ffr_LFDFT in a nutshell

- a poor man's program to do electronic structure calculation based on **density functional theory** (DFT)
- basis set: **Lagrange functions** (LF)
- ffr: my initials (to distinguish between several LFDFT's)

What can I do with `ffr_LFDFT`?

Not much currently:

- total energy calculations
- electronic density and orbitals

Getting started

- Clone the repository:

```
git clone https://github.com/f-fathurrahman/ffr-LFDFT f
```

- Build

```
cd ffr-LFDFT
cd src
cp ../make.inc.gfortran make.inc
make main
make postproc
```

How to use it

It uses very similar input file with `PWSCF` from Quantum Espresso package.
Currently, only HGH pseudopotentials are supported.

Why wrote another package DFT code?

Several reasons not to do it:

- time-consuming
- need devotion

Several reasons to do it:

- to learn the "technology", knowing the nitty-gritty

My personal motivation

- To develop a code to solve Kohn-Sham equation with fast convergence with respect to number of basis set. The convergence should be easy to control, with only few adjustable parameters.
- Education