PWDFT.jl: Density Functional Theory Calculations with Julia

Introduction and Current Status

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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

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.

Introducing PWDFT.jl

- A package (more or less like a library, no executable) for electronic structure calculations based on DFT.
- Available at `https://github.com/f-fathurrahman/PWDFT.jl`
- Using plane wave basis functions.
- Implemented using Julia programming language.
- My latest attempt to implement DFT softwares, previous attempts:
  - `ffr-LFDFT`: `https://github.com/f-fathurrahman/ffr-LFDFT`, using Lagrange basis functions, implemented in Fortran.
  - `ffr-PWDFT`: `https://github.com/f-fathurrahman/ffr-PWDFT` also using plane wave basis functions, implemented in Fortran.
- Starting point is my Julia implementation of the code by Prof. Tomas Arias described in his Practical DFT course. I extended the code to handle nonlocal pseudopotentials and multiple k-points.
- Taking many ideas from Quantum ESPRESSO, KSSOLV, ELK, etc.
- No logo yet.

Why I write another DFT package?

Writing a DFT package from scratch is not the solution for all problems.

[Rant mode ON]

Several questions appeared during my early days with DFT:

- Why my calculations are slow? What makes my calculations slow?
- Is this slowness justified? How can I make it faster?
- What are actually calculated by the DFT packages?

Learn by doing: how DFT or Kohn-Sham equations are solved (beyond described in textbooks or research papers)

Frustation when trying to extend functionalities of available packages.

Educational purpose: the secret art of writing a DFT code is not yet documented extensively in a book.

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!

Aims of PWDFT.jl

- 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.

Julia installation

I am assuming familiarity with command line.

Download Julia the current stable of Julia at `https://julialang.org/downloads` for your operating system.

Unpack the tarball. Usually after unpacking the tarball you should see a new directory created: `julia-1.x.x`, where `1.x.x` is the version of Julia.

```
julia-1.x.x/
├── bin
├── etc
├── include
├── lib
├── libexec
├── LICENSE.md
└── share
```

The Julia binary resides within the `bin` directory. You can launch Julia interpreter by executing the `bin/julia` executable. After executing the binary you can see the the following output:

```
               _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.3.1 (2019-12-30)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

julia>
```

Title

Examples

Typical steps

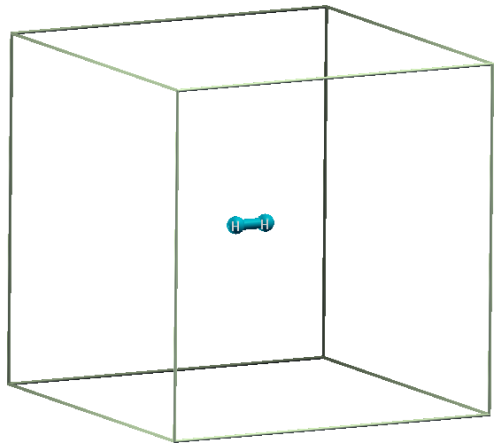
Write Julia code not an input file.

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