PWDFT.jl: Density Functional Theory Calculations with Julia

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24 September 2019

Software packages for DFT calculations

There are a lot of software packages for DFT calculations, for examples:

- Quantum ESPRESSO
- VASP
- ABINIT
- Gaussian series: G03, G09, G16
- NWchem

Test math:

$$\alpha + \beta \oint \tag{1}$$

More extensive list:

`https://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid-state_physics_software`

Problems

- These packages are very helpful for doing various calculations based on DFT. These packages are suitable for black-box-type calculations where we are only concerned about the results.
- However they are generally rather difficult to extend.
  - New development on the DFT functionals: users generally need to wait for the next release of the package to use them (if these functionals are to be implemented at all).
  - Custom calculations or post-processing steps: Users need to know in some detail about how the data they are interested in is represented or implemented in the package's source code.

Write another DFT package?

Personal motivation:

learning how DFT or Kohn-Sham equations are solved

frustation when trying to extend available package

Programming languages for DFT

Programming languages used:

- Fortran and/or C/C++: ABINIT, VASP, Quantum Espresso, ...
- Python: GPAW
- MATLAB: KSSOLV, RESCU

Static languages: Fortran, C/C++

Dynamic languages: Python and MATLAB

Julia programming language

A rather new programming language (2012)

Syntax is familar to MATLAB or Python users

support for multidimensional array and linear algebra

Loop is fast!

Introducing PWDFT.jl

- A program package for doing DFT calculations using Julia
- plane wave basis + pseudopotentials (norm-conserving)
- LDA and GGA functionals can be used (via LibXC)
- symmetry detection (via SPGLIB)
- algorithms for solving KS problem: SCF and Emin (PCG and DCM)

Aims

- Friendly-to-developers DFT package: enables quick implementation of various algorithms
- educational purpose: simple yet powerful enough to carry out practical DFT calculations for molecular and crystalline systems.

Examples

Typical steps

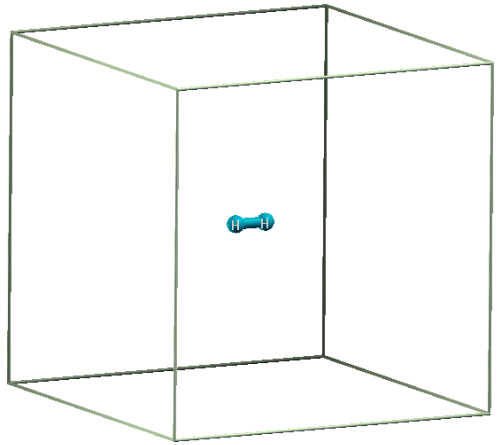
Write Julia code not an input file.

Typical steps:

- Initialize Atoms
- Initialize Hamiltonian with the given Atoms
- Solve the Hamiltonian

Atomic units are used (energy: Hartree, length: bohr)

Example: hydrogen molecule in a box



```
using PWDFT # activate PWDFT package

# Initialize an H2 molecule in cubic box (simple cubic lattice)
# The coordinates are read from
atoms = Atoms( xyz_file="H2.xyz",
               LatVecs=gen_lattice_sc(16.0) )

pspfiles = ["H-q1.gth"] # pseudopotential parameters

ecutwfc = 15.0 # cutoff energy for wave function expansion

# initialize Hamiltonian
Ham = Hamiltonian( atoms, pspfiles, ecutwfc )

# solve the Kohn-Sham problem (using SCF algorithm)
KS_solve_SCF!( Ham )
```

Output

```
$ julia run.jl

Self-consistent iteration begins ...
update_psi = LOBPCG
mix_method = simple
Density mixing with betamix =    0.20000

-------------------------------------------------------------
       iter            E            ΔE           Δρ
-------------------------------------------------------------
SCF:     1      -0.9088890376  9.08889e-01  1.36287e-04
SCF:     2      -0.9197780666  1.08890e-02  1.17877e-04
SCF:     3      -0.9589404606  3.91624e-02  9.53668e-05
SCF:     4      -0.9975511159  3.86107e-02  7.60953e-05
.... # snipped
```

Converged Kohn-Sham energy components

PWDFT.jl's result:

```
-------------------------
Final Kohn-Sham energies:
-------------------------

Kinetic    energy:       1.0100082069
Ps_loc     energy:      -2.7127851088
Ps_nloc    energy:       0.0000000000
Hartree    energy:       0.9015229089
XC         energy:      -0.6314259148
PspCore    energy:      -0.0000012675
------------------------------------
Electronic energy:      -1.4326811753
NN         energy:       0.3131700043
------------------------------------
Total      energy:      -1.1195111709
```

ABINIT's result:

```
 Components of total free energy (in Hartree) :

    Kinetic energy  =  1.01004059294567E+00
    Hartree energy  =  9.01545039301481E-01
    XC energy       = -6.31436384237843E-01
    Ewald energy    =  3.13170052325859E-01
    PspCore energy  = -1.26742500464741E-06
    Loc. psp. energy= -2.71283243086241E+00
    NL   psp  energy=  0.00000000000000E+00
    >>>>>>>>> Etotal= -1.11951439795224E+00
```

SCF solvers

Kohn-Sham problem is solved using self-consistent field (SCF) iterations. This is the most popular method.

In PWDFT.jl we can set various options to SCF algorithm:

- `betamix`: linear mixing parameters (between 0 and 1)
- `mix_method`: linear, adaptive linear, Anderson, Pulay, restarted Pulay, periodic Pulay, and Broyden.
- `update_psi`: how to update the wave functions (iterative diagonalization or Chebyshev subspace filtering).

Direct energy minimization

For systems with band gaps:

Conjugate gradient

Direct minimization