurations. The nonrelativistic configurations are the same as at NIST and are simply hardcoded in the subroutine for each atom. The relativistic configuration is then calculated from the nonrelativistic by splitting the occupancy according to the degeneracy (see the comments in the `get_atomic_states_rel` subroutine of this module for more technical information).

drivers.f90

This module contains high level drivers for atomic SCF calculations. The idea is to use these drivers to do most frequent calculations with an exponential mesh and to get an idea how things work. They can be used as a starting point/template to write a custom solver for a particular problem, or to use a different mesh.

energies.f90

Calculates Hydrogen nonrelativistic and relativistic energies (exact), Thomas-Fermi (TF) energies (only very approximate), TF potential and charge density (very accurate).

dftatom.f90

This module contains the high level public API (application programming interface) for dftatom. One should only be using this module from external programs (as long as only the high level functionality is needed). For a low level usage, one can always call the individual modules directly.

c_dftatom.f90/.h

The C API to dftatom that wraps the API exposed by the `dftatom` module and the corresponding C header file.

rschroed_other.f90

Other Schroedinger integrators, not directly used by dftatom, but available for reuse. This module contains various rk4 integrators and Adams predictor-corrector integrators (both for outward and inward integration).

rdirac_other.f90

Other Dirac integrators, not directly used by dftatom, but available for reuse. This module contains various Adams predictor-corrector integrators (both for outward and inward integration) and functions to calculate analytic asymptotic.

rpoisson_other.f90

Other Poisson integrators, not directly used by dftatom, but available for reuse. This module contains various Adams predictor-corrector integrators (both for outward and inward integration).

ode1d_other.f90

General utilities for solving 1D ODEs, not used directly by dftatom. They are available here for reuse.

types.f90

This module defines the `dp` double precision type.

constants.f90

Contains the mathematical constant `pi`.

utils.f90

Various utilities for general use in Fortran programs.