User Guide for `ffr-PWDFT`

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1 Introduction

Welcome to `ffr-PWDFT` documentation.
`ffr-PWDFT` is a poor man's program (or collection of subroutines, as of now) to carry out electronic structure calculations based on density functional theory and plane wave basis set.

2 Theory

Kohn-Sham equations
Plane wave basis set
Pseudopotential

3 Implementation

Description of unit cell and atomic structures
Description of plane wave basis set: G-vectors and real space basis set

```
PROGRAM testprog
  IMPLICIT NONE
END PROGRAM
```