

# Implementation Notes of `ffr`-LFDFT

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# Chapter 1

## Lagrange functions in one dimension

### 1.1 Introduction

There are various ways to derive what will be referred to as Lagrange basis functions (LBFs) or Lagrange functions (LFs) below. In some references, they are also referred to as discrete variable representation (DVR) basis functions, especially in papers by Tuckerman's research group [references needed].

In summary, this is the parameters that are needed to specify a specific LBFs:

- For periodic and cluster/box LBFs we need to specify:
  - number of basis functions  $N$
  - two end points  $a$  and  $b$
- For sinc LBFs, we need to specify:
  - number of basis functions  $N$
  - grid spacing  $h$

### 1.2 Implementation

Currently, there is only special module to handle global variables related to 1D LFs. However, there is a special module to handle 3D LFs, namely the module `m_LF3d` defined in file `m_LF3d.f90`. The relevant global variables for our current discussion are the following.

```
INTEGER :: LF3d_NN(3)
REAL(8) :: LF3d_LL(3)
REAL(8) :: LF3d_AA(3), LF3d_BB(3)
REAL(8) :: LF3d_hh(3)
```

Note that, these arrays are of size 3, for each  $x$ ,  $y$ , and  $z$  component. We will restrict ourself to 1D, and will take only the first element, i.e. the  $x$  direction. The grid points are stored in array:

```
REAL(8), ALLOCATABLE :: LF3d_grid_x(:)
```

In the actual code, if there is no name-clash (i.e. no two or more variables with the same name), we usually use the aliases for these global variables, e.g.:

```
USE m_LF3d, ONLY : NN => LF3d_NN, hh => LF3d_hh
```

### 1.3 Example: initializing LFs

Example code can be found in directory: `tests/init/ex_init.f90`.

### 1.4 Example: plotting the basis functions

Code to

Python

### 1.5 Example: basis function expansion

### 1.6 Example: integrals