User Guide for `ffr-ElectronicStructure.jl`

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Contents

1 Introduction

`ffr-ElectronicStructure.jl` is a collection of programs[1] for learning electronic structure calculations.
Design of the package
Introduction to electronic structure calculation based on DFT

2 Why using Julia?

I consider it to be close to Fortran, my favorite programming language.
The code is easier to translate to Fortran.
Why not Fortran ?
Why not MATLAB, Octave or Scilab ?
Why not Python ?
Why not C ?
Why not C++ ?

3 Short introduction to Julia programming languange

Common program structure that is employed in `ffr-ElectronicStructure.jl`.
I tried to make it simple to follow, although the design is clearly not considered good practice in software engineering.
Tried to make it modular, but no serious attempts to make the generic code this result in a lot of code repetition
Using include, instead of module

```julia
# file main.jl

include(”func1.jl”)
include(”func2.jl”)

function main()
  # do something here
end
```

[1] or scripts

```
# call main function
main()
```

4 Background

My background:

My first introduction to ab initio methods.

Gaussian03,

ABINIT

QuantumEspresso