A FORTRAN 90 numerical library

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Generalities

This is the documentation of a total of fourteen `FORTRAN 2003` modules with different utilities. This code is well documented, and can be useful for several people, although the idea is *not* to produce fast, high performance code, but to have nice data structures and `INTERFACE` definitions so that complex problems can be solved fast, writing only a couple of lines of code.

The code of all these modules is *free software*, this means that you can redistribute and/or modify all the code under the terms of the GNU General Public License[1] as published by the Free Software Foundation; either version 2 of the License, or (at your option) any later version. Note that the code is distributed in the hope that it will be useful, but **without any warranty; without even the implied warranty of merchantability or fitness for a particular purpose**. See the GNU General Public License for more details.

The code has been written using standard `FORTRAN 2003`, this means that it should run on any machine and with any compiler that conforms the standard. In particular the code of all these modules has been compiled using `GNU gfortran`, `INTEL ifort`.

Traditionally the source of the code hass been hosted in `http://www.sourceforge.net`. Due to the access blocking of some countries the code has been moved to `http://github.com`.

To obtain a copy of the source code and documentation, follow one of the following two options

- If you have `git` installed in your system, simply type

```
user@pc  $ git clone git://github.com/ramos/afnl.git
```

- In any other case, go to `http://github.com/ramos/afnl/downloads` and get the latest version of the library.

Minuit minimisation routines

The library includes an API to minuit minimisation routines. If you want to use this routines, you should have the fortran version of minuit available in your system. There is the option of building the `afnl` library without minuit support (see next section).

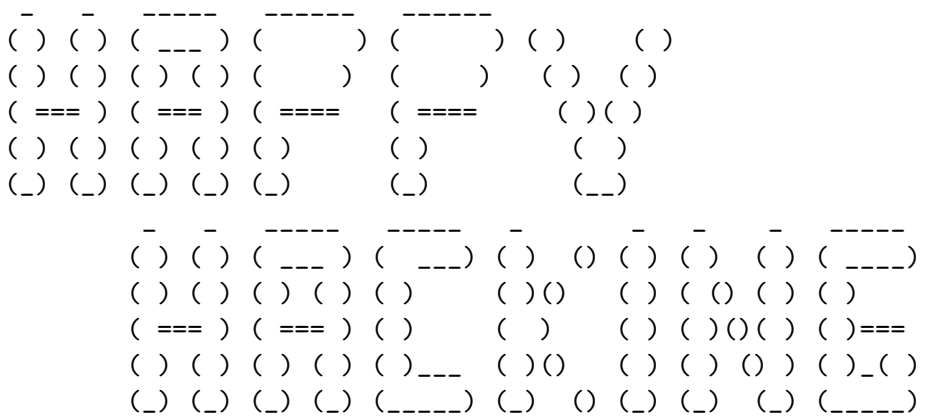
[1] `http://www.gnu.org/copyleft/gpl.html`

Installation

To install this library in a Unix/Linux environment, simply edit the `Makefile` file, and set the `F90` and `F90OPT` variables to whatever your compiler and your favourite optimisation flags are. After running `make` you should obtain a file called `libafnl.a`, and probably (that depends on the particular compiler) some `.mod` files. Copy the `libafnl.a` library and the `.mod` files to any place you like, and compile and link your program to that files. With `GNU gfortran` this is done using the flags `-I<path> -L<path> -lf90`, where `<path>` has to be substituted by the path you have chosen.

In case that you do not have a version of the fortran minuit library in your system, use `make lib-no-minuit` to build a version of `afnl` without the minuit API.

In other environments, you should ask the local guru/administrator about how to generate a library. In particular in a Windows environment the best option is to repartition you hard drive, eliminate Windows and install any Unix like free operating system, like Linux or FreeBSD.



One

MODULE NumTypes

This is the documentation of the `MODULE NumTypes`, that contaions the definition of Single Precision, and Double Precision data. All the other numerical modules uses this data type definitions.

1.1 Description

The `MODULE NumTypes` provides the definition of the Single Precision and Double Precision real and complex data in a potable way. When we want to define a single precision real we *will* do it with a statement like `Real (kind=DP)`, instead of `Real (kind=4)`. What we mean with `DP` is defined in this module. The different data types are:

SP: Single precision real.

DP: Double precision real.

SPC: Single precision complex.

DPC: Double precision complex.

To make all the code as portable as possible, all the data definitions should make use of this module.

1.2 Examples

Here we will define `A` as a single precision real, `D` as a double precision real, `Ac` as a single precision complex, and `Dc` as a double precision complex.

Listing 1.1: Definition of data types.

```
1  Program Types_of_Data
   USE NumTypes
3


5  Real (kind=SP) :: A
   Real (kind=DP) :: D
```

```
7     Complex (kind=SPC) :: Ac
      Complex (kind=DPC) :: Dc
9
      Write(*,*)Kind(A), Kind(Aa)
11
13    End Program Types_of_Data
```

Two

MODULE Constants

This is the documentation of the MODULE Constants, that contains the definition of the most used mathematical constants. This module uses numerical types defined in the MODULE NumTypes.

2.1 Name conventions

All the real simple precision constants ends with _SP, the real double precision constants with _DP, the complex simple precision with _SPC and the complex double precision with _DPC.

If a there exist a real or complex constant of simple precison defined, then it exist other with the same name (except for the sufix) of double precision and viceversa.

2.2 π-related constants

2.2.1 Real

The complex π-related defined in this module and its values can be seen in the table (2.1)

SP Name	DP Name	Value
PI_SP	PI_DP	π
TWOPI_SP	TWOPI_DP	2π
HALFPI_SP	HALFPI_DP	$\frac{\pi}{2}$

Table 2.1: π-related real constants defined in the MODULE constants.

2.2.2 Complex

The complex π-related defined in this module and its values can be seen in the table (2.2)

2.3 Square roots and log related constants

We have only real constants defined here. We can see a list of names-vlues in the table (2.3)

SPC Name	DPC Name	Value
UNITIMAG_SPC	UNITIMAG_DPC	ι
PI_IMAG_SPC	PI_IMAG_DPC	$\pi\iota$
TWOPI_IMAG_SPC	TWOPI_IMAG_DPC	$2\pi\iota$
HALFPI_IMAG_SPC	HALFPI_IMAG_SDC	$\frac{\pi}{2}\iota$

Table 2.2: π-related complex constants defined in the MODULE constants.

SP Name	DP Name	Value
SR2_SP	SR2_DP	$\sqrt{2}$
SR3_SP	SR3_DP	$\sqrt{3}$
SRe_SP	SRe_DP	$\sqrt{e}$
SRpi_SP	SRpi_DP	$\sqrt{\pi}$
LG102_SP	LG102_DP	$\log_{10} 2$
LG103_SP	LG103_DP	$\log_{10} 3$
LG10e_SP	LG10e_DP	$\log_{10} e$
LG10pi_SP	LG10pi_DP	$\log_{10} \pi$
LGe2_SP	LGe2_DP	$\log_e 2$
LGe3_SP	LGe3_DP	$\log_e 3$
LGe10_SP	LGe10_DP	$\log_e 10$

Table 2.3: Square roots and log related constants defined in the MODULE constants.

2.4 Other mathematical constants

In this section we have only the Euler γ constant. We can see the name-value pair in the table (2.4)

SP Name	DP Name	Value
GEULER_SP	GEULER_DP	$\gamma(= 0.5772\ldots)$

Table 2.4: Other mathematical constants defined in the MODULE constants.

Three

MODULE Error

This is the documentation of the MODULE Error, a set of FORTRAN 90 routines that allow to write errors.

3.1 Defined variables

3.1.1 stderr

Description

This variable has the unit number of standard error.

Examples

Listing 3.1: Standard error unit.

```
1 Program Test
    USE Error
3
    Write(stderr,*)''This is printed in standard error.''
5
    Stop
7 End Program Test
```

3.2 Subroutine perror([routine], msg)

3.2.1 Description

Prints the error message msg in standard error. If the optional argument routine is given, it is used as the routine where the program has crashed.

3.2.2 Arguments

routine: Character string with arbitrary length. It should be the routine or program name where the error has ocurred. It is an optional argument.

msg: Character string with arbitrary length. It should be the message that you want to print.

3.2.3 Examples

Listing 3.2: Print error message.

```
1  Program Test
     USE Error
3
     Integer :: N1, N2
5
     Write(*,*) 'Two integer numbers:'
7    Read(*,*)N1,N2

9    If (N2 == 0) Then
       CALL Perror('Test', 'Division by cero. See the product: ')
11     Write(*,*)N1*N2
     Else
13     Write(*,*)N1/N2
     End If
15
     Stop
17 End Program Test
```

3.3 Subroutine `abort([routine], msg)`

3.3.1 Description

Prints the error message `msg` in standard error, and stops the program. If the optional argument `routine` is given, it is used as the routine where the program has crashed.

3.3.2 Arguments

routine: Character string with arbitrary length. It should be the routine or program name where the error has ocurred. It is an optional argument.

msg: Character string with arbitrary length. It should be the message that you want to print.

3.3.3 Examples

Listing 3.3: Print error message and stop a program.

```
1  Program Test
     USE Error
3
     Integer :: N1, N2
5
     Write(*,*) 'Two integer numbers:'
7    Read(*,*)N1,N2

9    If (N2 == 0) Then
```

```
    CALL abort('Test', 'Division by cero')
  Else
    Write(*,*)N1/N2
  End If

  Stop
End Program Test
```

Four

MODULE Integration

This is the documentation of the `MODULE Integration`, a set of `FORTRAN 90` routines that performs numerical integration and solves the initial value problem for a specified system of first-order ordinary differential equations. This module make use of the `MODULE NumTypes`, so please read the documentation of this module *before* reading this.

4.1 Function `Trapecio(a, b, Func, [Tol])`

4.1.1 Description

Calculates the integral of the function `Func` between `a` and `b` with precision `Tol` (optional) using the trapezoid rule.

4.1.2 Arguments

`a, b`: Real single or double precision. The limits of the integral.

`Func`: The function to be integrated. It must be a function of only one argument of the same type as the function itself. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Fint(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X
     Real (kind=DP) :: Fint
   End Function Fint
End Interface
```

`Tol`: Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter, and the default is `Tol` = 0.01.

4.1.3 Output

If the arguments are real of single (double) precision, the result will also be a real of single (double) precision. The value of the integral.

4.1.4 Examples

Listing 4.1: Example of integration of a function using `Trpecio`.

```
Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol

  Interface
     Function Fint(X)
       USE NumTypes

       Real (kind=DP), Intent (in) :: X
       Real (kind=DP) :: Fint
     End Function Fint
  End Interface

  Tol = 1.0E-6_DP
  Write(*,*) 'Integral of x**2 between 0 and 1:'
  Write(*,*) Trapecio(0.0_DP, 1.0_DP, Fint, Tol)

  Stop
End Program Test

! ********************************************
! *
Function Fint(X)
! *
! ********************************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: X
  Real (kind=DP) :: Fint

  Fint = X**2

  Return
End Function Fint
```

4.2 Function Simpson(a, b, Func, [Tol])

4.2.1 Description

Calculates the integral of the function `Func` between `a` and `b` with precision `Tol` (optional) using the Simpson's rule.

In general this routine is better than `Trapecio`.

4.2.2 Arguments

`a, b`: Real single or double precision. The limits of the integral.

`Func`: The function to be integrated. It must be a function of only one argument of the same type as the function itself. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Fint(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X
     Real (kind=DP) :: Fint
   End Function Fint
End Interface
```

`Tol`: Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter, and the default is `Tol` = 0.01.

4.2.3 Output

If the arguments are reals of single (double) precision, the result will also be a real of single (double) precision. The value of the integral.

4.2.4 Examples

Listing 4.2: Exmaple of integration of a function using `Simpson`.

```
1  Program Test
     USE NumTypes
3    USE Integration

5    Real (kind=DP) :: Tol

7    Interface
       Function Fint(X)
9        USE NumTypes

11       Real (kind=DP), Intent (in) :: X
         Real (kind=DP) :: Fint
13     End Function Fint
```

```
  End Interface

  Tol = 1.0E-6_DP
  Write(*,*) 'Integral of x**2 between 0 and 1:'
  Write(*,*) Simpson(0.0_DP, 1.0_DP, Fint, Tol)

  Stop
End Program Test

! ***********************************************
! *
Function Fint(X)
! *
! ***********************************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: X
  Real (kind=DP) :: Fint

  Fint = X**2

  Return
End Function Fint
```

4.3 Function `TrapecioAb(a, b, Func, [Tol])`

4.3.1 Description

Calculates the integral of the function `Func` between `a` and `b` with precision `Tol` (optional) using the open trapezoid rule.

4.3.2 Arguments

`a, b`: Single (SP) or double (DP) precision. They are the limits of the integral.

`Func`: The function to be integrated. It must be a function of only one argument of the same type as the function itself. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Fint(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X
     Real (kind=DP) :: Fint
   End Function Fint
End Interface
```

`Tol`: Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter, and the default is `Tol` = 0.01.

4.3.3 Output

If the arguments are single (double) precision, the result will also be of single (double) precision. The value of the integral.

4.3.4 Examples

Listing 4.3: Integrating a function using the open trapezoid rule.

```
Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol

  Interface
     Function Fint(X)
       USE NumTypes

       Real (kind=DP), Intent (in) :: X
       Real (kind=DP) :: Fint
     End Function Fint
  End Interface

  Tol = 1.0E-6_DP
  Write(*,*)'Integral of x**2 between 0 and 1:'
  Write(*,*)TrapecioAb(0.0_DP, 1.0_DP, Fint, Tol)

  Stop
End Program Test

! ********************************************
! *
Function Fint(X)
! *
! ********************************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: X
  Real (kind=DP) :: Fint

  Fint = X**2

  Return
End Function Fint
```

4.4 Function SimpsonAb(a, b, Func, [Tol])

4.4.1 Description

Calculates the integral of the function `Func` between `a` and `b` with precision `Tol` (optional) using the open Simpson's rule.

In general better than `TrapecioAb`

4.4.2 Arguments

`a, b:` Single (SP) or double (DP) precision. They are the limits of the integral.

`Func:` The function to be integrated. It must be a function of only one argument of the same type as the function itself. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Fint(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X
     Real (kind=DP) :: Fint
   End Function Fint
End Interface
```

`Tol:` Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter, and the default is `Tol` = 0.01.

4.4.3 Output

If the arguments are single (double) precision, the result will also be of single (double) precision. The value of the integral.

4.4.4 Examples

Listing 4.4: Exmaple of integration using the open Simpson rule.

```
1  Program Test
     USE NumTypes
3    USE Integration

5    Real (kind=DP) :: Tol

7    Interface
        Function Fint(X)
9         USE NumTypes

11        Real (kind=DP), Intent (in) :: X
          Real (kind=DP) :: Fint
13      End Function Fint
```

```
  End Interface

  Tol = 1.0E-6_DP
  Write(*,*) 'Integral of x**2 between 0 and 1:'
  Write(*,*) SimpsonAb(0.0_DP, 1.0_DP, Fint, Tol)

  Stop
End Program Test

! ***********************************************
! *
Function Fint(X)
! *
! ***********************************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: X
  Real (kind=DP) :: Fint

  Fint = X**2

  Return
End Function Fint
```

4.5 Function SimpsonInfUp(a, Func, [Tol])

4.5.1 Description

Calculates the integral of the function `Func` between `a` and ∞ with precision `Tol` (optional) using the Simpson rule and a change of variables.

4.5.2 Arguments

a: Single (SP) or double (DP) precision. They are the limits of the integral.

Func: The function to be integrated. It must be a function of only one argument of the same type as the function itself. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Fint(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X
     Real (kind=DP) :: Fint
   End Function Fint
End Interface
```

This routine does not check if the integral exist, so the function must obviously decay fast for large x to obtain a finite value.

`Tol`: Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter, and the default is `Tol` = 0.01.

4.5.3 Output

If the arguments are single (double) precision, the result will also be of single (double) precision. The value of the integral.

4.5.4 examples

Listing 4.5: Integration of a function between 0 and ∞.

```
Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol

  Interface
     Function Fint(X)
       USE NumTypes

       Real (kind=DP), Intent (in) :: X
       Real (kind=DP) :: Fint
     End Function Fint
  End Interface

  Tol = 1.0E-6_DP
  Write(*,*)'Integral of e**(-x**2) between 0 and infinity:'
  Write(*,*)SimpsonInfUp(0.0_DP, Fint, Tol)

  Stop
End Program Test

! ********************************************
! *
Function Fint(X)
! *
! ********************************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: X
  Real (kind=DP) :: Fint

  Fint = exp(-X**2)

  Return
End Function Fint
```

4.6 Function SimpsonInfDw(a, Func, [Tol])

4.6.1 Description

Calculates the integral of the function `Func` between $-\infty$ and `a` with precision `Tol` (optional) using the Simpson rule and a change of variables.

4.6.2 Arguments

a: Single (SP) or double (DP) precision. They are the limits of the integral.

Func: The function to be integrated. It must be a function of only one argument of the same type as the function itself. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Fint(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X
     Real (kind=DP) :: Fint
   End Function Fint
End Interface
```

This routine does not check if the integral exist, so the function must obviously decay fast for large $-x$ to obtain a finite value.

Tol: Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter, and the default is `Tol` = 0.01.

4.6.3 Output

If the arguments are single (double) precision, the result will also be of single (double) precision. The value of the integral.

4.6.4 examples

Listing 4.6: Integrating a function between $-\infty$ and 0.

```
1  Program Test
     USE NumTypes
3    USE Integration

5    Real (kind=DP) :: Tol

7    Interface
       Function Fint(X)
9        USE NumTypes

11       Real (kind=DP), Intent (in) :: X
```

```
      Real (kind=DP) :: Fint
    End Function Fint
  End Interface

  Tol = 1.0E-6_DP
  Write(*,*) 'Integral of e**(-x**2) between -infinity and 0:'
  Write(*,*) SimpsonInfDw(0.0_DP, Fint, Tol)

  Stop
End Program Test

! ********************************************
! *
Function Fint(X)
! *
! ********************************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: X
  Real (kind=DP) :: Fint

  Fint = exp(-X**2)

  Return
End Function Fint
```

4.7 Function `SimpsonSingUp(a, b, Func, [Tol], gamma)`

4.7.1 Description

Calculates the integral of the function `Func` between `a` and `b` with precision `Tol` (optional) using the Simpson's rule. The function may have an integrable singularity of the type:

$$f(x+b) \approx \frac{c}{(x-b)^{\gamma}} + \dots$$

with $0 < \gamma < 1$.

4.7.2 Arguments

`a, b`: Single (SP) or double (DP) precision. They are the limits of the integral.

`Func`: The function to be integrated. It must be a function of only one argument of the same type as the function itself. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Fint(X)
     USE NumTypes
```

```
        Real (kind=DP), Intent (in) :: X
        Real (kind=DP) :: Fint
      End Function Fint
    End Interface
```

`Tol`: Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter, and the default is `Tol` = 0.01.

`gamma`: The "degree of divergence" of the function in $x \approx b$.

4.7.3 Output

If the arguments are single (double) precision, the result will also be of single (double) precision. The value of the integral.

4.7.4 Examples

Listing 4.7: Integrating functions with singularities in the upper limit.

```
Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol

  Interface
     Function Fint(X)
       USE NumTypes

       Real (kind=DP), Intent (in) :: X
       Real (kind=DP) :: Fint
     End Function Fint
  End Interface

  Tol = 1.0E-6_DP
  Write(*,*)'Integral of 1/sqrt(-x) between -1 and 0:'
  Write(*,*)SimpsonSingUp(-1.0_DP, 0.0_DP, Fint, Tol, 0.5_DP)

  Stop
End Program Test

! ********************************************
! *
Function Fint(X)
! *
! ********************************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: X
  Real (kind=DP) :: Fint

```

```
    Fint = Sqrt(-X)
35
    Return
37  End Function Fint
```

4.8 Function SimpsonSingDw(a, b, Func, [Tol], gamma)

4.8.1 Description

Calculates the integral of the function `Func` between `a` and `b` with precision `Tol` (optional) using the Simpson's rule. The function may have an integrable singularity of the type:

$$f(x+a) \approx \frac{c}{(x-a)^{\gamma}} + \dots$$

with $0 < \gamma < 1$.

4.8.2 Arguments

`a, b`: Single (SP) or double (DP) precision. They are the limits of the integral.

`Func`: The function to be integrated. It must be a function of only one argument of the same type as the function itself. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Fint(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X
     Real (kind=DP) :: Fint
   End Function Fint
End Interface
```

`Tol`: Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter, and the default is `Tol` = 0.01.

`gamma`: The "degree of divergence" of the function in $x \approx a$.

4.8.3 Output

If the arguments are single (double) precision, the result will also be of single (double) precision. The value of the integral.

4.8.4 Examples

Listing 4.8: Integrating functions with singularities in the lower limit.

```
Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol

  Interface
     Function Fint(X)
       USE NumTypes

       Real (kind=DP), Intent (in) :: X
       Real (kind=DP) :: Fint
     End Function Fint
  End Interface

  Tol = 1.0E-6_DP
  Write(*,*)'Integral of 1/sqrt(x) between 0 and 1:'
  Write(*,*)SimpsonSingDw(0.0_DP, 1.0_DP, Fint, Tol, 0.5_DP)

  Stop
End Program Test

! ***********************************************
! *
Function Fint(X)
! *
! ***********************************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: X
  Real (kind=DP) :: Fint

  Fint = Sqrt(X)

  Return
End Function Fint
```

4.9 Function Euler(Init, Xo, Xfin, Feuler, [Tol])

4.9.1 Description

Integrate the first order set of ODE defined by the function `Feuler`, with initial conditions given by the vector `Init` in `Xo`, until `Xfin`, with a precision given by `Tol` (optional).

A set of first order ODE's is given by the first derivatives of the variables involved:

$$\frac{\mathrm{y}_i(x)}{\mathrm{x}} = f_i(y_j, x)$$

and the initial conditions:

$$y_i(x_0)$$

After the integration we get:

$$y_i(x_{\text{fin}})$$

So to define a set of first order ODE's we need the value of the derivative of the variable i in te point x (this is done by `Feuler`), a vector of initial conditions (`Init`) and the point where this initial conditions are defined (`Xo`), and finally the point where we want the solution (`Xfin`)

4.9.2 Arguments

`Init(:)`: Single (SP) or double (DP) precision vector of one dimension with the initial conditions.

`Xo`: Single (SP) or double (DP) precision. The point where the initial conditions are defined.

`Xfin`: Single (SP) or double (DP) precision. The point where we want the value of the functions.

`Feuler`: The function that defines the set of first order ODE's. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Feuler(X, Y) Result (Func)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X, Y(:)
     Real (kind=DP) :: Func(Size(Y))
   End Function Feuler
End Interface
```

The function must return a vector with the values of the first derivatives of the functions $y_i(x)$ in the point `X`.

`Tol`: Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter.

4.9.3 Output

Real single or double precision (same as input) one dimensional array. The array contains the values of the functions y_i in the point `Xfin`.

4.9.4 Examples

This example below will integrate the set of first order ODE's defined by the equations:

$$\frac{\dot{y}_1(x)}{\dot{x}} = y_2(x); \qquad \frac{\dot{y}_2(x)}{\dot{x}} = -y_1(x)$$

whose solution is:

$$y_1(x) = A\cos(x) + B\sin(x)$$

With the initial conditions $y_1(0) = 0; y_2(0) = 1$, the solution is:

$$y_1(x) = \sin(x); \qquad y_2(x) = \cos(x)$$

so if we plot $y_1(1)$ and $y_2(1)$ we will obtain the values $\sin(1)$ and $y_2(1)$. In the following example, we will compare the result of integrating the differential equations with the exact values.

Listing 4.9: Integrating differential equations with Euler.

```
Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol, In(2)

  Interface
    Function Feuler(X, Y) Result (Func)
      USE NumTypes

      Real (kind=DP), Intent (in) :: X, Y(:)
      Real (kind=DP) :: Func(Size(Y))
    End Function Feuler
  End Interface


  Tol = 1.0E-2_DP
  In(1) = 0.0_DP
  In(2) = 1.0_DP
  Write(*,*) 'Values of sin(1) and cos(1): '
  Write(*,*) Euler(In, 0.0_DP, 1.0_DP, Feuler, Tol)
  Write(*,*) Sin(1.0_DP), Cos(1.0_DP)

  Stop
End Program Test

! ******************************************
! *                                        *
  Function FEuler(X, Y) Result (Func)
! *                                        *
! ******************************************

    Real (kind=8), Intent (in) :: X, Y(:)
    Real (kind=8) :: Func(Size(Y))

    Func(1) = Y(2)
    Func(2) = -Y(1)

    Return
  End Function FEuler
```

4.10 Function Rgnkta(Init, Xo, Xfin, Feuler, [Tol])

4.10.1 Description

Integrate the first order set of ODE defined by the function `Feuler`, with initial conditions given by the vector `Init` in `Xo`, until `Xfin`, with a precision given by `Tol` (optional). This method uses a Runge-Kutta algorithm and is much more exact than the previous `Euler` function.

A set of first order ODE's is given by the first derivatives of the variables involved:

$$\frac{\dot{y}_i(x)}{\dot{x}} = f_i(y_j, x)$$

and the initial conditions:

$$y_i(x_0)$$

After the integration we get:

$$y_i(x_{\text{fin}})$$

So to define a set of first order ODE's we need the value of the derivative of the variable i in te point x (this is done by `Feuler`), a vector of initial conditions (`Init`) and the point where this initial conditions are defined (`Xo`), and finally the point where we want the solution (`Xfin`)

4.10.2 Arguments

`Init(:)`: Single (SP) or double (DP) precision vector of one dimension with the initial conditions.

`Xo`: Single (SP) or double (DP) precision. The point where the initial conditions are defined.

`Xfin`: Single (SP) or double (DP) precision. The point where we want the value of the functions.

`Feuler`: The function that defines the set of first order ODE's. If it is an external function an interface block like the following should be declared:

```
Interface
   Function Feuler(X, Y) Result (Func)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X, Y(:)
     Real (kind=DP) :: Func(Size(Y))
   End Function Feuler
End Interface
```

The function is the same as in the previos function.

`Tol`: Single (SP) or double (DP) precision. An estimation of the desired accuracy of the result. It is an optional parameter.

4.10.3 Output

Real single or double precision (same as input) one dimensional array. The array contains the values of the functions y_i in the point `Xfin`.

4.10.4 Examples

This example below will integrate the set of first order ODE's defined by the equations:

$$\frac{\dot{y}_1(x)}{\dot{x}} = y_2(x); \qquad \frac{\dot{y}_2(x)}{\dot{x}} = -y_1(x)$$

whose solution is:

$$y_1(x) = A\cos(x) + B\sin(x)$$

With the initial conditions $y_1(0) = 0; y_2(0) = 1$, we have:

$$y_1(x) = \sin(x); \qquad y_2(x) = \cos(x)$$

so if we plot $y_1(1)$ and $y_2(1)$ we will obtain the values $\sin(1)$ and $y_2(1)$. In the following example, we will compare the values obtained with `Euler`, with `Rgnkta` and the exact ones.

Listing 4.10: Integrating differential equations with the Runge-Kutta method

```
Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol, In(2)

  Interface
    Function Feuler(X, Y) Result (Func)
      USE NumTypes

      Real (kind=DP), Intent (in) :: X, Y(:)
      Real (kind=DP) :: Func(Size(Y))
    End Function Feuler
  End Interface


  Tol = 1.0E-3_DP
  In(1) = 0.0_DP
  In(2) = 1.0_DP
  Write(*,*) 'Values of sin(1) and cos(1): '
  Write(*,*) '  Euler: '
  Write(*,*) Euler(In, 0.0_DP, 1.0_DP, Feuler, Tol)
  Write(*,*) '  Runge-Kutta: '
  Write(*,*) Rgnkta(In, 0.0_DP, 1.0_DP, Feuler, Tol)
  Write(*,*) '  Exact: '
  Write(*,*) Sin(1.0_DP), Cos(1.0_DP)

  Stop
End Program Test

```

```
! ********************************************
! *                                          *
  Function FEuler(X, Y) Result (Func)
! *                                          *
! ********************************************

    Real (kind=8), Intent (in) :: X, Y(:)
    Real (kind=8) :: Func(Size(Y))

    Func(1) = Y(2)
    Func(2) = -Y(1)

    Return
  End Function FEuler
```

4.11 Function `IntQuadrilateral(P1,P2,P3,P4,Fval)`

4.11.1 Description

Given four 2D points (`P1(2), P2(2), P3(2), P4(2)`), and the values of a function in this points, this routine computes the bilineal interpolation polynomial, and returns the value of this polynomial in the quadrilateral.

4.11.2 Arguments

`P1(:), P2(:), P3(:), P4(:):` Real single or double precision two component vectors. Four points that delimitate a quadrilateral. The corners of the quadrilateral must be given in (counter-)clock wise order.

`Fval:` Real singler or double precision one dimensional array of four elements. The value of a functio in the four corners of the quadrilateral.

4.11.3 Output

Real single or double precision (same as input). An aproximation of the value of the integral of the function over the quadrilateral.

4.11.4 Examples

Listing 4.11: Computing the area of a quadrilateral.

```
Program TQ

  USE NumTypes
  USE Integration
  USE SpaceGeometry

  Real (kind=DP) :: P1(3), P2(3), P3(3), P4(3), F(4), Tp(3)

  P1(:) = (/-2.0_DP, -1.4.0_DP, 0.0_DP/)
```

```
10    P2(:) = (/1.2_DP, 0.0_DP, 0.0_DP/)
      P3(:) = (/2.0_DP, 3.0_DP, 0.0_DP/)
12    P4(:) = (/0.0_DP, 2.5_DP, 0.0_DP/)

14    F(:)  = (/1.0_DP, 1.0_DP, 1.0_DP, 1.0_DP/)


16
      Write(*,*) IntQuadrilateral(P1(1:2),P2(1:2),P3(1:2),P4(1:2),F)
18    Tp(:) = Cross_Product(P1,P2)
      Tp(:) = Tp + Cross_Product(P2,P3)
20    Tp(:) = Tp + Cross_Product(P3,P4)
      Tp(:) = Tp + Cross_Product(P4,P1)
22    Write(*,*) Dot_Product((/0.0_DP,0.0_DP,0.5_DP/),Tp)


24
      Stop
26  End Program TQ
```

Five

MODULE Optimization

This is the documentation of the MODULE `Optimization`, a set of routines to Optimise (maximise or minimise) functions of one or several variables. Lot of work is needed to improve this module (simplex, quasi-Newton methods, etc...).

5.1 Subroutine `Bracket(X1, X2, X3, Func)`

5.1.1 Description

The routine `Bracket(X1, X2, X3, FStep)` "brackets" a minimum of the function `Func`. That is to say, after calling, '`X1, X2` and `X3` obey

$$\texttt{X1} < \texttt{X2} < \texttt{X3} \tag{5.1}$$

and

$$\texttt{Func}(\texttt{X1}) > \texttt{Func}(\texttt{X2}) \quad \text{and} \quad \texttt{Func}(\texttt{X3}) > \texttt{Func}(\texttt{X2}) \tag{5.2}$$

This assures that `Func` has a minimum in the interval $(\texttt{X1}, \texttt{X3})$. The bracketing of the minimum obey the golden rule, that is to say

$$(\texttt{X2} - \texttt{X1}) = \Phi(\texttt{X3} - \texttt{X2}) \tag{5.3}$$

where Φ is the golden number

$$\Phi = \frac{1+\sqrt{5}}{2} \tag{5.4}$$

5.1.2 Arguments

`X1,X2,X3:` Real single or double precision. At output, they bracket a minimum of `Func`. If you have a guess of the minimum of `Func`, introduce it in `X2`. of the minimum.

`Func:` The function whose minimum we want to bracket. An interface like the following should be declared

```
Interface
   Function Func(Xo)
```

```
      USE NumTypes

      Real (kind=DP), Intent (in) :: Xo
      Real (kind=DP) :: Func
    End Function Func
  End Interface
```

5.1.3 Example

Listing 5.1: Bracketing a minimum.

```
Program TestMin

  USE NumTypes
  USE Optimization

  Real (kind=DP) :: X1, X2, X3

  Interface
     Function FstepM(Xo)
       USE NumTypes

       Real (kind=DP), Intent (in) :: Xo
       Real (kind=DP) :: FstepM
     End Function FstepM
  End Interface


  ! Initial guess of the position of the minimum
  X2 = 2.0_DP

  CALL Bracket(X1,X2,X3, FstepM)
  Write(*,*)
  Write(*,*) 'Minimum bracketed: '

  Write(*,'(1A,1ES33.25)') 'X1: ', X1
  Write(*,'(1A,1ES33.25)') 'X2: ', X2
  Write(*,'(1A,1ES33.25)') 'X3: ', X3

  Stop
End Program TestMin

! ******************************
! *
Function FstepM(Xo)
! *
! ******************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: Xo
  Real (kind=DP) :: FstepM
```

```
42
44    FstepM = Sin(Xo)
46
    Return
48  End Function FstepM
```

5.2 Subroutine LineSrch(X, Func[, Tol])

5.2.1 Description

The function `LineSrch(X, FStep, Tol)` returns the position of the minimum of the Function `Fstep` with an optional precision `Tol`. This routine does not need the values of the derivative(s) of the function to work.

5.2.2 Arguments

`X[(:)]`: Real single or double precision. An initial guess of the position of the minimum when input. At output, the position of the minimum.

`Func`: The function that we want to minimise. It can be a function of one or several variables. In the case of one variable functions an interface like the following should be declared

```
Interface
   Function Func(Xo)
     USE NumTypes

     Real (kind=DP), Intent (in) :: Xo
     Real (kind=DP) :: Func
   End Function Func
End Interface
```

In the case of a function of several variables, the interface block should be like the following

```
Interface
   Function Func(Xo)
     USE NumTypes

     Real (kind=DP), Intent (in) :: Xo(:)
     Real (kind=DP) :: Func
   End Function Func
End Interface
```

`Tol`: Real single or double precision. As estimation of the precision of the result. The dafult value is 10^{-3}.

5.2.3 Example

Listing 5.2: Minimising a function.

```
Program TestMin

  USE NumTypes
  USE Optimization

  Integer, Parameter :: Ndim = 4
  Real (kind=DP) :: XoM(Ndim)

  Interface
     Function FstepM(Xo)
       USE NumTypes

       Real (kind=DP), Intent (in) :: Xo(:)
       Real (kind=DP) :: FstepM
     End Function FstepM
  End Interface


  ! Initial guess of the position of the minimum
  XoM(1) = 1.373_DP
  XoM(2) = 1.373_DP
  XoM(3) = 1.373_DP
  XoM(4) = 1.373_DP


  Write(*,*) 'Initial Position: '
  Do I = 1, Ndim
     Write(*,'(1A,1I4,1A,1ES33.25)') 'Variable ', I, " : ", XoM(I)
  End Do

  CALL LineSrch(XoM, FstepM, 1.0E-7_DP)
  Write(*,*)
  Write(*,*) 'Position of the minimum: '
  Do I = 1, Ndim
     Write(*,'(1A,1I4,1A,1ES33.25)') 'Variable ', I, " : ", XoM(I)
  End Do

  Stop
End Program TestMin

! ******************************
! *
Function FstepM(Xo)
! *
! ******************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: Xo(:)
```

```
50   Real (kind=DP) :: FstepM

52

   FstepM = (Xo(1)-1.0_DP)**2 + &
54        & (Xo(2)-2.0_DP)**2 + &
          & (Xo(3)+3.0_DP)**4 + &
56        & (Xo(4)-4.0_DP)**8

58

   Return
60 End Function FstepM
```

5.3 Subroutine ConjGrad(X, F, Fd[, Tol])

5.3.1 Description

The function ConjGrad(X, F, Fd[, Tol]) returns the position of the minimum of the Function F with an optional precision Tol. This routine uses the conjugate gradient method, and should be much faster that LineSrch, but you must be able to compute the derivatives of F

5.3.2 Arguments

X(:): Real single or double precision. An initial guess of the position of the minimum when input. At output, the position of the minimum.

F: The function that we want to minimise. An interface block like the following should be defined.

```
Interface
   Function F(Xo)
     USE NumTypes

     Real (kind=DP), Intent (in) :: Xo(:)
     Real (kind=DP) :: F
   End Function F
End Interface
```

Fd: The gradient of the function that we want to minimise. An interface block like the following should be defined.

```
Interface
   Subroutine Fd(X, D)
     USE NumTypes
     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP), Intent (out) :: D(Size(X))
   End Subroutine Fd
End Interface
```

where the vector D returns the value of the derivatives.

`Tol`: Real single or double precision. As estimation of the precision of the result. The dafult value is 10^{-3}.

5.3.3 Example

Listing 5.3: Minimising a function.

```
Program TestMin

Program OOOO

  USE NumTypes
  USE Optimization

  Real (kind=DP) Xx(2)

  Interface
     Function F(X)
       USE NumTypes
       Real (kind=DP), Intent (in) :: X(:)
       Real (kind=DP) :: F
     End Function F
  End Interface

  Interface
     Subroutine Fd(X, D)
       USE NumTypes
       Real (kind=DP), Intent (in) :: X(:)
       Real (kind=DP), Intent (out) :: D(Size(X))
     End Subroutine Fd
  End Interface


  Xx = 112.0_DP

  CALL ConjGrad(Xx, F, Fd, 1.E-10_DP)
  Write(*,*) 'Minimo: ', Xx

  Stop
End Program Test


Function F(X)

  USE NumTypes

  Real (kind=DP), Intent (in) :: X(:)
  Real (kind=DP) :: F


  F = (X(1)-2.23_DP)**2 + (X(2)+1.23_DP)**2 + X(1)*X(2) + Sin(X(1)*X(2))
```

```
46
  Return
48 End Function F

50
Subroutine Fd(X, D)
52   USE NumTypes

54   Real (kind=DP), Intent (in) :: X(:)
   Real (kind=DP), Intent (out) :: D(Size(X))
56
   D(1) = (X(1)-2.23_DP)*2 + X(2) + Cos(X(1)*X(2))*X(2)
58   D(2) = (X(2)+1.23_DP)*2 + X(1) + Cos(X(1)*X(2))*X(1)

60   Return
End Subroutine Fd
```

5.4 Function Step(X, FStep[, Tol])

5.4.1 Description

The function Step(X, FStep, Tol) returns the position of the minimum of the Function Fstep with an optional precision Tol. Unless you know very well what you are doing, you should use LineSrch or ConjGrad to minimize functions.

5.4.2 Arguments

X: Real single or double precision. An initial guess of the position of the minimum.

Fstep: The function that we want to minimise. It can be a function of one or several variables. In the case of one variable functions an interface like the following should be declared

```
Interface
   Function Fstep(Xo)
     USE NumTypes

     Real (kind=DP), Intent (in) :: Xo
     Real (kind=DP) :: Fstep
   End Function Fstep
End Interface
```

In the case of a function of several variables, the interface block should be like the following

```
Interface
   Function Fstep(Xo)
     USE NumTypes
```

```
        Real (kind=DP), Intent (in) :: Xo(:)
        Real (kind=DP) :: Fstep
      End Function Fstep
    End Interface
```

Tol: Real single or double precision. As estimation of the precision of the result. The dault value is 10^{-3}.

5.4.3 Output

Real Single or double precision (same as the output). The position of a minimum of **Fstep**.

5.4.4 Example

Listing 5.4: Minimising a function.

```
Program TestMin

  USE NumTypes
  USE Optimization

  Integer, Parameter :: Ndim = 4
  Real (kind=DP) :: XoM(Ndim), Xmin(Ndim)

  Interface
     Function FstepM(Xo)
       USE NumTypes

       Real (kind=DP), Intent (in) :: Xo(:)
       Real (kind=DP) :: FstepM
     End Function FstepM
  End Interface


  ! Initial guess of the position of the minimum
  XoM(1) = 1.373_DP
  XoM(2) = 1.373_DP
  XoM(3) = 1.373_DP
  XoM(4) = 1.373_DP


  Write(*,*) 'Initial Position: '
  Do I = 1, Ndim
     Write(*,'(1A,1I4,1A,1ES33.25)') 'Variable ', I, " : ", XoM(I)
  End Do

  Xmin = Step(XoM, FstepM, 1.0E-7_DP)
  Write(*,*)
  Write(*,*) 'Position of the minimum: '
  Do I = 1, Ndim
     Write(*,'(1A,1I4,1A,1ES33.25)') 'Variable ', I, " : ", Xmin(I)
  End Do
```

```
37
  Stop
39 End Program TestMin

41 ! ******************************
   ! *
43 Function FstepM(Xo)
   ! *
45 ! ******************************

47   USE NumTypes

49   Real (kind=DP), Intent (in) :: Xo(:)
     Real (kind=DP) :: FstepM
51

53   FstepM = (Xo(1)-1.0_DP)**2 + &
          & (Xo(2)-2.0_DP)**2 + &
55        & (Xo(3)+3.0_DP)**4 + &
          & (Xo(4)-4.0_DP)**8
57

59   Return
   End Function FstepM
```

5.5 Function MaxPosition(FVal, IpX, IpY)

5.5.1 Description

Given a two dimensional array of values `FVal(:,:)`, the function `MaxPosition(FVal, IpX, IpY)` returns the number of local maxima of `FVal(:,:)` and its positions in the one dimensional arrays `IpX(:)`and `IpY(:)`.

5.5.2 Arguments

`Fval(:,:)`: Real single or double precision. The values of a function in a two dimensional grid of points.

`IpX(:)`: Integer. A one dimensional array that contains the value of X for the positions of the maxima.

`IpY(:)`: Integer. A one dimensional array that contains the value of Y for the positions of the maxima.

5.5.3 Output

Integer. The number of local maxima of the input. `FVal(:,:)`.

5.5.4 Example

Listing 5.5: Example of the usage of the routine MaxPosition.

```
Program MaxLoc

  USE NumTypes
  USE Constants
  USE Optimization
  USE Error

  IMPLICIT NONE

  Integer :: I, J, IsX, IsY, Nmax
  Character (len=200) :: Filename
  Real (kind=DP) :: DnullX, DnullY
  Real (kind=DP), Allocatable :: F(:,:)
  Integer :: IpX(10), IpY(10)

  Write(stderr,*)"SizeX, SizeY, Filename"
  Read(*,*)IsX, IsY, Filename

  Allocate(F(IsX,IsY))
  Open (Unit=666, File=Trim(Filename), Action="READ")
  Do I = 1, IsX
     Do J = 1, IsY
        Read(666,*)DnullX, DnullY, F(I,J)
        Write(stderr,*)DnullX, DnullY, F(I,J)
     End Do
  End Do
  Close(666)

  Nmax = MaxPosition(F, IpX, IpY)
  Write(*,*)"# Number of maxima: ", Nmax
  Write(*,*)"# Positions of the maxima: "
  Do I = 1, Nmax
     Write(*,*)IpX(I), IpY(I)
  End Do

  Stop
End Program MaxLoc
```

Six

MODULE MinuitAPI

This is the documentation of the MODULE MinuitAPI, a set of routines to Optimise (maximise or minimise) functions of one or several variables. This module is a simple API to the CERN minuit library[1].

6.1 Subroutine Minimize(Func, X, Fval, [Bound], [Release], [logfile])

6.1.1 Description

The routine Minimize, minimises the function of several variables Func. As an output you get the position of the minima in the vector X(:), and the value of the function in the minima in the variable Fval. It uses a series of minimization calls to different minuit strategies: MINIMIZE → SEEK → MIGRAD. This is a safe and robust minimizer for almost everything.

Several optional parameters can be used to put boundaries in the values of the parameters, or to specify a release order for the parameters.

6.1.2 Arguments

Func: The function we want to minimise. An interface like the following should be declared

```
Interface
   Function Func(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP) :: Func
   End Function Func
End Interface
```

X(:): Real double precision one dimensional array. As input an estimate of the position of the minima. As output the position of the minima.

[1] http://lcgapp.cern.ch/project/cls/work-packages/mathlibs/minuit/home.html

`Fval`: Real double precision. Output. The value of the function at the minima.

`Bound(:)`: Real double precision one dimensional array. Optional. Parameter limits. The minimum value for parameter n is given by `Bound(2n-1)`, and the maximum value is given by `Bound(2n)`. If both limits are `0.0D0` the parameter has no limits.

`Release(0:,:)`: Integer two dimensional array. Optional. The integer two dimensional array can be used to specify a release order of parameters. The first dimension of `Release(0:,:)` contains the steps in which you want to release the parameters. The vector `Release(0,:)` contains the number of parameters released in each step. `Release(1,:)` contains the parameters released in the first step. `Release(2,:)` contains the parameters released in the second step, etc...

For example, the array (an $*$ means that the value of this element of the array is irrelevant).

$$R_{ij} = \begin{pmatrix} 2 & 2 & 3 & * \\ 1 & 2 & * & * \\ 3 & 4 & * & * \\ 5 & 6 & 7 & * \end{pmatrix} \tag{6.1}$$

Means that parameters $1, 2$ are free in the first step of the fit. Parameters $(1, 2, 3, 4)$ are free in the second step, and finally parameters $(1, 2, 3, 4, 5, 6, 7)$ are released in the last step of the fit.

`logfile`: Character (len=*). Optional. A file name where MINUIT will write some information about the minimisation process.

6.1.3 Example

Listing 6.1: Using minuit library to minimize a function.

```
Program TestAPI

  USE MinuitAPI
  USE Statistics
  USE Constants

  Integer, Parameter :: N = 2
  Real (kind=8) :: X(N), Y(N), Ye(N), C(2), Ch

  Interface
     Function Func(X)
       Real (kind=8), Intent (in) :: X(:)
       Real (kind=8) :: Func
     End Function Func
  End Interface


  X(:) = -23.0D0
  CALL Minimize(Func, X, Ch)
  Write(*,*)Ch
  Write(*,*)X
```

```
  Write(*,*)Tan(X(1)), Cos(X(2))
23
  Stop
25 End Program TestAPI

27 Function Func(X)

29   Real (kind=8), Intent (in) :: X(:)
  Real (kind=8) :: Func
31
  Func = (X(1)-tan(X(1)))**2 + (X(2) - Cos(X(2)))**2
33
  Return
35 End Function Func
```

6.2 Subroutine Migrad(Func, X, Fval, [Bound], [Release], [logfile])

6.2.1 Description

The routine Migrad, minimises the function of several variables Func using Minuit MIGRAD minimizer. As an output you get the position of the minima in the vector X(:), and the value of the function in the minima in the variable Fval.

From the minuit documentation:

> This is the best minimizer for nearly all functions. It is a variable-metric method with inexact line search, a stable metric updating scheme, and checks for positive-definiteness.

Several optional parameters can be used to put boundaries in the values of the parameters, or to specify a release order for the parameters.

6.2.2 Arguments

Func: The function we want to minimise. An interface like the following should be declared

```
Interface
   Function Func(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP) :: Func
   End Function Func
End Interface
```

X(:): Real double precision one dimensional array. As input an estimate of the position of the minima. As output the position of the minima.

Fval: Real double precision. Output. The value of the function at the minima.

`Bound(:)`: Real double precision one dimensional array. Optional. Parameter limits. The minimum value for parameter n is given by `Bound(2n-1)`, and the maximum value is given by `Bound(2n)`. If both limits are `0.0D0` the parameter has no limits.

`Release(0:,:)`: Integer two dimensional array. Optional. The integer two dimensional array can be used to specify a release order of parameters. The first dimension of `Release(0:,:)` contains the steps in which you want to release the parameters. The vector `Release(0,:)` contains the number of parameters released in each step. `Release(1,:)` contains the parameters released in the first step. `Release(2,:)` contains the parameters released in the second step, etc...

For example, the array (an $*$ means that the value of this element of the array is irrelevant).

$$R_{ij} = \begin{pmatrix} 2 & 2 & 3 & * \\ 1 & 2 & * & * \\ 3 & 4 & * & * \\ 5 & 6 & 7 & * \end{pmatrix} \tag{6.2}$$

Means that parameters $1, 2$ are free in the first step of the fit. Parameters $(1, 2, 3, 4)$ are free in the second step, and finally parameters $(1, 2, 3, 4, 5, 6, 7)$ are released in the last step of the fit.

`logfile`: Character (len=*). Optional. A file name where MINUIT will write some information about the minimisation process.

6.2.3 Example

Listing 6.2: Using minuit library to minimize a function.

```
Program TestAPI

  USE MinuitAPI
  USE Statistics
  USE Constants

  Integer, Parameter :: N = 2
  Real (kind=8) :: X(N), Y(N), Ye(N), C(2), Ch

  Interface
     Function Func(X)
       Real (kind=8), Intent (in) :: X(:)
       Real (kind=8) :: Func
     End Function Func
  End Interface


  X(:) = -23.0D0
  CALL Migrad(Func, X, Ch)
  Write(*,*)Ch
  Write(*,*)X
  Write(*,*)Tan(X(1)), Cos(X(2))

```

```
  Stop
End Program TestAPI

Function Func(X)

  Real (kind=8), Intent (in) :: X(:)
  Real (kind=8) :: Func

  Func = (X(1)-tan(X(1)))**2 + (X(2) - Cos(X(2)))**2

  Return
End Function Func
```

6.3 Subroutine Misimplex(Func, X, Fval, [Bound], [Release], [logfile])

6.3.1 Description

The routine **Misimplex**, minimises the function of several variables Func using Minuit **SIMPLEX** minimizer. As an output you get the position of the minima in the vector **X(:)**, and the value of the function in the minima in the variable **Fval**.

From the minuit documentation:

> This genuine multidimensional minimization routine is usually much slower than MIGRAD, but it does not use first derivatives, so it should not be so sensitive to the precision of the FCN calculations, and is even rather robust with respect to gross fluctuations in the function value. However, it gives no reliable information about parameter errors, no information whatsoever about parameter correlations, and worst of all cannot be expected to converge accurately to the minimum in a finite time. Its estimate of EDM is largely fantasy, so it would not even know if it did converge.

Several optional parameters can be used to put boundaries in the values of the parameters, or to specify a release order for the parameters.

6.3.2 Arguments

Func: The function we want to minimise. An interface like the following should be declared

```
Interface
   Function Func(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP) :: Func
   End Function Func
End Interface
```

X(:): Real double precision one dimensional array. As input an estimate of the position of the minima. As output the position of the minima.

`Fval:` Real double precision. Output. The value of the function at the minima.

`Bound(:):` Real double precision one dimensional array. Optional. Parameter limits. The minimum value for parameter n is given by `Bound(2n-1)`, and the maximum value is given by `Bound(2n)`. If both limits are `0.0D0` the parameter has no limits.

`Release(0:,:):` Integer two dimensional array. Optional. The integer two dimensional array can be used to specify a release order of parameters. The first dimension of `Release(0:,:)` contains the steps in which you want to release the parameters. The vector `Release(0,:)` contains the number of parameters released in each step. `Release(1,:)` contains the parameters released in the first step. `Release(2,:)` contains the parameters released in the second step, etc...

For example, the array (an $*$ means that the value of this element of the array is irrelevant).

$$R_{ij} = \begin{pmatrix} 2 & 2 & 3 & * \\ 1 & 2 & * & * \\ 3 & 4 & * & * \\ 5 & 6 & 7 & * \end{pmatrix} \tag{6.3}$$

Means that parameters $1, 2$ are free in the first step of the fit. Parameters $(1, 2, 3, 4)$ are free in the second step, and finally parameters $(1, 2, 3, 4, 5, 6, 7)$ are released in the last step of the fit.

`logfile:` Character (len=*). Optional. A file name where MINUIT will write some information about the minimisation process.

6.3.3 Example

Listing 6.3: Using minuit library to minimize a function.

```
Program TestAPI

  USE MinuitAPI
  USE Statistics
  USE Constants

  Integer, Parameter :: N = 2
  Real (kind=8) :: X(N), Y(N), Ye(N), C(2), Ch

  Interface
     Function Func(X)
       Real (kind=8), Intent (in) :: X(:)
       Real (kind=8) :: Func
     End Function Func
  End Interface


  X(:) = -23.0D0
  CALL Misimplex(Func, X, Ch)
  Write(*,*)Ch
  Write(*,*)X
```

```
  Write(*,*)Tan(X(1)), Cos(X(2))
23
  Stop
25 End Program TestAPI

27 Function Func(X)

29   Real (kind=8), Intent (in) :: X(:)
  Real (kind=8) :: Func
31
  Func = (X(1)-tan(X(1)))**2 + (X(2) - Cos(X(2)))**2
33
  Return
35 End Function Func
```

6.4 Subroutine Miseek(Func, X, Fval, [Bound], [Release], [logfile])

6.4.1 Description

The routine Miseek, minimises the function of several variables Func using Minuit SEEK minimizer. As an output you get the position of the minima in the vector X(:), and the value of the function in the minima in the variable Fval.

From the minuit documentation:

> We have retained this Monte Carlo search mainly for sentimental reasons, even though the limited experience with it is less than spectacular. The method now incorporates a Metropolis algorithm which always moves the search region to be centred at a new minimum, and has probability $e^{-F/F_{\text{min}}}$ of moving the search region to a higher point with function value F. This gives it the theoretical ability to jump through function barriers like a multidimensional quantum mechanical tunneler in search of isolated minima, but it is widely believed by at least half of the authors of Minuit that this is unlikely to work in practice (counterexamples are welcome) since it seems to depend critically on choosing the right average step size for the random jumps, and if you knew that, you wouldn't need Minuit.

Several optional parameters can be used to put boundaries in the values of the parameters, or to specify a release order for the parameters.

6.4.2 Arguments

Func: The function we want to minimise. An interface like the following should be declared

```
Interface
   Function Func(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP) :: Func
   End Function Func
End Interface
```

`X(:)`: Real double precision one dimensional array. As input an estimate of the position of the minima. As output the position of the minima.

`Fval`: Real double precision. Output. The value of the function at the minima.

`Bound(:)`: Real double precision one dimensional array. Optional. Parameter limits. The minimum value for parameter n is given by `Bound(2n-1)`, and the maximum value is given by `Bound(2n)`. If both limits are `0.0D0` the parameter has no limits.

`Release(0:,:)`: Integer two dimensional array. Optional. The integer two dimensional array can be used to specify a release order of parameters. The first dimension of `Release(0:,:)` contains the steps in which you want to release the parameters. The vector `Release(0,:)` contains the number of parameters released in each step. `Release(1,:)` contains the parameters released in the first step. `Release(2,:)` contains the parameters released in the second step, etc...

For example, the array (an $*$ means that the value of this element of the array is irrelevant).

$$R_{ij} = \begin{pmatrix} 2 & 2 & 3 & * \\ 1 & 2 & * & * \\ 3 & 4 & * & * \\ 5 & 6 & 7 & * \end{pmatrix} \tag{6.4}$$

Means that parameters $1, 2$ are free in the first step of the fit. Parameters $(1, 2, 3, 4)$ are free in the second step, and finally parameters $(1, 2, 3, 4, 5, 6, 7)$ are released in the last step of the fit.

`logfile`: Character (len=*). Optional. A file name where MINUIT will write some information about the minimisation process.

6.4.3 Example

Listing 6.4: Using minuit library to minimize a function.

```
Program TestAPI

  USE MinuitAPI
  USE Statistics
  USE Constants

  Integer, Parameter :: N = 2
  Real (kind=8) :: X(N), Y(N), Ye(N), C(2), Ch

  Interface
     Function Func(X)
       Real (kind=8), Intent (in) :: X(:)
       Real (kind=8) :: Func
     End Function Func
  End Interface


  X(:) = -23.0D0
```

```
19    CALL Miseek(Func, X, Ch)
      Write(*,*)Ch
21    Write(*,*)X
      Write(*,*)Tan(X(1)), Cos(X(2))
23
      Stop
25  End Program TestAPI

27  Function Func(X)

29    Real (kind=8), Intent (in) :: X(:)
      Real (kind=8) :: Func
31
      Func = (X(1)-tan(X(1)))**2 + (X(2) - Cos(X(2)))**2
33
      Return
35  End Function Func
```

6.5 Subroutine Miscan(Func, X, Fval, [Bound], [Release], [logfile])

6.5.1 Description

The routine Miscan, minimises the function of several variables Func using Minuit SCAN minimizer. As an output you get the position of the minima in the vector X(:), and the value of the function in the minima in the variable Fval.

From the minuit documentation:

> This is not intended to minimize, and just scans the function, one parameter at a time. It does however retain the best value after each scan, so it does some sort of highly primitive minimization.

Several optional parameters can be used to put boundaries in the values of the parameters, or to specify a release order for the parameters.

6.5.2 Arguments

Func: The function we want to minimise. An interface like the following should be declared

```
Interface
   Function Func(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP) :: Func
   End Function Func
End Interface
```

X(:): Real double precision one dimensional array. As input an estimate of the position of the minima. As output the position of the minima.

`Fval:` Real double precision. Output. The value of the function at the minima.

`Bound(:):` Real double precision one dimensional array. Optional. Parameter limits. The minimum value for parameter n is given by `Bound(2n-1)`, and the maximum value is given by `Bound(2n)`. If both limits are `0.0D0` the parameter has no limits.

`Release(0:,:):` Integer two dimensional array. Optional. The integer two dimensional array can be used to specify a release order of parameters. The first dimension of `Release(0:,:)` contains the steps in which you want to release the parameters. The vector `Release(0,:)` contains the number of parameters released in each step. `Release(1,:)` contains the parameters released in the first step. `Release(2,:)` contains the parameters released in the second step, etc...

For example, the array (an $*$ means that the value of this element of the array is irrelevant).

$$R_{ij} = \begin{pmatrix} 2 & 2 & 3 & * \\ 1 & 2 & * & * \\ 3 & 4 & * & * \\ 5 & 6 & 7 & * \end{pmatrix} \tag{6.5}$$

Means that parameters $1, 2$ are free in the first step of the fit. Parameters $(1, 2, 3, 4)$ are free in the second step, and finally parameters $(1, 2, 3, 4, 5, 6, 7)$ are released in the last step of the fit.

`logfile:` Character (len=*). Optional. A file name where MINUIT will write some information about the minimisation process.

6.5.3 Example

Listing 6.5: Using minuit library to minimize a function.

```
Program TestAPI

  USE MinuitAPI
  USE Statistics
  USE Constants

  Integer, Parameter :: N = 2
  Real (kind=8) :: X(N), Y(N), Ye(N), C(2), Ch

  Interface
     Function Func(X)
       Real (kind=8), Intent (in) :: X(:)
       Real (kind=8) :: Func
     End Function Func
  End Interface


  X(:) = -23.0D0
  CALL Miscan(Func, X, Ch)
  Write(*,*)Ch
  Write(*,*)X
```

```
  Write(*,*)Tan(X(1)), Cos(X(2))
23
  Stop
25 End Program TestAPI

27 Function Func(X)

29   Real (kind=8), Intent (in) :: X(:)
  Real (kind=8) :: Func
31
  Func = (X(1)-tan(X(1)))**2 + (X(2) - Cos(X(2)))**2
33
  Return
35 End Function Func
```

Seven

MODULE LapackAPI

This is the documentation of the MODULE `LapackAPI`, a set of routines to perform calls to the Linear Algebra PACKage.

7.1 Subroutine `SVD(A, L [, U, VT])`

7.1.1 Description

The routine `SVD`, performs the singular value decomposition of the matrix $A(:,:)$, optionally returning the right and left eigenvectors.

7.1.2 Arguments

`A:` Real double precision two dimensional array. The matrix whose singular value decomposition we want to know.

`L(:):` Real double precision one dimensional array. A vector containing the singular values of A.

`U(:,:):` Real double precision two dimensional array. Output. Optional. The left eigenvectors as columns.

`VT(:,:):` Real double precision two dimensional array. Output. Optional. The right eigenvectors as columns.

7.1.3 Example

Listing 7.1: Using lapack library to perform a SVD decomposition.

```
1 Program SVDtest
3   USE NumTypes
    USE LapackAPI
5
    Real (kind=DP), Allocatable :: A(:,:), U(:,:), VT(:,:), Sv(:),&
7        & SA(:,:)
```

```
 9    Real (kind=DP), Allocatable :: Work(:)
      Integer :: NWork
11    Character (len=100) :: foo

13    Write(*,*) 'Enter matrix size: '
      Read(*,*)N
15    M = N

17    ALLOCATE(A(N,N), SA(N,N), U(N,N), VT(N,N), Sv(N))
      CALL Random_Number(A)
19    A(:,N) = A(:,1)
      Write(*,*) 'A = ['
21    Do K1 = 1, N
         Write(foo,*) '(1X, ', N, 'ES13.5,1A1)'
23       Write(*,foo)(A(K1,K2), K2=1, N), ';'
      End Do
25    Write(*,*) ']'

27    CALL SVD(A, Sv, U, VT)
      Write(*,*)Sv
29
      Write(*,*) 'U = ['
31    Do K1 = 1, N
         Write(foo,*) '(1X, ', N, 'ES13.5,1A1)'
33       Write(*,foo)(U(K1,K2), K2=1, N), ';'
      End Do
35    Write(*,*) ']'

37    Write(*,*) 'VT = ['
      Do K1 = 1, N
39       Write(foo,*) '(1X, ', N, 'ES13.5,1A1)'
         Write(*,foo)(VT(K1,K2), K2=1, N), ';'
41    End Do
      Write(*,*) ']'
43
      Stop
45  End Program SVDtest
```

7.2 Function `PseudoInverse(A [, Ikeep])`

7.2.1 Description

This function returns the pseudo-inverse of the matrix A.

7.2.2 Arguments

`A`: Real double precision two dimensional array. The matrix whose pseudo-inverse we want to know.

`Ikeep:` Integer. Optional. Number of singular values that we want to keep to perform the pseudo inversion. If not present the inverse matrix is computed.

7.2.3 Output

A two dimensional array. Contains the pseudo-inverse of $A(:,:)$.

7.2.4 Example

Listing 7.2: Using lapack library to compute the inverse.

```
Program SVDtest

  USE NumTypes
  USE LapackAPI

  Real (kind=DP), Allocatable :: A(:,:), B(:,:)
  Character (len=100) :: foo


  Write(*,*) 'Enter matrix size: '
  Read(*,*)N

  ALLOCATE(A(N,N), B(N,N))
  CALL Random_Number(A)
  Write(*,*) 'A = ['
  Do K1 = 1, N
     Write(foo,*) '(1X, ', N, 'ES13.5,1A1)'
     Write(*,foo)(A(K1,K2), K2=1, N), ';'
  End Do
  Write(*,*) ']'

  B = PseudoInverse(A)

  Write(*,*) 'B = ['
  Do K1 = 1, N
     Write(foo,*) '(1X, ', N, 'ES13.5,1A1)'
     Write(*,foo)(B(K1,K2), K2=1, N), ';'
  End Do
  Write(*,*) ']'

  A = MatMul(A,B)
  Write(*,*) 'A = ['
  Do K1 = 1, N
     Write(foo,*) '(1X, ', N, 'ES13.5,1A1)'
     Write(*,foo)(A(K1,K2), K2=1, N), ';'
  End Do
  Write(*,*) ']'

  Stop
End Program SVDtest
```

Eight

MODULE Linear

This is the documentation of the MODULE Linear, a set of FORTRAN 90 routines to solve linear systems of equations. This module make use of the MODULE NumTypes, and MODULE Error so please read the documentation of these modules *before* reading this.

8.1 Subroutine Pivoting(M,Ipiv,Idet)

8.1.1 Description

Permute the rows of M so that the biggest elements (in absolute value) of M are in the diagonal.

8.1.2 Arguments

M(:,:): Real or complex single or double precision two dimensional array. Initially it contains the matrix to permute, after calling the routine, it contains the permuted matrix. *Note that M is overwritten when calling this routine.*

Ipiv(:): Integer one dimensional array. It returns the permutation of rows made to M.

Idet: Integer. If the number of permutations is odd, Idet $= 1$, if it is even Idet $= -1$

8.1.3 Examples

Listing 8.1: Pivoting data of a matrix label

```
Program TestLinear

  USE NumTypes
  USE Linear

  Integer, Parameter :: Nord = 4

  Real (kind=DP) :: M(Nord,Nord), L(Nord,Nord), U(Nord,Nord), &
       & Mcp(Nord,Nord)
  Integer :: Ipiv(Nord), Iperm
```

```
12
   ! Fill M of random numbers
14 CALL Random_Number(M)

16 Write(*,*) 'Original M:  '
   Do I = 1, Nord
18    Write(*, '(100ES10.3) ')(M(I,J), J = 1, Nord)
   End Do
20
   CALL Pivoting (M, Ipiv, Iperm)
22 Write(*,*) 'Permuted M:  '
   Do I = 1, Nord
24    Write(*, '(100ES10.3) ')(M(I,J), J = 1, Nord)
   End Do
26
   Stop
28 End Program TestLinear
```

8.2 Subroutine `LU(M, Ipiv, Idet)`

8.2.1 Description

Make the LU decomposition of matrix M. That is to say, given a matrix M, this function returns two matrix L and U, such that

$$M = LU \tag{8.1}$$

where L is lower triangular, and U upper triangular.

$$L = \begin{pmatrix} 1 & 0 & 0 & \dots \\ L_{21} & 1 & 0 & \dots \\ L_{31} & L_{32} & 1 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}; \quad U = \begin{pmatrix} U_{11} & U_{12} & U_{13} & \dots \\ 0 & U_{22} & U_{23} & \dots \\ 0 & 0 & U_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{8.2}$$

The rows of M are permuted so that the biggest possible elements are on the diagonal (this makes the problem more stable). The two matrices L and U are returned *overwriting* M.

8.2.2 Arguments

`M(:,:)`: Real or complex single or double precision two dimensional array. Initially it contains the matrix to decompose, after calling the routine, it contains L in its lower part, and U in its upper part. *Note that M is overwritten when calling this routine.*

`Ipiv(:)`: Integer one dimensional array. It returns the permutation of rows made to M.

`Idet`: Integer. If the number of permutations is odd, `Idet` $= 1$, if it is even `Idet` $= -1$

8.2.3 Examples

Listing 8.2: Making the LU decomposition.

```
Program TestLinear

  USE NumTypes
  USE Linear

  Integer, Parameter :: Nord = 4

  Real (kind=DP) :: M(Nord,Nord), L(Nord,Nord), U(Nord,Nord), &
       & Mcp(Nord,Nord)
  Integer :: Ipiv(Nord), Iperm


  ! Fill M of random numbers, and make a copy
  CALL Random_Number(M)
  Mcp = M
  L = 0.0_DP
  U = 0.0_DP

  ! Make the LU decomposition and fill the matrices
  ! L and U
  CALL Lu(M, Ipiv, Iperm)
  Do I = 1, Nord
     L(I,I) = 1.0_DP
     U(I,I) = M(I,I)
     Do J = I+1, Nord
        L(J,I) = M(J,I)
        U(I,J) = M(I,J)
     End Do
  End Do

  ! Now Make the product and see that it is the original matrix with
  ! some rows permuted
  Write(*,*) 'M:  '
  Do I = 1, Nord
     Write(*,'(100ES10.3)')(Mcp(I,J), J = 1, Nord)
  End Do

  Write(*,*) 'L:  '
  Do I = 1, Nord
     Write(*,'(100ES10.3)')(L(I,J), J = 1, Nord)
  End Do
  Write(*,*) 'U:  '
  Do I = 1, Nord
     Write(*,'(100ES10.3)')(U(I,J), J = 1, Nord)
  End Do

  M = MatMul(L,U)
  Write(*,*) 'LU (Same as M with some rows permuted):  '
  Do I = 1, Nord
```

```
50      Write(*,'(100ES10.3)')(M(I,J), J = 1, Nord)
    End Do
52
54  Stop
End Program TestLinear
```

8.3 Subroutine LUsolve(M, b)

8.3.1 Description

Solves the linear system of equations

$$\begin{aligned} M_{11}x_1 + M_{12}x_2 + M_{13}x_3 + M_{14}x_4 + \ldots &= b_1 \\ M_{21}x_1 + M_{22}x_2 + M_{23}x_3 + M_{24}x_4 + \ldots &= b_2 \\ &\vdots \end{aligned} \tag{8.3}$$

8.3.2 Arguments

`M(:,:)`: Real or complex single or double precision two dimensional array. The matrix of coefficients. *M is overwritten when solving the system.*

`b(:)`: Real or complex single or double precision one dimensional array. The independent terms before calling the routine, and the solution of the linear system of equations after calling it. *Note that b is overwritten when calling this routine.*

8.3.3 Examples

Listing 8.3: Solving systems of linear equations.

```
1  Program TestLinear
3    USE NumTypes
     USE Linear
5
     Integer, Parameter :: Nord = 10
7
     Real (kind=DP) :: M(Nord,Nord), L(Nord,Nord), U(Nord,Nord), &
9         & Mcp(Nord,Nord), b(Nord), bcp(Nord)
     Integer :: Ipiv(Nord), Iperm
11
     ! Fill M and b of random numbers, and make a copy of both
13   CALL Random_Number(M)
     CALL Random_Number(b)
15   Mcp = M
     bcp = b
17
     ! Solve the linear system
19   CALL LUsolve(M,b)
```

```
21    ! Check that it is a solution:
      b = MatMul(Mcp,b)
23    Write(*,*) 'b: '
      Write(*,'(100ES10.3)')(Abs(bcp(I)-b(I)), I = 1, Nord)
25
27    Stop
End Program TestLinear
```

8.4 Function Det(M)

8.4.1 Description

Computes the determinant of the matrix M.

8.4.2 Arguments

`M(:,:)`: Real or complex, simple or double precision two dimensional array. The matrix whose determinant we want to know.

8.4.3 Output

The value of the determinant. Same precision as the input argument.

8.4.4 Examples

Listing 8.4: Computing the determinant of a matrix.

```
Program TestLinear
2
  USE NumTypes
4 USE Linear

6 Integer, Parameter :: Nord = 10

8 Real (kind=DP) :: M(Nord,Nord), L(Nord,Nord), U(Nord,Nord), &
       & Mcp(Nord,Nord), b(Nord), bcp(Nord)
10 Integer :: Ipiv(Nord), Iperm

12
  ! Fill M of randoms numbers
14 CALL Random_Number(M)

16 ! Now compute the determinant.
  Write(*,'(ES15.8)')Det(M)
18

20 Stop
End Program TestLinear
```

Nine

MODULE NonNum

This is the documentation of the `MODULE NonNum`, a set of `FORTRAN 90` routines to sort and search. This module make use of the `MODULE NumTypes`, and `MODULE Error` so please read the documentation of these modules *before* reading this.

9.1 Subroutine `Swap(X,Ind1,Ind2)`

9.1.1 Description

Swaps elements `Ind1` and `Ind2` of the array `X(:)`.

9.1.2 Arguments

`X(:)`: Integer, real single or real double precision one dimensional array. *Note that X is overwritten when calling this routine.*

`Ind1, Ind2`: Integer. The elements that we want to permute.

9.1.3 Examples

Listing 9.1: Sorting data.

```
1  Program TestNN

3    USE NumTypes
     USE NonNumeric
5
     Integer, Parameter :: Nmax = 10
7    Integer :: Ima(Nmax), I

9
     ! Fill Ima(:)
11   Forall (I=1:Nmax) Ima(I) = I

13   ! Plot the numbers
     Do I = 1, Nmax
15      Write(*,'(1000I10)')Ima(I)
```

```
  End Do

  ! Swap first and last elemetns of Ima(:) and plot them.
  CALL Swap(Ima, 1, Nmax)
  Write(*,*) '# With first and last elements permuted: '
  Do I = 1, Nmax
     Write(*, '(1000I10)')Ima(I)
  End Do


  Stop
End Program TestNN
```

9.2 Subroutine `Insrt(X[, Ipt])`

9.2.1 Description

Sort the elements of `X(:)` in ascendant order[1].

9.2.2 Arguments

`X(:)`: Integer, real single or real double precision one dimensional array. Initially it contains unsorted numbers, and after calling the routine, it contains the sorted elements. *Note that X is overwritten when calling this routine.*

`Ipt(:)`: Integer vector, Optional. It returns the permutation made to `X(:)` to sort it.

9.2.3 Examples

Listing 9.2: Sorting data.

```
Program TestNN

  USE NumTypes
  USE NonNumeric

  Integer, Parameter :: Nmax = 10
  Integer :: Ima(Nmax)
  Real (kind=DP) :: X(Nmax), Y(Nmax)


  ! Fill X(:) with random data, and define Y(:)
  CALL Random_Number(X)
  Y = Sin(12.34_DP*(X-0.5_DP))

  ! Plot an unsorted data table
  Do I = 1, Nmax
     Write(*, '(1000ES13.5)')X(I), Y(I)
```

[1] This routine uses *insertion sort*, and is much slower than `Qsort`. To sort more than 10 elements, use `Qsort` unless you know what you are doing.

```
  End Do

  ! Sort them, and plot the table again. Same points, but this time
  ! sorted
  CALL Insrt(X, Ima)
  Write(*,*) '# Again, this time sorted: '
  Do I = 1, Nmax
     Write(*, '(1000ES13.5)')X(I), Y(Ima(I))
  End Do


  Stop
End Program TestNN
```

9.3 Subroutine Qsort(X[, Ipt])

9.3.1 Description

Sort the elements of `X(:)` in ascendant order.

9.3.2 Arguments

`X(:)`: Integer, real single or real double precision one dimensional array. Initially it contains unsorted numbers, and after calling the routine, it contains the sorted elements. *Note that X is overwritten when calling this routine.*

`Ipt(:)`: Integer vector, Optional. It returns the permutation made to `X(:)` to sort it.

9.3.3 Examples

Listing 9.3: Sorting data.

```
Program TestNN

  USE NumTypes
  USE NonNumeric

  Integer, Parameter :: Nmax = 10
  Integer :: Ima(Nmax)
  Real (kind=DP) :: X(Nmax), Y(Nmax)


  ! Fill X(:) with random data, and define Y(:)
  CALL Random_Number(X)
  Y = Sin(12.34_DP*(X-0.5_DP))

  ! Plot an unsorted data table
  Do I = 1, Nmax
     Write(*, '(1000ES13.5)')X(I), Y(I)
  End Do
```

```
20    ! Sort them, and plot the table again. Same points, but this time
      ! sorted
22    CALL Qsort(X, Ima)
      Write(*,*) '# Again, this time sorted: '
24    Do I = 1, Nmax
         Write(*, '(1000ES13.5)')X(I), Y(Ima(I))
26    End Do


28
      Stop
30  End Program TestNN
```

9.4 Function `Locate(X, X0[, Iin])`

9.4.1 Description

Given a *sorted* vector of elements `X(:)`, and a point $\mathtt{X}_0$, `Locate` returns the position n such that $\mathtt{X(n)} < \mathtt{X}_0 < \mathtt{X(n+1)}$. If $\mathtt{X}_0$ is less than all the elements of `X(:)`, `Locate` returns 0, and if it is greater than all the elements of `X(:)`, it returns the number of elements of `X(:)`

9.4.2 Arguments

`X(:)`: Integer, real single or real double precision one dimensional *sorted* array.

$\mathtt{X}_0$: Integer, real single or real double precision number, but the same type as `X(:)`. Point that we want to locate in the sorted vector `X(:)`.

`Iin`: Integer, Optional. Initial guess of the position.

9.4.3 Output

Integer. The position n such that

$$\mathtt{X(n)} < \mathtt{X}_0 < \mathtt{X(n+1)}$$

9.4.4 Examples

Listing 9.4: Searching data position in an ordered list.

```
Program TestNN
2
  USE NumTypes
4 USE NonNumeric

6 Integer, Parameter :: Nmax = 100
  Integer :: Ima(Nmax), Idx
8 Real (kind=DP) :: X(Nmax), Y(Nmax), X0


10
  ! Fill X(:) with random data, and set X0 to some arbitrary value.
12 CALL Random_Number(X)
```

```
  X0 = 0.276546754_DP

  ! Sort X(:), find the position of X0, and plot the neightborr
  ! elements.
  CALL Qsort(X)
  Idx = Locate(X, X0)
  Write(*,'(1A,1ES33.25)') 'Searched element: ', X0
  Write(*,'(1A,1ES33.25)') 'Previous element in the list: ', X(Idx)
  Write(*,'(1A,1ES33.25)') 'Next element in the list:     ', X(Idx+1)

  Stop
End Program TestNN
```

Ten

MODULE SpecialFunc

This is the documentation of the `MODULE SpecialFunc`, a set of `FORTRAN 90` routines to compute the value of some functions. This module make use of the `MODULE NumTypes`, `MODULE Constants`, `MODULE Error` so please read the documentation of these modules *before* reading this.

10.1 Function `GammaLn(X)`

10.1.1 Description

Compute $\log(\Gamma(X))$.

10.1.2 Arguments

`X:` Double (DP) precision. The point in which we want to know the value of $\Gamma(X)$.

10.1.3 Output

A real Double precision (DP).

10.1.4 Examples

This program should write the factorial of the first 100 numbers.

Listing 10.1: Computing the Gamma Function.

```
Program TestSpecialFunc

  USE NumTypes
  USE SpecialFunc

  Integer :: q


  Do q = 1, 100
     Write(*,'(1A13,1I4,1A3,1ES33.25)') 'Factorial of:', q, ' = ',&
          & exp(GammaLn(Real(q+1,kind=DP)))
```

```
12    End Do

14
    Stop
16  End Program TestSpecialFunc
```

10.2 Function erf(X)

10.2.1 Description

Compute values of the error function erf(X). A high precision algorithm by W. J. Candy [2] is used.

10.2.2 Arguments

X: Single (SP) or double (DP) precision. The point in which we want to know the value of erf(X).

10.2.3 Output

Same type as input.

10.2.4 Examples

This program should compute the erf(X) and its complementary in an given point.

Listing 10.2: Computing the Error Function.

```
  Program TestSpecialFunc
2
    USE NumTypes
4   USE SpecialFunc

6   Real (kind=DP) :: X

8   Write(*,*) 'Enter a number: '
    Read(*,*)X
10  Write(*,'(ES33.25)')erf(X)
    Write(*,'(ES33.25)')erfc(X)
12
    Stop
14  End Program TestSpecialFunc
```

10.3 Function erfc(X)

10.3.1 Description

Compute values of the complementary error function erf(X). A high precision algorithm by W. J. Candy [2] is used.

10.3.2 Arguments

`X`: Single (SP) or double (DP) precision. The point in which we want to know the value of erfc(X).

10.3.3 Output

Same type as input.

10.3.4 Examples

This program should compute the erf(X) and its complementary in an given point.

Listing 10.3: Computing the complementary Error Function.

```
Program TestSpecialFunc

  USE NumTypes
  USE SpecialFunc

  Real (kind=DP) :: X

  Write(*,*) 'Enter a number: '
  Read(*,*)X
  Write(*, '(ES33.25)') erf(X)
  Write(*, '(ES33.25)') erfc(X)

  Stop
End Program TestSpecialFunc
```

10.4 Function `inverf(X)`

10.4.1 Description

Compute values of the inverse error function inverf(X). A combination of a rational approximation by Peter John Acklam, and Halley's rational method is used to attain double precision.

10.4.2 Arguments

`X`: Single (SP) or double (DP) precision. The point in which we want to know the value of inverf(X).

10.4.3 Output

Same type as input.

10.4.4 Examples

This program should use the inverf(X) function and test it is ok.

Listing 10.4: Computing the Inverse Error Function.

```
Program Test

  USE NumTypes
  USE SpecialFunc

  Real (kind=DP) :: X = 0.6783457843_DP, Y

  Write(*,'(ES33.25)')inverf(-0.998_DP)
  Write(*,'(ES33.25)')inverf(-0.5_DP)
  Write(*,'(ES33.25)')inverf(0.988_DP)

  Y = inverf(X)
  Write(*,*)'Same number two times!'
  Write(*,'(ES33.25)')X
  Write(*,'(ES33.25)')erf(Y)

  Stop
End Program Test
```

10.5 Function `Theta(i, z, tau[, Prec])`

10.5.1 Description

Compute the value of the i^{th} Jacobi theta function ($i = 1, 2, 3, 4$) with nome $q = e^{i\pi\tau}$

$$\vartheta_i(z|\tau) \tag{10.1}$$

For a definition and properties of these functions take a look [3], here we will only say that following the conventions of the cited reference, our Theta functions have quasi-periods π and $\tau\pi$.

10.5.2 Arguments

`i`: Integer. Which theta function we want to compute. i must have one of the following values: $1, 2, 3, 4$.

`z`: Complex Double Precision (DPC) or Complex Single Precision (SPC). The point in which we want to compute the Theta function.

`tau`: Complex, with the same precision as `z`. is the quasi period of the Theta function. must be in the upper half plane ($Im(\tau) > 0$).

`Prec`: Real, Optional. If `z` is DPC (SPC), `Prec` must be double precision (single precision). An estimation of the desired precision of the result. The default value is 1×10^{-3}

10.5.3 Output

If `z` is Double Precision Complex (SPC), the the result will be Double Precision Complex (SPC).

10.5.4 Examples

Listing 10.5: Computing the Jacobi Theta functions.

```
Program TestSpecialFunc

  USE NumTypes
  USE SpecialFunc

  Complex (DPC) :: Z, tau


  Z = Cmplx(0.546734, 2.76457643, kind=DPC)
  tau = Cmplx(0.0_DP, 3.76387540_DP)

  ! Check the quasi-periodicity of the Third
  ! Jacobi Theta function.
  Write(*,*)Theta(3, Z          , tau)
  Write(*,*)Theta(3, Z+Cmplx(PI_DP), tau)
  Write(*,*)Theta(3, Z+PI_DP*tau, tau) * &
       &exp(PI_IMAG_DPC*tau + 2.0_DP*UNITIMAG_DPC*Z)


  Stop
End Program TestSpecialFunc
```

10.6 Function ThetaChar(a, b, z, tau[, Prec])

10.6.1 Description

Computes the value of the Theta function with Characteristics (a, b) and quasi-periods $(\pi, \pi\tau)$ in the point z:

$$\vartheta \begin{bmatrix} a \\ b \end{bmatrix} (z|\tau) \tag{10.2}$$

10.6.2 Arguments

a, b: Complex or Real, Single or double precision. The two characteristics of the Theta function.

z: Complex (Single or Double precision). The point in the complex plane.

tau: Complex (Single or Double precision). The quasi-period of the theta function. Must have $(\mathrm{Im}(\tau) > 0)$.

Prec: Real (Single or Double precision). Optional. An estimation of the desired precision of the value of the theta function.

10.6.3 Output

Complex Single or Double precision, the same as the input values.

10.6.4 Examples

Listing 10.6: Computing the Jacobi Theta functions with characteristics.

```
Program TestSpecialFunc

  USE NumTypes
  USE SpecialFunc

  Real(kind=DP) :: Deriv, X1, X2
  Complex (DPC) :: Wmas, Wmenos, Z, tau
  Integer :: q, s


  Z = Cmplx(0.546734, 2.76457643, kind=DPC)
  tau = Cmplx(0.0_DP, 3.76387540_DP)


  Write(*,*) 'Theta 1:'
  Write(*,*)Theta(1, Z, tau)
  Write(*,*)-ThetaChar(0.5_DP,0.5_DP, Z, tau)
  Write(*,*) 'Theta 2:'
  Write(*,*)Theta(2, Z, tau)
  Write(*,*)ThetaChar(0.5_DP,0.0_DP, Z, tau)
  Write(*,*) 'Theta 3:'
  Write(*,*)Theta(3, Z, tau)
  Write(*,*)ThetaChar(0.0_DP,0.0_DP, Z, tau)
  Write(*,*) 'Theta 4:'
  Write(*,*)Theta(4, Z, tau)
  Write(*,*)ThetaChar(0.0_DP,0.5_DP, Z, tau)


  Stop
End Program TestSpecialFunc
```

10.7 Function `Hermite(n,x[, Dval])`

10.7.1 Description

Returns the value of the $n^{\underline{\text{th}}}$ Hermite polynomial in the point X. If `Dval` is specified, the value of the Derivative of the $n^{\underline{\text{th}}}$ Hermite polynomial in the point X is also returned.

10.7.2 Arguments

`n`: Integer. Which Hermite polynomial wants to compute.

`X`: Real (Single or Double precision). The point in which we want to compute the Polynomial.

`Dval`: Real (Single or Double precision). Optional. If specified, it stores the value of the Derivative of the Polynomials.

10.7.3 Output

Real single or double precision (same as input). The value of the $n^{\underline{\text{th}}}$ Hermite Polynomial in the point X.

10.7.4 Examples

Listing 10.7: Computing the first 31 Hermite numbers.

```
Program TestSpecialFunc

  USE NumTypes
  USE SpecialFunc

  Integer :: q


  Write(*,*) 'The first 31 Hermite Numbers'
  Write(*,*) 'http://www.research.att.com/~njas/sequences/A067994'
  Do q = 1, 31
     Write(*,'(1I4,1ES33.25)')q, Hermite(q, 0.0_DP)
  End Do

  Stop
End Program TestSpecialFunc
```

10.8 Function HermiteFunc(n, x[, Dval])

10.8.1 Description

Returns the value of the $n^{\underline{\text{th}}}$ Hermite function

$$\frac{1}{\sqrt{n!2^n\sqrt{\pi}}}e^{-x^2/2}H_n(x) \tag{10.3}$$

in the point X. If `Dval` is specified, the value of the Derivative of the $n^{\underline{\text{th}}}$ Hermite function in the point X is also returned.

10.8.2 Arguments

n: Integer. Which Hermite function wants to compute.

X: Real (Single or Double precision). The point in which we want to compute the Polynomial.

Dval: Real (Single or Double precision). Optional. If specified, it stores the value of the Derivative of the function.

10.8.3 Output

Real single or double precision (same as input). The value of the $n^{\underline{\text{th}}}$ Hermite function in the point X.

10.8.4 Examples

Listing 10.8: Compute the Hermite functions.

```
Program TestSpecialFunc

  USE NumTypes
  USE SpecialFunc

  Real(kind=DP) :: Deriv, X1, X2, Sum
  Complex (DPC) :: Wmas, Wmenos, Z, tau
  Integer :: q, s


  Write(*,*) 'A (really bad) proof of orthonormality:'
  X1 = -10.0_DP
  Sum = 0.0_DP
  Do q = -1000, 1000
     Sum = Sum + HermiteFunc(6,X1)**2
     X1 = X1 + 0.01_DP
  End Do

  Write(*, '(1ES33.25)')Sum*0.01_DP

  Stop
End Program TestSpecialFunc
```

10.9 Function `Basis(X1, X2, n, s, q, itau[, Prec])`

10.9.1 Description

Return the value of the basis elements of the Hilbert space $\mathcal{H}_q$ of quasi-periodic functions

$$|\, n, s\rangle = e^{\imath \frac{f}{2} x_1 x_2} \sum_{k \in s+q\mathbb{Z}} e^{-u^2/2} H_n(u) e^{2\pi \imath k \frac{x_1}{l_1}} \qquad n = 0, \ldots \infty; s = 1, \ldots, q \tag{10.4}$$

defined in the appendix of [1] (look there for more details and properties).

10.9.2 Arguments

`X1,X2`: Real (Single or Double precision). The point in the Torus.

`n,s`: Integer. Specify which element of the basis.

`q`: Integer. Specify the Hilbert space $\mathcal{H}_q$.

`itau`: Real (Single or Double precision). Specify the ratio of quasi-periods: `itau` $= l_2/l_1$.

`Prec`: Real (Single or Double precision). Optional. An estimation of the desired precision.

10.9.3 Output

Complex single or double precision, depends of the input arguments.

10.9.4 Examples

Listing 10.9: Computing the bassi of a special Hilbert space (details in [1]).

```
Program TestSpecialFunc

  USE NumTypes
  USE SpecialFunc

  Real(kind=DP) :: X1, X2
  Complex (DPC) :: Wmas, Wmenos,
  Integer :: I, q, s


  Write(*,*) 'Looking at the quasi-periodicity properties:'
  X1 = 0.97834D0
  X2 = 0.873873D0
  q = 4
  s = 3
  Do I = 0, 8
     Wmas   = Basis( X1,  X2+1.0_DP, I, s, q, 1.0_DP, 1.0D-15) * &
          & exp(PI_IMAG_DPC*X1*q)
     Wmenos = Basis( X1+1.0_DP,  X2, I, s, q, 1.0_DP, 1.0D-15) * &
          & exp(-PI_IMAG_DPC*X2*q)
     Write(*, '(1I3,2ES33.25)')I, Basis( X1,  X2, I, s, q, 1.0_DP, 1.0D-15)
     Write(*, '(1I3,2ES33.25)')I, Wmas
     Write(*, '(1I3,2ES33.25)')I, Wmenos
  End Do


  Stop
End Program TestSpecialFunc
```

10.10 Function Factorial(N)

10.10.1 Description

Compute $N!$. Better (faster and more accurate for small numbers) than the use of `GammaLn` to compute the factorial of a number.

10.10.2 Arguments

`N`: Integer. The number to compute the factorial.

10.10.3 Output

A real Double precision (DP).

10.10.4 Examples

This program should write the factorial of the first 100 numbers.

Listing 10.10: Computing the factorial.

```
Program TestSpecialFunc

  USE NumTypes
  USE SpecialFunc

  Integer :: q


  Do q = 1, 100
     Write(*,'(1A13,1I4,1A3,1ES33.25)') 'Factorial of:', q, ' = ',&
          & Factorial(q)
  End Do


  Stop
End Program TestSpecialFunc
```

10.11 Function `Legendre(l, m, X)`

10.11.1 Description

Computes the value at X of the (l, m) Legendre polynomial $P_l^m(X)$.

10.11.2 Arguments

`l,m`: Integer. Specifies which Legendre polynomial we want to compute.

`X`: Real sinple or double precision. The point at which we want to compute the polinomial.

10.11.3 Output

A real simple or double precision (same as `X`).

10.11.4 Examples

This program writes the values of the Legendre polynomials $P_l^m(0.5)$ for $0 \leq m \leq l$.

Listing 10.11: Computing some legendre polynomials.

```
Program TestLeg


  USE NumTypes
  USE SpecialFunc

  Real (kind=DP) :: Y

  Read(*,*)L

  Do I = 0, L
```

```
12      Y = Legendre(L, I, 0.50_DP)
        Write(*,*)I, Y, Legendre(L, I, 0.5_SP)
14    End Do

16    Stop
End Program TestLeg
```

10.12 Function SphericalHarmonics(l, m, th,ph)

10.12.1 Description

Computes the value at (θ, ϕ) of the (l, m) spherical harmonic $Y_l^m(\theta, \phi)$.

10.12.2 Arguments

l,m: Integer. Specifies which spherical harmonic we want to compute.

th,ph: Real single or double precision. (θ, ϕ) coordinates of the point at which we we want to compute the vlue of the spherical harmonic.

10.12.3 Output

A complex simple or double precision (same as th).

10.12.4 Examples

This program checks the relation $Y_l^m(\theta, phi) = (-)^m Y_l^{*-m}(\theta, \phi)$ for $\theta = 0.5, \phi = 0.35$.

Listing 10.12: Computing some spherical harmonics.

```
1  Program TestSph


3
     USE NumTypes
5    USE SpecialFunc

7    Complex (kind=DPC) :: Y

9    Read(*,*)L

11   Do I = 0, L
       Y = SphericalHarmonic(L, I, 0.50_DP, 0.35_DP)
13     Write(*,'(1A,1I4,1A,1I4)')'Spherical Harmonic l=', L, ' m=+-', I
       Write(*,*) '  +m ', Y
15     Write(*,*) '  -m ', SphericalHarmonic(L, -I, 0.5_DP, 0.35_DP)
     End Do
17
     Stop
19 End Program TestSph
```

Eleven

MODULE Statistics

This is the documentation of the `MODULE Statistics`, a set of `FORTRAN 90` routines to perform statistical description of data. This module make use of the `MODULE NumTypes`, `MODULE Constants`, `MODULE Error` and `MODULE Linear` so please read the documentation of these modules *before* reading this.

11.1 Function `Mean(X)`

11.1.1 Description

Compute the mean value of the numbers stored in `X(:)`.

11.1.2 Arguments

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The values whose mean we want to compute.

11.1.3 Output

A real double or simple precision (same type as the input). The mean of the values.

11.1.4 Examples

Listing 11.1: Computing the Mean of a vector of numbers.

```
1  Program Tests
2
3    USE NumTypes
4    USE Error
5    USE Statistics
6
7    Integer, Parameter :: Nmax = 100
8    Real (kind=DP) :: X(Nmax)
9
10   CALL Random_Number(X)
11   Write(*,'(ES33.25)')Mean(X)
```

```
13    Stop
End Program Tests
```

11.2 Function Median(X)

11.2.1 Description

Compute the median value of the numbers stored in `X(:)`.

11.2.2 Arguments

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The values whose median we want to compute.

11.2.3 Output

A real double or simple precision (same type as the input). The median of the values.

11.2.4 Examples

Listing 11.2: Computing the Median of a vector of numbers.

```
Program Tests
2
  USE NumTypes
4 USE Error
  USE Statistics
6
  Integer, Parameter :: Nmax = 5
8 Real (kind=SP) :: X(Nmax) = (/1.0, 1.0, 2.0, 4.0, 1.5/)

10 Write(*,'(ES33.25)')Median(X)

12
  Stop
14 End Program Tests
```

11.3 Function WMedian(X, w)

11.3.1 Description

Compute the weighted median of the numbers stored in `X(:)` with weights `w(:)`.

11.3.2 Arguments

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The values whose median we want to compute.

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The weights.

11.3.3 Output

A real double or simple precision (same type as the input). The weighted median of the values.

11.3.4 Examples

Listing 11.3: Computing the Weighted Median of a vector of numbers.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 5
  Real (kind=SP) :: X(Nmax) = (/1.0, 1.0, 2.0, 4.0, 1.5/)
  Real (kind=SP) :: w(Nmax) = (/10.0, 2.0, 3.0, 4.0, 1.5/)

  Write(*,'(ES33.25)')WMedian(X, w)


  Stop
End Program Tests
```

11.4 Function WPercentile(X, w, p)

11.4.1 Description

Compute the weighted percentile `p` of the numbers stored in `X(:)` with weights `w(:)`.

11.4.2 Arguments

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The values whose median we want to compute.

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The weights.

`p`: Double (DP) or simple (SP) precision number. The percentile (should be between 0 and 100).

11.4.3 Output

A real double or simple precision (same type as the input). The weighted percentile `p` of the values.

11.4.4 Examples

Listing 11.4: Computing the Weighted Median in two ways.

```
Program Tests
```

```
  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 5
  Real (kind=SP) :: X(Nmax) = (/1.0, 1.0, 2.0, 4.0, 1.5/)
  Real (kind=SP) :: w(Nmax) = (/10.0, 2.0, 3.0, 4.0, 1.5/)

  Write(*,'(ES33.25)')WMedian(X, w)
  Write(*,'(ES33.25)')WPercentile(X, w, 50.0_DP)


  Stop
End Program Tests
```

11.5 Subroutine `WConfInt(X, w, Xmin, Xmax)`

11.5.1 Description

Compute the weighted 16^{th} and 84^{th} percentiles f the numbers stored in `X(:)` with weights `w(:)`, and return the values in `Xmin` and `Xmax`.

11.5.2 Arguments

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The values whose median we want to compute.

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The weights.

`Xmin`: Double (DP) or simple (SP) precision number. Output. The 16^{th} percentile.

`Xmax`: Double (DP) or simple (SP) precision number. Output. The 84^{th} percentile.

11.5.3 Examples

Listing 11.5: Computing the 1 sigma confidence interval in two ways.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 500
  Real (kind=SP) :: X(Nmax), w(Nmax), X1, X2

  CALL Normal(X)
  CALL Random_Number(w)

  Write(*,'(ES33.25)')WPercentile(X, w, 16.0_DP)
  Write(*,'(ES33.25)')WPercentile(X, w, 84.0_DP)
```

```
  CALL WConfInt(X, W, X1, X2)
  Write(*,'(ES33.25)')X1, X2

  Stop
End Program Tests
```

11.6 Function Var(X)

11.6.1 Description

Compute the variance of a vector of numbers `X(:)`

11.6.2 Arguments

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The values whose variance we want to compute.

11.6.3 Output

A real double or simple precision (same type as the input). The variance of the values.

11.6.4 Examples

Listing 11.6: Computing the Variance of a set of numbers.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 100, Npinta = 100, Npar = 4
  Real (kind=DP) :: X(Nmax), Y(Nmax), Yer(Nmax), &
       & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax,2)


  CALL Random_Number(X)
  Write(*,'(ES33.25)')Var(X)


  Stop
End Program Tests
```

11.7 Function Stddev(X)

11.7.1 Description

Computes the standard deviation of the numbers stored in the vector `X(:)`.

11.7.2 Arguments

`X(:)`: Double (DP) or simple (SP) precision one dimensional array. The values whose standard deviation we want to compute.

11.7.3 Output

Real Single or Double precision, the same as the input values. The standard deviation of the values.

11.7.4 Examples

Listing 11.7: Compputing the standard deviation.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 100, Npinta = 100, Npar = 4
  Real (kind=DP) :: X(Nmax), Y(Nmax), Yer(Nmax), &
       & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax,2)


  CALL Random_Number(X)
  Write(*,'(ES33.25)')Stddev(X)


  Stop
End Program Tests
```

11.8 Function `Moment(X, k)`

11.8.1 Description

Returns the $k^{\underline{th}}$ moment of the values stored in the vector `X(:)`.

11.8.2 Arguments

`X(:)`: Real (Single or Double precision). The numbers whose $k^{\underline{th}}$ moment we want to compute.

`k`: Integer. Which moment we want to compute.

11.8.3 Output

Real single or double precision. The $k^{\underline{th}}$ moment of the numbers.

11.8.4 Examples

Listing 11.8: Computing the k$^{\underline{th}}$ moment of a data set.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 100, Npinta = 100, Npar = 4
  Real (kind=DP) :: X(Nmax), Y(Nmax), Yer(Nmax), &
       & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax,2)


  CALL Random_Number(X)
  Write(*,*) 'We should obtain the same numbers twice: '
  Write(*,'(ES33.25)')Moment(X,2), Var(X)

  Stop
End Program Test
```

11.9 Subroutine Histogram(Val, Ndiv, Ntics, Vmin, Vmax, h)

11.9.1 Description

Given a set of points `Val(:)`, this routine makes `Ndiv` divisions between the minimum and the greatest value of `Val` (respectively returned in `Vmin` and `Vmax`), each of size `h` (also returned), and returns in the integer vector `Nticks(:)` the number of points that are in each interval.

11.9.2 Arguments

`Val(:)`: Real (Single or Double precision) one dimensional array. The original values.

`Ndiv`: Integer. The number of divisions.

`Nticks`: Integer one dimensional array. `Ndiv(I)` Tells how many points of `Val(:)` are between `Vmin` + (`I` − 1)`h` and `Vmin` + `Ih`.

`Vmin, Vmax`: Real (Single or Double precision). The minimum and maximum values of `Val`.

`h`: Real (Single or Double precision). After calling the routine has the step of the division.

11.9.3 Examples

Listing 11.9: Making Histograms.

```
Program Tests

  USE NumTypes
  USE Error
```

```
  USE Statistics

  Integer, Parameter :: Nmax = 500000, Npinta = 100, Npar = 4, Ndiv = 100
  Real (kind=DP) :: X(Nmax), Y(Nmax), Yer(Nmax), &
       & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax,2), &
       & Xmin, Xmax, h, Xac
  Integer :: Ntics(Ndiv)

  CALL Normal(X, 1.23_DP, 0.345_DP)
  CALL Histogram(X, Ndiv, Ntics, Xmin, Xmax, h)

  Do I = 1, Ndiv
     Xac = Xmin + (I-1)*h
     Write(*,'(1ES33.25,1I)')Xac, Ntics(I)
  End Do

  Stop
End Program Tests
```

11.10 Subroutine `LinearReg(X, Y, Yerr, [Func], Coef, Cerr, ChisqrV)`

11.10.1 Description

Given a set of points `X(:)` and `Y(:)`, this routine performs a linear fit to a set of functions defined by `Func`.

$$Y = \sum_i a_i f_i(X)$$

This routine also performs multi-dimensional fitting, in which case the points are specified as `X(:,:)`, where the first argument tells which point, and the second which variable.

11.10.2 Arguments

`X(:[,:])`: Real single or double precision one dimensional array (for a one dimensional fit) or two dimensional array (for a multidimensional fit). The independent variables. For a multidimensional fit, the first argument tells which point, and the second which variable. So the size of the array should be `X(Npoints,Ndim)`.

`Y(:)`: Real single or double precision one dimensional array. The dependent variable.

`Yerr(:[,:])`: Real single or double precision one or two dimensional array. If a one dimensional array is inserted, they are the errors of the points (if you don't have them, you should put all of them to some non-zero value). If a two dimensional array is given, it is treated as the correlation matrix.

`Func`: Optional. This routine define the functions to fit. An interface like this should be provided

```
Interface
```

```
   Function Func(Xx, i)

     USE NumTypes

     Real (kind=SP), Intent (in) :: Xx
     Integer, Intent (in) :: i
     Real (kind=SP) :: Func

   End Function Func
End Interface
```

if you want to perform a one dimensional fitting, and like this

```
Interface
   Function Func(Xx, i)

     USE NumTypes

     Real (kind=SP), Intent (in) :: Xx(:)
     Integer, Intent (in) :: i
     Real (kind=SP) :: Func

   End Function Func
End Interface
```

if it is a multidimensional fitting. Since you are making a fitting to a function of the type

$$Y = \sum_i a_i f_i(X)$$

the values $f_i(X)$ are given by this function as `Func(X, I)`. If the functions are not specified (i.e. you don't put this argument), a fit to a polynomial is made (this only work for one-dimensional fittings).

`Coef(:)`: Real single or double precision one dimensional array. The parameters that you want to determine.

`Cerr(:)`: Real single or double precision one dimensional array. The errors in the parameters.

`ChiSqr`: Real single or double precision. The χ^2 per degree of freedom of the fit.

11.10.3 Examples

Listing 11.10: Doing linear regressions.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics
```

```
6
   Integer, Parameter :: Nmax = 200, Npinta = 100, Npar = 4, Ndiv = 100
8  Real (kind=DP) :: X(Nmax), Y(Nmax), Yer(Nmax), &
        & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax,2), &
10      & Xmin, Xmax, h, Xac
   Integer :: Ntics(Ndiv)
12
   Interface
14    Function Fd(Xx, i)

16      USE NumTypes

18      Real (kind=DP), Intent (in) :: Xx(:)
        Integer, Intent (in) :: i
20      Real (kind=DP) :: Fd

22    End Function FD
   End Interface
24

26 CALL Random_Number(Xd)
   Xd(:,:) = 10.0_DP*(Xd(:,:) - 0.8_DP)
28
   CALL Normal(Yer, 0.0_DP, 1.0E-3_DP)
30 Y(:) = 12.34_DP*Xd(:,1)*sin(Xd(:,2)) - 2.23_DP + &
        & 0.67_DP*Xd(:,1)**2*Xd(:,2) + 0.23_DP*Xd(:,1) + Yer(:)
32

34 CALL LinearReg(Xd, Y, Yer, Fd, Coef, Cerr, Corr)

36 ! This should print the adjusted parameters,
   ! that have values: 12.34, -2.23, 0.67, 0.23
38 Do I = 1, Npar
      Write(*,'(2ES33.25)')Coef(I), Cerr(I)
40 End Do

42 ! This prints the ChiSqr, that should be very
   ! close to 1.
44 Write(*,'(1A,1ES33.25)') 'ChiSqr of the Fit: ', Corr

46
   Stop
48 End Program Tests

50 ! ***********************************
   ! *
52 Function Fd(X, i)
   ! *
54 ! ***********************************

56 USE NumTypes

58 Real (kind=DP), Intent (in) :: X(:)
```

```
  Integer, Intent (in) :: i
  Real (kind=DP) :: Fd

  If (I==1) Then
     Fd = 1.0_DP
  Else If (I==2) Then
     Fd = X(1)*sin(X(2))
  Else If (I==3) Then
     Fd = X(1)**2*X(2)
  Else If (I==4) Then
     Fd = X(1)
  End If

  Return
End Function FD
```

11.11 Subroutine NonLinearReg(X, Y, Yerr, Func, Coef, Cerr, ChisqrV)

11.11.1 Description

Given a set of points `X(:)` and `Y(:)`, this routine performs a non-linear fit to a set of functions defined by `Func`.

This routine also performs multi-dimensional fitting, in which case the points are specified as `X(:,:)`, where the first argument tells which point, and the second which variable.

This routine uses the Levenberg-Marquardt algorithm to perform the optimisation[1].

11.11.2 Arguments

`X(:[,:])`: Real single or double precision one dimensional array (for a one dimensional fit) or two dimensional array (for a multidimensional fit). The independent variables. For a multidimensional fit, the first argument tells which point, and the second which variable. So the size of the array should be `X(Npoints,Ndim)`.

`Y(:)`: Real single or double precision one dimensional array. The dependent variable.

`Yerr(:[,:])`: Real single or double precision one or two dimensional array. If a one dimensional array is inserted, they are the errors of the points (if you don't have them, you should put all of them to some non-zero value). If a two dimensional array is given, it is treated as the correlation matrix.

`Func`: This routine define the functions to fit. An interface like this should be provided

```
Interface
   Subroutine Func(X, Cf, Valf, ValD)

     USE NumTypes
```

[1] http://en.wikipedia.org/wiki/Levenberg-Marquardt_algorithm

```
      Real (kind=SP), Intent (in) :: X, Cf(:)
      Real (kind=SP), Intent (out) :: Valf, ValD(Size(Cf))

   End Subroutine Func
End Interface
```

if you want to perform a one dimensional fitting, and like this

```
Interface
   Subroutine Func(X, Cf, Valf, ValD)

     USE NumTypes

     Real (kind=SP), Intent (in) :: X(:), Cf(:)
     Real (kind=SP), Intent (out) :: Valf, ValD(Size(Cf))

   End Subroutine Func
End Interface
```

if it is a multidimensional fitting.

This routine returns the values of the function at X for some values of the parameters given in `Cf` in the variable `Valf`, and a vector with the derivatives (respect with the parameters) in `ValD`(:).

`Coef(:):` Real single or double precision one dimensional array. Output. The parameters that you want to determine.

`Cerr(:):` Real single or double precision one dimensional array. Outpue. The errors in the parameters.

`ChiSqr:` Real single or double precision. The χ^2 per degree of freedom of the fit.

11.11.3 Examples

In this example we will fit some generated data, with a Normal noise to the function

$$f(x_1, x_2; a, b) = \sin(ax_1) + bx_1x_2$$

We will generate the data with the values $a = 2.0$ and $b = 0.2$, so our fitting routine *should* return this values within errors.

The derivatives of the function (repect the parameters a and b), as well as the value of function are given by the user routine `Func`. The derivatives are:

$$\begin{aligned} \frac{\partial f(x_1, x_2; a, b)}{\partial a} &= x_1 \cos ax_1 \\ \frac{\partial f(x_1, x_2; a, b)}{\partial b} &= x_1x_2 \end{aligned}$$

Listing 11.11: Doing non linear regressions.

```
Program NLFit

  USE NumTypes
  USE Statistics

  Interface
     Subroutine Func(X, Cf, Valf, ValD)

       USE NumTypes

       Real (kind=DP), Intent (in) :: X(:), Cf(:)
       Real (kind=DP), Intent (out) :: Valf, ValD(Size(Cf))

     End Subroutine Func
  End Interface

  Integer, Parameter :: Np = 20, Ndim = 2
  Real (kind=DP) :: X(Np, Ndim), Y(Np), Ye(Np), Co(2), Vd(2), Ce(2), Ch

  ! First Fill the data
  CALL Random_Number(X)
  X = 2.0_DP*(X - 0.5_DP)
  Co(1) = 2.0_DP
  Co(2) = 0.2_DP
  CALL Normal(Ye, 0.0_DP, 0.5_DP)
  Do I = 1, Np
     CALL Func(X(I,:), Co, Y(I), Vd)
     Y(I) = Y(I) + Ye(I)
  End Do


  ! Now Perform the non linear fit
  Co = 1.0_DP
  CALL NonLinearReg(X, Y, Abs(Ye), Func, Co, Ce, Ch)
  Do I = 1, Npar
    Write(*,'(1A,100ES33.25)') 'Parameter and error: ', Co(I), Ce(I)
  End Do
  Write(*,'(1A,100ES33.25)')&
  & 'Chi Square per degree of freedom of the Fit: ', Ch


  Stop
End Program NLFit

Subroutine Func(X, Cf, Valf, ValD)

  USE NumTypes

  Real (kind=DP), Intent (in) :: X(:), Cf(:)
  Real (kind=DP), Intent (out) :: Valf, ValD(Size(Cf))

```

```
    Valf = Sin(Cf(1)*X(1)) + Cf(2)*X(1)*X(2)
53  ValD(1) = X(1)*Cos(Cf(1)*X(1))
    ValD(2) = X(1)*X(2)
55

57  End Subroutine Func
```

11.12 Subroutine `SetLuxLevel(Ilevel)`

11.12.1 Description

This function changes the behaviour of the "intrinsic" `Random_Number` subroutine. To call the intrinsic `FORTRAN 90` routine, you should set the Luxury level to zero. Other values makes the `Random_Number` subroutine use the Marsaglia and Zaman algorithm modified by M. Lüscher [4]. This part of the code has some inspiration in the `FORTRAN 90` implementation of Allan Miller. **Note:** This routine affects the way all the other routines that use pseudo random number generators works. That is to say, all the routines of this module that follow this one.

11.12.2 Arguments

`Ilevel`: Integer. Set the way the random number generator works. We have the following options:

- `Ilevel` = 0. The default intrinsic `FROTRAN 90` routine is used. This is usually considered a *bad*, non portable pseudo-random number generator, that you do not want to use when correlations are important.
- `Ilevel` = 1. This is the original Marsaglia and Zaman algorithm. Probably better than the intrinsic procedure, but still with large correlations.
- `Ilevel` = 2. The M. Lüscher modified version of the algorithm with $p = 48$. Still fail many tests, but a very good pseudo-number generator for many things.
- `Ilevel` = 3. The M. Lüscher modified version of the algorithm with $p = 97$. Theoretically still defective (fail the serial correlation test).
- `Ilevel` = 4. The M. Lüscher modified version of the algorithm with $p = 218$. Any theoretically possible correlation has a very small probability of being observed. A value very similar to this has been used for large scale high precision lattice gauge theory computations. This corresponds with the Lüscher recommended level 0.
- `Ilevel` = 5. The M. Lüscher modified version of the algorithm with $p = 404$. Good for anything you need the pseudo-random numbers (but cryptography, of course). It seems completely pointless to use values of p higher than this. This corresponds with the Lüscher recommended level 1. This is the **default value**.
- `Ilevel` = 6. The M. Lüscher modified version of the algorithm with $p = 794$. Good for anything you need the pseudo-random numbers (but cryptography, of course). Probably waste of computer resources. This corresponds with the Lüscher recommended level 2.
- Other values of `Ilevel` (> 24). Sets the value of p in the M. Lüscher modified version of the algorithm. Don't use it, unless you know what you are doing.

11.12.3 Examples

Listing 11.12: Setting the Luxury level of the pseudo random number generator.

```
Program Tests

  USE NumTypes
  USE Statistics

  Integer, Parameter :: NN = 70
  Real (kind=SP) :: rr(NN)

  CALL SetLuxLevel(5)
  CALL Random_Number(rr)
  Write(*,*) rr


  Stop
End Program Tests
```

11.13 Subroutine PutLuxSeed([ISeed(25)])

11.13.1 Description

Restarts the position in the Luxury pseudo-random number generator.

11.13.2 Arguments

ISeed(25): Integer one dimensional array of 25 elements. Optional. If present, restarts the generator from an output of GetLuxSeed. If not present, initialises the random number generator.

11.13.3 Examples

Listing 11.13: Using a previously saved point in the generating process.

```
Program Tests

  USE NumTypes
  USE Statistics

  Integer, Parameter :: NN = 70
  Real (kind=SP) :: rr(NN)
  Integer :: Sd(25)


  Open(Unit=69, File="seed.dat")
  Read(69,*)Sd
  CALL PutLuxSeed(Sd)
  CALL Random_Number(rr)
  Write(*,*) rr
```

```
17
  Stop
19 End Program Tests
```

11.14 Subroutine GetLuxSeed(ISeed(25))

11.14.1 Description

Saves the position in the Luxury pseudo-random number generator.

11.14.2 Arguments

ISeed(25): Integer one dimensional array of 25 elements. Saves the position in the random number generator.

11.14.3 Examples

Listing 11.14: Saving a point in the generating process.

```
1  Program Tests

3    USE NumTypes
     USE Statistics
5
     Integer, Parameter :: NN = 70
7    Real (kind=SP) :: rr(NN)
     Integer :: Sd(25)
9


11   CALL Random_Number(rr)
     CALL GetLuxSeed(Sd)
13   Open(Unit=69, File="seed.dat")
     Write(69,*)Sd
15


17   Stop
End Program Tests
```

11.15 Subroutine Normal(X, [Rm], [Rsig])

11.15.1 Description

Fills X(:) with numbers from a normal distribution with mean Rm, and standard deviation Rsig. The parameters Rm and Rsig are optional. If they are not given the mean will be 0, and the standard deviation 1.

11.15.2 Arguments

X(:): Real (Single or Double precision) one dimensional array. A vector that will be filled with numbers according to the normal distribution.

Rm: Real (Single or Double precision), Optional. The mean of the normal distribution. If not present the default value is 0.

Rsig: Real (Single or Double precision), Optional. The standard deviation of the normal distribution. If not present the default value is 1.

11.15.3 Examples

Listing 11.15: Obtaining numbers with a normal distribution.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 100
  Real (kind=DP) :: X(Nmax)


  CALL Normal(X, 1.23_DP, 0.345_DP)
  ! Now compute the mean and standard deviation of the data
  Write(*,*) 'We should obtain 1.23 and 0.345: '
  Write(*, '(ES33.25)')Mean(X), Stddev(X)


  Stop
End Program Tests
```

11.16 Subroutine Levy(X, α, [β], [c], [μ])

11.16.1 Description

Fills X(:) with numbers from a Levy stable distribution with mean μ, scale c and exponent α. The probability distribution is defined via

$$\rho(x) = \frac{1}{\pi}\Re\int_{-\infty}^{+\infty} dt \exp\left\{-\imath t(x-\mu) - c|t|^{\alpha}\left[1 + \imath\frac{t\beta}{|t|}\tan\left(\frac{\pi\alpha}{2}\right)\right]\right\} \tag{11.1}$$

For $\alpha = 1$ the distribution reduces to the Cauchy distribution. For $\alpha = 2$ it is a Gaussian distribution with $\sigma = \sqrt{2}c$ and mean μ.

The algorithm only works for $0 < \alpha \leq 2$.

11.16.2 Arguments

X(:): Real (Single or Double precision) one dimensional array. A vector that will be filled with numbers according to the normal distribution.

α: Real (Single or Double precision). The characteristic exponent (or Levy index).

β: Real (Single or Double precision), Optional. The skewness parameter.

c: Real (Single or Double precision), Optional. The scale factor.

μ: Real (Single or Double precision), Optional. The translation factor.

11.16.3 Examples

Listing 11.16: Obtaining numbers with a Levy skew stable distribution.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 100
  Real (kind=DP) :: X(Nmax)


  CALL Levy(X, 1.23_DP)
  ! Now compute the mean and standard deviation of the data
  Write(*,*) 'We should obtain 0.0 and something without sense!: '
  Write(*, '(ES33.25)')Mean(X), Stddev(X)


  Stop
End Program Tests
```

11.17 Subroutine FishTipp(X, Rm, Rb)

11.17.1 Description

Fills X(:) with numbers from a Fisher-Tippet distribution with parameters[2] Rm, and 2Rb[2].

11.17.2 Arguments

X(:): Real (Single or Double precision) one dimensional array. A vector that will be filled with numbers according to the normal distribution.

Rm: Real (Single or Double precision).

Rb: Real (Single or Double precision).

[2] More info about this distribution in the Wikipedia: http://en.wikipedia.org/wiki/Fisher-Tippett_distribution

11.17.3 Examples

Listing 11.17: Obtaining numbers with a Fisher-Tippet distribution.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 100
  Real (kind=DP) :: X(Nmax)


  CALL FishTipp(X, 2.00_DP, 1.00_DP)
  ! Now compute the mean and standard deviation of the data
  Write(*,*) 'We should obtain 2.57721... and 1.2782...: '
  Write(*, '(ES33.25)')Mean(X), Stddev(X)


  Stop
End Program Tests
```

11.18 Subroutine Laplace(X, Rm, Rb)

11.18.1 Description

Fills `X(:)` with numbers from a Laplace distribution with mean `Rm`, and variance $2\texttt{Rb}^2$.

11.18.2 Arguments

`X(:)`: Real (Single or Double precision) one dimensional array. A vector that will be filled with numbers according to the Laplace distribution.

`Rm`: Real (Single or Double precision). The mean of the Laplace distribution.

`Rb`: Real (Single or Double precision). The width of the Laplace distribution (i.e. The variance is $2\texttt{Rb}^2$).

11.18.3 Examples

Listing 11.18: Obtaining numbers with a Laplace distribution.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 100
  Real (kind=DP) :: X(Nmax)
```

```
10
   CALL Laplace(X, 1.23_DP, 1.0_DP)
12 ! Now compute the mean and standard deviation of the data
   Write(*,*) 'We should obtain 1.23 and sqrt(2): '
14 Write(*,'(ES33.25)')Mean(X), Stddev(X)

16
   Stop
18 End Program Tests
```

11.19 Subroutine/Function `Irand([Irnd], N, M)`

11.19.1 Description

If present, fills `Irnd(:)` with random integer numbers between `N` and `M` with an uniform distribution. If `Irnd(:)` is not present returns a integer random number between `N` and `M`.

11.19.2 Arguments

`Irnd(:)`: Integer, Optional. A vector that will be filled with integer numbers according to a uniform distribution.

`N`: Integer. The minimum number that we can obtain.

`M`: Integer. The maximum number that we can obtain.

11.19.3 Examples

Listing 11.19: Obtaining integer random numbers.

```
Program Tests
2
   USE NumTypes
4  USE Error
   USE Statistics
6
   Integer, Parameter :: Nmax = 100
8  Integer :: Irnd(Nmax)

10
   CALL Irand(Irnd, 0, 1)
12 ! Now compute the mean
   Write(*,*) 'We should obtain 0.5: '
14 Write(*,'(ES33.25)')Mean(Real(Irnd(:),kind=DP))

16
   Stop
18 End Program Tests
```

11.20 Subroutine Permutation(Idx)

11.20.1 Description

Returns a random permutation of N elements. It uses the Knuth shuffle algorithm[3].

11.20.2 Arguments

Idx(:): Integer one dimensional array. Output. The random permutation.

Listing 11.20: Obtaining a permutation.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 10
  Integer :: Id(Nmax)


  CALL Permutation(Id)
  Write(*,'(100I3)')(Id(I), I = 1, Nmax)

  Stop

End Program Tests
```

11.21 Subroutine BootStrap(Ibt)

11.21.1 Description

Generates N_b bootstrap sequence of N numbers each. These bootstraps are returned in the two dimensional integer array Ibt(:,:) of size $N \times N_b$.

11.21.2 Arguments

Ibt(:): Integer. A two dimensional array of size $N \times N_b$, where N_b is the number of bootstraps, and N is the range of each bootstrap.

11.21.3 Examples

Listing 11.21: Resampling some data.

```
Program Tests

  USE NumTypes
  USE Error
```

[3] http://en.wikipedia.org/wiki/Knuth_shuffle

```
  USE Statistics
6
  Integer, Parameter :: Nmax = 8, Nbt = 5
8 Real (kind=DP) :: X(Nmax)
  Integer :: Ib(Nmax, Nbt), I, J
10


12 CALL Random_Number(X)
  ! Generate 5 bootstraps
14 CALL BootStrap(Ib)

16 ! Write the original sample, and the bootstraps
  Write(*,'(1000ES33.25)')(X(J), J=1, Nmax)
18 Do I = 1, Nbt
     Write(*,'(1000ES33.25)')(X(Ib(J)), J=1, Nmax)
20 End Do

22 Stop
End Program Tests
```

11.22 Subroutine SaveBstrp(Ibt, Filename)

11.22.1 Description

Saves the bootstrap stored in `Ibt` and saves it in the file `Filename`.

11.22.2 Arguments

`Ibt(:)`: Integer. A two dimensional array of size $N \times N_b$, where N_b is the number of bootstraps, and N is the range of each bootstrap.

`Filename`: Character (len=*). A file name to save the resampling data.

11.22.3 Examples

Listing 11.22: Reading the resampling info.

```
1 Program Tests

3   USE NumTypes
    USE Error
5   USE Statistics

7   Integer, Parameter :: Nmax = 8, Nbt = 5
    Integer :: Ib(Nmax, Nbt)
9


11  ! Generate 5 bootstraps
    CALL BootStrap(Ib)
13

    ! Save it
```

```
15    SaveBstrp(Ibt, 'example.bst')

17    Stop
End Program Tests
```

11.23 Subroutine ReadBstrp(Ibt, Filename)

11.23.1 Description

Reads the bootstrap stored in the file `Filename`, and returns it in `Ibt`.

11.23.2 Arguments

`Ibt(:)`: Integer. A two dimensional array of size $\mathtt{N} \times \mathtt{N_b}$, where $\mathtt{N_b}$ is the number of bootstraps, and `N` is the range of each bootstrap.

`Filename`: Character (len=*). A file name to read the resampling data.

11.23.3 Examples

Listing 11.23: Saving the resampling info.

```
Program Tests
2
  USE NumTypes
4 USE Error
  USE Statistics
6
  Integer, Parameter :: Nmax = 8, Nbt = 5
8 Integer :: Ib(Nmax, Nbt)

10

  ! Read a saved Bootstrap.
12 ReadBstrp(Ibt, 'example.bst')

14  Stop
End Program Tests
```

11.24 Subroutine EstBstrp(Data, Ibt, Func, Val, Err[, Rest])

11.24.1 Description

Estimates using the Bootstrap method the average and error of an estimator given as a user supplied function.

11.24.2 Arguments

`Data(:)`: Double precision Real. A one dimensional array with the original sampling.

`ibt(:,:)`: Integer two dimensional array. The bootstrap that we want to use to make the estimation.

`Func`: A user suplied function that returns the value of the estimator. An interface block of the following type should be defined.

```
Interface
   Function Func(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP) :: Func

   End Function Func
End Interface
```

`Val`: Double precision real. Output. The value of the estimation of the parameter.

`Err`: Double precision real. Output. An estimation of the error in the estimation of the parameter.

`Rest`: Double precision real one dimensional array (same dimension as the number of bootstraps in `Ibt`). Output. The value of the estimator for each resampling.

11.24.3 Examples

Listing 11.24: Estimating the average.

```
1  Program Tests
2
3    USE NumTypes
4    USE Error
5    USE Statistics
6
7    Integer, Parameter :: Nmax = 100, Nbt = 50
8    Integer :: Ib(Nmax, Nbt)
9    Real (kind=DP) :: Avg, Err, Data(Nmax), Rest(Nbt)
10
11   Interface
12      Function F(X)
13        USE NumTypes
14
15        Real (kind=DP), Intent (in) :: X(:)
16        Real (kind=DP) :: F
17
18      End Function F
19   End Interface
```

```
21    ! Read a saved Bootstrap, and the data from a file
      ReadBstrp(Ibt, 'example.bst')
23    Open (Unit=22, File="data.dat")
      Read(22,*)Data
25    Close(22)

27    ! And estimate the average
      CALL EstBstrp(Data, Ibt, F, Avg, Err, Rest)
29
      ! Print the Average of each resampling
31    Do I = 1, Nbt
        Write(*,*)I, Rest(I)
33    End Do

35    Stop
End Program Tests
37
Function F(X)
39    USE NumTypes
      USE Statistics
41


43    Real (kind=DP), Intent (in) :: X(:)
      Real (kind=DP) :: F
45
      F = Mean(X)
47
End Function F
```

11.25 Subroutine BstrpConfInt(Data, Ibt, alpha, Func, dmin, dpls))

11.25.1 Description

Gives an Confidence interval for the estimator given as the user supplied function `Func`, such that

$$\mathcal{P}(dmin < Func(Data) < dpls) = 1 - 2\alpha$$

11.25.2 Arguments

`Data(:)`: Double precision Real. A one dimensional array with the original sampling.

`ibt(:,:)`: Integer two dimensional array. The bootstrap that we want to use to make the estimation.

`alpha`: Double precision real. The level of the confidence interval.

`Func`: A user suplied function that returns the value of the estimator. An interface block of the following type should be defined.

```
Interface
   Function Func(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP) :: Func

   End Function Func
End Interface
```

dmin: Double precision real. Output. The lower limit of the confidence interval.

dpls: Double precision real. Output. The higher limit of the confidence interval.

11.25.3 Examples

Listing 11.25: Giving a confidence interval.

```
Program Tests

  USE NumTypes
  USE Error
  USE Statistics

  Integer, Parameter :: Nmax = 1000, Nb = 10000, Ndiv = 50
  Real (kind=DP) :: Rdata(Nmax), Rmean(Nb), avg, Xmin, Xmax, h, Xac,&
       & err, dmin, dpls
  Integer :: Id(Nmax), Ib(Nb, Nmax), Ntics(Ndiv)

  Interface
     Function F(X)
       USE NumTypes

       Real (kind=DP), Intent (in) :: X(:)
       Real (kind=DP) :: F

     End Function F
  End Interface

  CALL Normal(Rdata)

  avg = Mean(Rdata)
  ! Now create the resamples
  CALL Bootstrap(Ib)

  CALL EstBstrp(Rdata, Ib, F, avg, Err, Rmean)
  Write(*,*) '#', avg, Err, Mean(Rdata)

  CALL BstrpConfInt(Rdata, Ib, 0.1_DP, F, dmin, dpls)
  Write(*,*) 'Intervalo:', dmin, dpls
  Write(*,*)Avg - Dmin, Dpls - Avg
  Write(*,*)(dpls - dmin)/2.0_DP, 1.64485_DP/Sqrt(Real(Nmax,kind=DP))
```

```
35
  Stop
37
End Program Tests
39
Function F(X)
41  USE NumTypes
  USE Statistics
43
  Real (kind=DP), Intent (in) :: X(:)
45  Real (kind=DP) :: F

47  F = Mean(X)

49  Return
End Function F
```

11.26 Function Prop_Error(X, Dx, Func[, N])

11.26.1 Description

Being `Func` a function of one or several variables, and `X` a point known with accuracy given by `Dx`, this routine propagate the errors in the position of the point, to obtain the accuracy of `F(X)`.

11.26.2 Arguments

`X[(:)]`: Double (DP) or simple (SP) precision one dimensional array or number. The value(s) of the variables.

`Dx[(:)]`: Double (DP) or simple (SP) precision one dimensional array or number. The value(s) of the error in the variables.

`Func`: A user supplied function. The function of the variables whose errors you want to propagate. An interface block of the following type should be defined.

```
Interface
   Function Func(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP) :: Func

   End Function Func
End Interface
```

`N`: Integer, Optional. The number of samples used to propagate the error. The default value is 1000.

11.26.3 Output

A real double or simple precision (same type as the input). An stimate of the accuracy of the value `F(X)`.

11.26.4 Examples

Here we compare our method of propagating errors, with the traditional propagation of errors formula for the case of the function $f(x, y) = x^2 + y^2$.

Listing 11.26: Propagating errors in a function.

```
Program Tests

  USE NumTypes
  USE Statistics

  Real (kind=DP) :: Xm(2), Em(2)

  Interface
     Function F2(X)
       USE NumTypes
       Real (kind=DP), Intent (in) :: X(:)
       Real (kind=DP) :: F2
     End Function F2
  End Interface


  Xm(1) = 1.23_DP
  Xm(2) = 1.62_DP
  Em(1) = 0.02_DP
  Em(2) = 0.03_DP
  Write(*,*) 'Value of the function at Xm: ', F2(Xm)
  Write(*,*) '  Error estimate:            ', Prop_Error(Xm, Em, F2)
  Write(*,*) '  Error estimate by hand:    ', &
       & Sqrt((Em(1)/Xm(1))**2 + (Em(2)/Xm(2))**2)*F2(Xm)

  Stop
End Program Tests


Function F2(X)
  USE NumTypes

  Real (kind=DP), Intent (in) :: X(:)
  Real (kind=DP) :: F2

  F2 = X(1)**2 + X(2)**2

  Return
End Function F2
```

11.27 Subroutine MCIntegration(X1, X2, Func, Val, Err[, Tol])

11.27.1 Description

Uses the Monte Carlo method to stimate the value of the integral of the several variables function `Func` between the limits (`X1(1)`, `X1(2)`, ..., `X1(Ndim)`) and (`X2(1)`, `X2(2)`, ..., `X2(Ndim)`). The value of the integral is returned in `Val`, and an estimation of the error in `Err`. The desired precision can be introduced via the optional argument `Tol`.

11.27.2 Arguments

`X1(:)`: Double or simple precision Real. A one dimensional array with the lower limits of the integrals.

`X2(:)`: Double or simple precision Real. A one dimensional array with the upper limits of the integrals.

`Func`: A user suplied function that returns the value of the function to integrate. An interface block of the following type should be defined.

```
Interface
   Function Func(X)
     USE NumTypes

     Real (kind=DP), Intent (in) :: X(:)
     Real (kind=DP) :: Func

   End Function Func
End Interface
```

`Val`: Double or simple precision real (same as input). Output. An estimation of the value of the integral.

`Err`: Double or simple precision real (same as input). Output. An estimation of the error.

`Tol`: Double or simple precision real. Optional. An estimation of the desired precision.

11.27.3 Examples

Listing 11.27: Integrating a two dimensional function.

```
1 MODULE ExtData

3   USE NumTypes

5   Real (kind=DP) :: Sig = 2.345763450_DP
    Real (kind=DP) :: X1 = -0.324563562345643650_DP, X2 = 1.623473_DP, &
7        & Y1 = 1.34764574570_DP, Y2 = 5.3476347634_DP
```

```
9
End MODULE ExtData
11
Program MonteCarlo
13
  USE NumTypes
15  USE Error
  USE Statistics
17
  USE ExtData
19

21  IMPLICIT NONE

23  Real (kind=DP) :: Res, Err

25  Interface
     Function F(X)
27      USE NumTypes

29      Real (kind=DP), Intent (in) :: X(:)
        Real (kind=DP) :: F
31    End Function F
  End Interface
33
  CALL MCintegration((/X1,Y1/), (/X2,Y2/), F, Res, Err, 1.0E-4_DP)
35  Write(*,'(1A,100ES33.25)')'# Value of the integral: ', Res, Err

37
  Stop
39 End Program Monte

41
Function F(X)
43
  USE NumTypes
45  USE ExtData

47  Real (kind=DP), Intent (in) :: X(:)
  Real (kind=DP) :: F
49

51  F = exp(-1.0_DP/(2.0_DP*Sig**2) * (Sum(X(:)**2)))*Sin(X(1)*X(2))

53  Return
End Function F
```

Twelve

MODULE Polynomial

This is the documentation of the `MODULE Polynomial`, a set of `FORTRAN 90` routines to work with polynomials. This module make use of the `MODULE NumTypes`, `MODULE Constants`, `MODULE Error` and `MODULE Linear` so please read the documentation of these modules *before* reading this.

12.1 Type Pol

12.1.1 Description

A new data type `Pol` is defined to work with polynomials. This type has two components: The coefficients of the polynomial, and the degree.

12.1.2 Components

`Coef(:):` Real double precision one dimensional array.

`dg:` Integer. The degree of the polynomial.

12.1.3 Examples

A small example showing how to define a polynomial.

Listing 12.1: Defining a polynomial.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Type (Pol) :: P1

  Stop
End Program TestPoly
```

12.2 Type CmplxPol

12.2.1 Description

A new data type `CmplxPol` is defined to work with complex polynomials. This type has two components: The coefficients of the polynomial, and the degree.

All the routines, operators, etc... defined in this module works for complex as well as for real polynomials.

12.2.2 Components

`Coef(:):` Complex double precision one dimensional array.

`dg:` Integer. The degree of the polynomial.

12.2.3 Examples

A small example showing how to define a polynomial of complex coefficients.

Listing 12.2: Defining a polynomial.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Type (CmplxPol) :: P1

  Stop
End Program TestPoly
```

12.3 Assignment

12.3.1 Description

You can directly assign one defined polynomial (complex or real) to another, or to an array of real numbers, that are interpreted as the coefficients.

12.3.2 Examples

Listing 12.3: Assigning polynomials.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Integer, Parameter :: Deg = 4
  Real (kind=DP) :: Hcoef(Deg+1)
```

```
  Type (Pol) :: Hermite4

  ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(1) =  3.0_DP
  Hcoef(3) = -6.0_DP
  Hcoef(5) =  1.0_DP

  Hermite4 = Hcoef

  ! Now Show what we have in our data type:
  Do I = 0, Hermite4%dg
     Write(*,'(1I5,ES33.25)')I, Hermite4%Coef(I)
  End Do

  Stop
End Program TestPoly
```

12.4 Operator +

12.4.1 Description

You can naturally sum `Pol` or `CmplxPol` data types.

12.4.2 Examples

Listing 12.4: Adding polynomials.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Integer, Parameter :: Deg = 4
  Real (kind=DP) :: Hcoef(Deg+1)
  Type (Pol) :: Hermite4, Hermite3, Sum

  ! The Third Hermite polynomial is x^3 - 3x, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(2) = -3.0_DP
  Hcoef(4) =  1.0_DP

  Hermite3 = Hcoef(1:4)

  ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(1) =  3.0_DP
```

```
  Hcoef(3) = -6.0_DP
  Hcoef(5) =  1.0_DP

  Hermite4 = Hcoef

  ! Now Add the two polynomials, and show the result.
  Sum = Hermite3 + Hermite4
  Do I = 0, Sum%dg
     Write(*,'(1I5,ES33.25)')I, Sum%Coef(I)
  End Do

  Stop
End Program TestPoly
```

12.5 Operator -

12.5.1 Description

You can subtract `Pol` or `CmplxPol` data types.

12.5.2 Examples

Listing 12.5: Substracting polynomials.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Integer, Parameter :: Deg = 4
  Real (kind=DP) :: Hcoef(Deg+1)
  Type (Pol) :: Hermite4, Hermite3, Sum

  ! The Third Hermite polynomial is x^3 - 3x, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(2) = -3.0_DP
  Hcoef(4) =  1.0_DP

  Hermite3 = Hcoef(1:4)

  ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(1) =  3.0_DP
  Hcoef(3) = -6.0_DP
  Hcoef(5) =  1.0_DP

  Hermite4 = Hcoef

```

```
  ! Now Subtract the two polynomials, and show the result.
  Sum = Hermite3 - Hermite4
  Do I = 0, Sum%dg
     Write(*,'(1I5,ES33.25)')I, Sum%Coef(I)
  End Do

  Stop
End Program TestPoly
```

12.6 Operator *

12.6.1 Description

You can naturally multiply `Pol` data types, `Pol` data types with double precision real numbers, `CmplxPol` data types and `CmplxPol` data types with real or complex numbers.

12.6.2 Examples

Listing 12.6: Computing the product of two polynomials.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Integer, Parameter :: Deg = 4
  Real (kind=DP) :: Hcoef(Deg+1)
  Type (Pol) :: Hermite4, Hermite3, Sum

  ! The Third Hermite polynomial is x^3 - 3x, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(2) = -3.0_DP
  Hcoef(4) =  1.0_DP

  Hermite3 = Hcoef(1:4)

  ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(1) =  3.0_DP
  Hcoef(3) = -6.0_DP
  Hcoef(5) =  1.0_DP

  Hermite4 = Hcoef

  ! Now multiply the two polynomials, and show the result.
  Sum = Hermite3 * Hermite4
  Do I = 0, Sum%dg
     Write(*,'(1I5,ES33.25)')I, Sum%Coef(I)
```

```
  End Do

  Stop
End Program TestPoly
```

12.7 Subroutine Init(P, Dgr)

12.7.1 Description

Allocate memory space for the coefficients of a Pol or a CmplxPol type.

12.7.2 Arguments

P: Type Pol or CmplxPol. The polynomial that you want to allocate space for.

Dgr: Integer. The degree of the polynomial.

12.7.3 Examples

Listing 12.7: Initialising a polynomial data type.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Integer, Parameter :: Deg = 4
  Real (kind=DP) :: Hcoef(Deg+1)
  Type (Pol) :: Hermite4, Hermite3, Sum


  ! An alternative way of setting the third Hermite
  ! polynomial.
  CALL Init(Hermite3, 3)
  Hermite3%Coef(0) =  0.0_DP
  Hermite3%Coef(1) = -3.0_DP
  Hermite3%Coef(2) =  0.0_DP
  Hermite3%Coef(3) =  1.0_DP
  Hermite3%dg = 3


  Stop
End Program TestPoly
```

12.8 Function Degree(P)

12.8.1 Description

Returns the degree of the polynomial P.

12.8.2 Arguments

P: Type Pol or CmplxPol. The polynomial whose degree we want to know.

12.8.3 Output

Integer. The degree of the polynomial P.

12.8.4 Examples

Listing 12.8: Returns the degree of a polynomial.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Integer, Parameter :: Deg = 4
  Real (kind=DP) :: Hcoef(Deg+1), X
  Type (Pol) :: Hermite4, Hermite3, Sum

  ! The Third Hermite polynomial is x^3 - 3x, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(2) = -3.0_DP
  Hcoef(4) =  1.0_DP

  Hermite3 = Hcoef(1:4)

  ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(1) =  3.0_DP
  Hcoef(3) = -6.0_DP
  Hcoef(5) =  1.0_DP

  Hermite4 = Hcoef

  ! Now Mutiply the two polynomials, and show the result.
  Sum = Hermite3 * Hermite4

  ! Show the degree of the product. It should be 4+3=7.
  Write(*,*)Degree(Sum)


  Stop
End Program TestPoly
```

12.9 Function Value(P, X)

12.9.1 Description

Computes the value of the polynomial P in the point X.

12.9.2 Arguments

P: Type Pol or CmplxPol. The polynomial.

X: Real double precision if P is of type Pol and Complex double precision if P is CmplxPol. The point in which you want to compute the value.

12.9.3 Output

Real double precision. The value of the polynomial P in the point X.

12.9.4 Examples

Listing 12.9: Computes the values of a polynomial at some points.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Integer, Parameter :: Deg = 4
  Real (kind=DP) :: Hcoef(Deg+1), X
  Type (Pol) :: Hermite4, Hermite3, Sum

  ! The Third Hermite polynomial is x^3 - 3x, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(2) = -3.0_DP
  Hcoef(4) =  1.0_DP

  Hermite3 = Hcoef(1:4)

  ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(1) =  3.0_DP
  Hcoef(3) = -6.0_DP
  Hcoef(5) =  1.0_DP

  Hermite4 = Hcoef

  ! Now Mutiply the two polynomials, and show the result.
  Sum = Hermite3 * Hermite4

  ! Compute the valuye of the product in some point in two
```

```
  ! different ways.
  X = 9.34564_DP
  Write(*,'(ES33.25)')Value(Sum, X)
  Write(*,'(ES33.25)')Value(Hermite3, X)*Value(Hermite4, X)


  Stop
End Program TestPoly
```

12.10 Function Deriv(P)

12.10.1 Description

Computes the derivative of the polynomial P.

12.10.2 Arguments

P: Type Pol or CmplxPol. The polynomial whose derivative we want to compute.

12.10.3 Output

Type Pol. Another polynomial: the derivative of P.

12.10.4 Examples

Listing 12.10: Computing the derivative of a polynomial.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Integer, Parameter :: Deg = 4
  Real (kind=DP) :: Hcoef(Deg+1), X
  Type (Pol) :: Hermite4, Hermite3, Res, Sum

  ! The Third Hermite polynomial is x^3 - 3x, so
  ! we first assign the values of the coefficients.
  Hcoef   =  0.0_DP
  Hcoef(2) = -3.0_DP
  Hcoef(4) =  1.0_DP

  Hermite3 = Hcoef(1:4)

  ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
  ! we first assign the values of the coefficients.
  Hcoef   =  0.0_DP
  Hcoef(1) =  3.0_DP
  Hcoef(3) = -6.0_DP
  Hcoef(5) =  1.0_DP
```

```
25
   Hermite4 = Hcoef
27
   ! Now compute the derivative of Hermite4
29 Res = Deriv(Hermite4)

31 ! From the recursion relation of the Hermite polynomials
   ! we should obtain twwice the same number:
33 X = 7.346582_DP
   Write(*,'(ES33.25)')Value(Res, X)
35 Write(*,'(ES33.25)')4.0_DP*Value(Hermite3, X)

37
   Stop
39 End Program TestPoly
```

12.11 Function Integra(P[, Cte])

12.11.1 Description

Computes the integral of the polynomial `P`. If `Cte` is present then it is used as *integration constant*.

12.11.2 Arguments

`P`: Type `Pol` or `CmplxPol`. The polynomial whose integral we want to compute.

`Cte`: Optional. Real double precision if `P` is of type `Pol` and Complex double precision if `P` is `CmplxPol`. If not present, the default value is 0.

12.11.3 Output

Type `Pol`. Another polynomial: the integral of `P`.

12.11.4 Examples

Listing 12.11: Computing the integral of a polynomial.

```
1  Program TestPoly

3    USE NumTypes
     USE Error
5    USE Polynomial

7    Integer, Parameter :: Deg = 4
     Real (kind=DP) :: Hcoef(Deg+1), X
9    Type (Pol) :: Hermite4, Hermite3, Res, Sum

11   ! The Third Hermite polynomial is x^3 - 3x, so
     ! we first assign the values of the coefficients.
13   Hcoef    =  0.0_DP
```

```
  Hcoef(2) = -3.0_DP
  Hcoef(4) =  1.0_DP

  Hermite3 = Hcoef(1:4)

  ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
  ! we first assign the values of the coefficients.
  Hcoef    =  0.0_DP
  Hcoef(1) =  3.0_DP
  Hcoef(3) = -6.0_DP
  Hcoef(5) =  1.0_DP

  Hermite4 = Hcoef

  ! Now compute the derivative of Hermite4
  Res = Integra(Hermite3, 3.0_DP/4.0_DP)

  ! From the recursion relation of the Hermite polynomials
  ! we should obtain twwice the same number:
  X = 7.346582_DP
  Write(*,'(ES33.25)')Value(Res, X)
  Write(*,'(ES33.25)')0.25_DP*Value(Hermite4, X)


  Stop
End Program TestPoly
```

12.12 Function InterpolValue(X, Y, Xo)

12.12.1 Description

Computes the value of the interpolation polynomial that pass trough (X(:), Y(:)) in the point Xo.

12.12.2 Arguments

X(:), Y(:): Real double precision or Complex double precision one dimensional arrays. Specify the points at which the interpolation polynomial should pass.

Xo: Same type as X(:) and Y(.). The point at which you want to compute the interpolation polynomial.

12.12.3 Output

Real double precision if input is real and complex double precision if input is complex. The value of the interpolation polynomial in Xo.

12.12.4 Examples

Listing 12.12: Compute values of the Interpolation polynomial.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial

  Integer, Parameter :: Deg = 4, Np = 7
  Real (kind=DP) :: Hcoef(Deg+1), X, Xp(Np), Yp(Np)
  Type (Pol) :: Hermite4, Hermite3, Res, Sum


  CALL Random_Number(Xp)
  Yp = 3.347234_DP*Xp - 2.475875_DP*Xp**3 - 7.23467_DP*Xp**4 + &
       & 1.47854_DP*Xp**6

  ! Now we compute the value of the interpolation polynomial
  ! at X, and compare it with the real value of the Polynomial
  X = -1.23899843_DP
  Write(*,'(ES33.25)')InterpolValue(Xp, Yp, X)
  Write(*,'(ES33.25)')3.347234_DP*X - 2.475875_DP*X**3 - &
       & 7.23467_DP*X**4 + 1.47854_DP*X**6


  Stop
End Program TestPoly
```

12.13 Function `Interpol(X, Y)`

Computes the interpolation polynomial that pass trough `(X(:), Y(:))`. **Note that using this function can be very unstable**.

12.13.1 Arguments

`X(:), Y(:)`: Real double precision or Complex double precision one dimensional arrays. Specify the points at which the interpolation polynomial should pass.

12.13.2 Output

Type `Pol` if input is real, and `CmplxPol` if input is complex. The interpolation polynomial.

12.13.3 Examples

Listing 12.13: Computes the interpolation polynomial.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial
```

```
  Integer, Parameter :: Deg = 4, Np = 7
  Real (kind=DP) :: Hcoef(Deg+1), X, Xp(Np), Yp(Np)
  Type (Pol) :: Hermite4, Hermite3, Res, Sum


  CALL Random_Number(Xp)
  Yp = 3.347234_DP*Xp - 2.475875_DP*Xp**3 - 7.23467_DP*Xp**4 + &
       & 1.47854_DP*Xp**6

  ! Now we compute the interpolation polynomial
  ! at X, and compare it with the real value of the Polynomial
  X = -1.23899843_DP
  Res = Interpol(Xp,Yp)
  Write(*,'(ES33.25)')Value(Res, X)
  Write(*,'(ES33.25)')3.347234_DP*X - 2.475875_DP*X**3 - &
       & 7.23467_DP*X**4 + 1.47854_DP*X**6


  Stop
End Program TestPoly
```

12.14 Subroutine Spline(X, Y, Ypp0, YppN, Pols)

12.14.1 Description

Compute the cubic spline interpolation polynomial that pass trough `(X(:), Y(:))`.

12.14.2 Arguments

`X(:), Y(:)`: Real double precision one dimensional arrays. Specify the points at which the cubic spline interpolation polynomial should pass.

`Ypp0, YppN`: The values of the second derivatives of the cubic spline interpolation polynomial in the first and last points.

`Pols(:)`: Type `Pol` one dimensional array. Returns the `N-1` cubic interpolation polynomials.

12.14.3 Examples

Listing 12.14: Computes the cubic spline interpolation polynomial.

```
Program TestPoly

  USE NumTypes
  USE Error
  USE Polynomial
  USE NonNumeric

  Integer, Parameter :: Deg = 4, Np = 7
  Real (kind=DP) :: Hcoef(Deg+1), X, Xp(Np), Yp(Np)
```

```
10    Type (Pol) :: Hermite4, Hermite3, Res, Sum, Spl(Np-1)

12

      CALL Random_Number(Xp)
14    ! Order Xp
      CALL Qsort(Xp)
16    Yp = 3.347234_DP*Xp - 2.475875_DP*Xp**3 - 7.23467_DP*Xp**4 + &
          & 1.47854_DP*Xp**6
18
      ! Now we compute the interpolation polynomial
20    ! at X, and compare it with the real value of the Polynomial, and
      ! the value of the spline cubic interpolation polynomial.
22    X = 0.23899843_DP
      Res = Interpol(Xp,Yp)
24    CALL Spline(Xp, Yp, 0.0_DP, 0.0_DP, Spl)
      Write(*,'(ES33.25)')Value(Res, X)
26    Write(*,'(ES33.25)')Value(Spl(Locate(Xp, X)), X)
      Write(*,'(ES33.25)')3.347234_DP*X - 2.475875_DP*X**3 - &
28        & 7.23467_DP*X**4 + 1.47854_DP*X**6

30

      Stop
32  End Program TestPoly
```

Thirteen

MODULE Root

This is the documentation of the MODULE Root, a set of FORTRAN 90 routines to compute roots of functions. This module make use of the MODULE NumTypes, MODULE Constants and MODULE Error so please read the documentation of these modules *before* reading this.

13.1 Subroutine RootPol(a, b, [c, d], z1, z2, [z3, z4])

13.1.1 Description

Returns the complex roots of a polynomial of degree 2, 3 or 4.

13.1.2 Arguments

a, b, c, d: The coefficients of the polynomial. The meaning of the coefficieents $\mathtt{a}, \mathtt{b}, \mathtt{c}, \mathtt{d}$ depends on the degree of the polynomial:

$$\begin{aligned} P(x) &= x^2 + \mathtt{a}x + \mathtt{b} \\ P(x) &= x^3 + \mathtt{a}x^2 + \mathtt{b}x + \mathtt{c} \\ P(x) &= x^4 + \mathtt{a}x^3 + \mathtt{b}x^2 + \mathtt{c}x + \mathtt{d} \end{aligned}$$

z1,z2,z3,z4: Complex simple or double precision. The roots of the polynomial.

13.1.3 Examples

Listing 13.1: Computing roots of polynomials.

```
Program TestRoot

  USE NumTypes
  USE Error
  USE Root

  Real (kind=DP) :: a, b, c, d
  Complex (kind=DPC) ::  z1, z2, z3, z4, ac, bc, cc, dc
```

```
10
   CALL Random_Number(a)
12 CALL Random_Number(b)
   CALL Random_Number(c)
14 CALL Random_Number(d)
   CALL RootPol(a,b,z1,z2)
16 Write(*,'(3ES20.12)')Z1, Abs(z1**2 + a*z1 + Cmplx(b,kind=DPC))
   Write(*,'(3ES20.12)')Z2, Abs(z2**2 + a*z2 + Cmplx(b,kind=DPC))
18
   CALL RootPol(a,b,c, z1,z2, z3)
20 Write(*,*)
   Write(*,'(3ES20.12)')Z1, Abs(z1**3+a*z1**2+b*z1+Cmplx(c,kind=DPC))
22 Write(*,'(3ES20.12)')Z2, Abs(z2**3+a*z2**2+b*z2+Cmplx(c,kind=DPC))
   Write(*,'(3ES20.12)')Z3, Abs(z3**3+a*z3**2+b*z3+Cmplx(c,kind=DPC))
24
   ac = Cmplx(a,kind=DPC)
26 bc = Cmplx(b,a,kind=DPC)
   cc = Cmplx(c,kind=DPC)
28 dc = Cmplx(d,kind=DPC)
   CALL RootPol(ac,bc,z1,z2)
30 Write(*,*)
   Write(*,'(3ES20.12)')Z1, Abs(z1**2 + ac*z1 + Cmplx(bc,kind=DPC))
32 Write(*,'(3ES20.12)')Z2, Abs(z2**2 + ac*z2 + Cmplx(bc,kind=DPC))
   CALL RootPol(ac,bc,cc, dc, z1,z2, z3, z4)
34 Write(*,*)
   Write(*,'(3ES20.12)')Z1, Abs(z1**4+ac*z1**3+bc*z1**2+cc*z1+dc)
36 Write(*,'(3ES20.12)')Z2, Abs(z2**4+ac*z2**3+bc*z2**2+cc*z2+dc)
   Write(*,'(3ES20.12)')Z3, Abs(z3**4+ac*z3**3+bc*z3**2+cc*z3+dc)
38 Write(*,'(3ES20.12)')Z4, Abs(z4**4+ac*z4**3+bc*z4**2+cc*z4+dc)

40
   Stop
42 End Program TestRoot
```

13.2 Function `Newton(Xo, Fnew, [Tol])`

13.2.1 Description

Compute a root of the function defined by the routine `Fnew`.

13.2.2 Arguments

`Xo`: Real simple or double precision. An initial guess of the position of the root.

`Fnew`: The function whose root we want to compute. It is defined as a subroutine that returns the value of the function and of its derivative. If it is an external function, an interface block like this should be defined

```
Interface
   Subroutine FNew(Xo, F, D)
```

```
        USE NumTypes

        Real (kind=DP), Intent (in) :: Xo
        Real (kind=DP), Intent (out) :: F, D
      End Subroutine FNew
    End Interface
```

where `F` is the value of the function in `Xo`, and `D` the value of the derivative in `Xo`. If the arguments are of simple precision, a similar interface should be provided, where the arguments of `Fnew` are of single precision.

`Tol`: Real single or double precision. Optional. An estimation of the desired accuracy of the position of the root.

13.2.3 Output

Real single or double precision. The position of the root.

13.2.4 Examples

Listing 13.2: Computing roots of non-linear functions with the Newton method.

```
Program TestRoot

  USE NumTypes
  USE Error
  USE Root

  Real (kind=DP) :: a, b, c, d, X
  Complex (kind=DPC) ::  z1, z2, z3, z4, ac, bc, cc, dc


  Interface
     Subroutine FNew(Xo, F, D)

       USE NumTypes

       Real (kind=DP), Intent (in) :: Xo
       Real (kind=DP), Intent (out) :: F, D
     End Subroutine FNew
  End Interface


  ! Compute the value such that cos(x) = x
  X = Newton(0.0_DP, Fnew, 1.0E-10_DP)
  Write(*,'(1A,ES33.25)') 'Point:          ', X
  Write(*,'(1A,ES33.25)') 'Value of Cos:  ', Cos(X)


  Stop
```

```
End Program TestRoot

! ********************************
! *
Subroutine FNew(Xo, F, D)
! *
! ********************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: Xo
  Real (kind=DP), Intent (out) :: F, D


  F = Xo - Cos(Xo)
  D = 1.0_DP + Sin(Xo)

  Return
End Subroutine FNew
```

13.3 Function `Bisec(a, b, Fbis, [Tol])`

13.3.1 Description

Compute the root of the function defined by `Fbis`.

13.3.2 Arguments

`a, b`: Real single or double precision. Initial points, such that `Fbis(a)Fbis(b)` < 0.

`Fbis`: The function whose root we want to compute. It is defined as a function that returns the value of the function. If it is an external function, an interface block like this should be defined

```
Interface
   Function F(X)

     USE NumTypes

     Real (kind=DP), Intent (in) :: X
     Real (kind=DP) :: F
   End Function F
End Interface
```

where `F` is the value of the function in `X`. If the arguments are of simple precision, a similar interface should be provided, where the arguments of `F` are of single precision.

`Tol`: Real single or double precision. Optional. An estimation of the desired accuracy of the position of the root.

13.3.3 Output

Real single or double precision. The position of the root of `Fbis`.

13.3.4 Examples

Listing 13.3: Computing roots with the bisection method.

```
Program TestRoot

  USE NumTypes
  USE Error
  USE Root

  Real (kind=DP) :: a, b, c, d, X
  Complex (kind=DPC) ::  z1, z2, z3, z4, ac, bc, cc, dc

  Interface
     Function Fbis(X)

       USE NumTypes

       Real (kind=DP), Intent (in) :: X
       Real (kind=DP) :: Fbis
     End Function Fbis
  End Interface

  ! Compute the value such that cos(x) = x
  X = Bisec(0.0_DP, 1.1_DP, Fbis, 1.0E-10_DP)
  Write(*,'(1A,ES33.25)') 'Point:          ', X
  Write(*,'(1A,ES33.25)') 'Value of Cos:  ', Cos(X)


  Stop
End Program TestRoot

! ********************************
! *
Function FBis(X)
! *
! ********************************

  USE NumTypes

  Real (kind=DP), Intent (in) :: X
  Real (kind=DP) :: Fbis


  Fbis = X - Cos(X)

  Return
End Function FBis
```

Fourteen

MODULE Fourier

This is the documentation of the `MODULE Fourier`, a set of `FORTRAN 90` routines to work with Fourier series. This module make use of the `MODULE NumTypes` and the `MODULE Constants` so please read the documentation of these modules *before* reading this.

14.1 Type Fourier_Serie

14.1.1 Description

A new data type `Fourier_Serie` is defined to work with Fourier series. This type has two components: The modes, and the number of modes.

14.1.2 Components

`Coef(:):` Complex double precision one dimensional array. The modes.

`Nterm:` Integer. The number of terms of the Fourier series.

14.1.3 Examples

A small example showing how to define a Fourier serie.

Listing 14.1: Defining a Fourier serie.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Type (Fourier_Serie) :: Ff

  Stop
End Program TestPoly
```

14.2 Type Fourier_Serie_2D

14.2.1 Description

A new data type `Fourier_Serie_2D` is defined to work with two dimensional Fourier series. This type has two components: The modes, and the number of modes.

14.2.2 Components

`Coef(:,:):` Complex double precision two dimensional array. The modes.

`Nterm:` Integer. The number of terms of the Fourier series.

14.2.3 Examples

A small example showing how to define a polynomial.

Listing 14.2: Defining a two-dimensional Fourier serie.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Type (Fourier_Serie_2D) :: Ff

  Stop
End Program TestPoly
```

14.3 Assignment

14.3.1 Description

You can directly assign one defined Fourier series (one or two dimensional) to another.

14.3.2 Examples

This example uses the `Init_Serie` subroutine. For details of the usage of this function look at the section (14.8), page (134).

Listing 14.3: Assigning Fourier series.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Type (Fourier_Serie) :: FS1, FS2

  CALL Init_Serie(FS1, 20)
  CALL Init_Serie(FS2, 20)
```

```
  FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
  FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

  FS2 = FS1

  Write(*,'(2ES33.25)')FS2%Coef( 1)
  Write(*,'(2ES33.25)')FS2%Coef(-1)

  Stop
End Program TestFourier
```

14.4 Operator +

14.4.1 Description

You can naturally sum one or two dimensional Fourier series. If they have different sizes, it is assumed that the non defined modes of the short Fourier Series are zero.

14.4.2 Examples

This example uses the `Init_Serie` subroutine. For details of the usage of this function look at the section (14.8), page (134).

Listing 14.4: Adding Fourier series.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Type (Fourier_Serie_2D) :: FS1, FS2, FS3
  Integer :: Nt

  Nt = 4
  CALL Init_Serie(FS1, Nt)
  CALL Init_Serie(FS2, Nt)

  FS1%Coef( 1,1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
  FS1%Coef(-1,1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

  FS2%Coef( 1,1) = Cmplx(-1.0_DP, 4.5_DP, kind=DPC)
  FS2%Coef(-1,1) = Cmplx(-1.0_DP, -6.78745_DP, kind=DPC)


  FS3 = FS1 + FS2
  Write(*,'(2ES33.25)')FS3%Coef( 1,1)
  Write(*,'(2ES33.25)')FS3%Coef(-1,1)

  Stop
End Program TestFourier
```

14.5 Operator -

14.5.1 Description

You can naturally subtract one or two dimensional Fourier series. If they have different sizes, it is assumed that the non defined modes of the short Fourier Series are zero.

14.5.2 Examples

Listing 14.5: Subtracting Fourier series.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Type (Fourier_Serie) :: FS1, FS2, FS3
  Integer :: Nt

  Nt = 4
  CALL Init_Serie(FS1, Nt)

  FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
  FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

  FS2 = FS1

  FS3 = FS1 - FS2
  Write(*,'(2ES33.25)')FS3%Coef( 1)
  Write(*,'(2ES33.25)')FS3%Coef(-1)

  Stop
End Program TestFourier
```

14.6 Operator *

14.6.1 Description

You can naturally multiply one or two dimensional Fourier series, in which case the convolution of the Fourier Modes is performed. If they have different sizes, it is assumed that the non defined modes of the short Fourier Series are zero.

14.6.2 Examples

Listing 14.6: Computing the convolution of Fourier series.

```
Program TestFourier

  USE NumTypes
  USE Constants
```

```
  USE Fourier

  Type (Fourier_Serie) :: FS1, FS2, FS3
  Integer :: Nt

  Nt = 4
  CALL Init_Serie(FS1, Nt)

  FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
  FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

  FS2 = FS1

  FS3 = FS1 * FS2
  Write(*,'(2ES33.25)')FS3%Coef( 0)

  Stop
End Program TestFourier
```

14.7 Operator **

14.7.1 Description

You can naturally compute the integer power of a one or two dimensional Fourier series, in which case the convolution of the Fourier modes with themselves are performed a certain number of times.

14.7.2 Examples

Listing 14.7: "Exponentiating" Fourier series.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Type (Fourier_Serie) :: FS1, FS2, FS3
  Integer :: Nt

  Nt = 4
  CALL Init_Serie(FS1, Nt)
  CALL Init_Serie(FS2, Nt)
  CALL Init_Serie(FS3, Nt)

  FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
  FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

  FS3%Coef(0) = Cmplx(1.0_DP, 0.0_DP, kind=DPC)

  FS2 = FS1**8
```

```
  Do I = 1, 8
22    FS3 = FS3 * FS1
  End Do
24
  Write(*,'(2ES33.25)')FS2%Coef( 0)
26  Write(*,'(2ES33.25)')FS3%Coef( 0)

28  Stop
End Program TestFourier
```

14.8 Subroutine `Init_Serie(FS,Ns)`

14.8.1 Description

Allocate memory space for the modes of a one or two dimensional Fourier series.

14.8.2 Arguments

`FS`: Type `Fourier_Serie` or type `Fourier_Serie_2D`. The Fourier series that you want to allocate space for.

`Ns`: Integer. The number of modes.

14.8.3 Examples

Any of the examples of some of the previous sections are aldo good examples of the use of the `Init_Serie` subroutine. Here we simply repeat one of them.

Listing 14.8: Initialising a Fourier series.

```
1  Program TestFourier

3    USE NumTypes
     USE Constants
5    USE Fourier

7    Type (Fourier_Serie) :: FS1, FS2, FS3
     Integer :: Nt
9
     Nt = 4
11   CALL Init_Serie(FS1, Nt)

13   FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
     FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)
15
     FS2 = FS1
17
     FS3 = FS1 * FS2
19   Write(*,'(2ES33.25)')FS3%Coef( 0)

21   Stop
End Program TestFourier
```

14.9 Function Eval_Serie(FS, X, [Y], Tx, [Ty])

14.9.1 Description

Compute the value of the Fourier series `FS` with periods `Tx,Ty` at the point `X,Y`.

14.9.2 Arguments

`FS`: Type `Fourier_Serie` or type `Fourier_Serie_2D`. The Fourier series that you want to evaluate.

`X,Y`: Real double precision. The point in which you want to evaluate the Fourier series. If `FS` is a two dimensional Fourier series, then `Y` must be present.

`Tx,Ty`: Real double precision. The period(s). If `FS` is a two dimensional Fourier series, then `Ty` must be present.

14.9.3 Output

Real double precision. The value of the function defined by the modes in `FS` at the point `(X[,Y])`.

14.9.4 Examples

Listing 14.9: Evaluating a Fourier series at a point.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Type (Fourier_Serie) :: FS1, FS2, FS3
  Integer :: Nt

  Nt = 4
  CALL Init_Serie(FS1, Nt)
  CALL Init_Serie(FS2, Nt)
  CALL Init_Serie(FS3, Nt)


  FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
  FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

  FS2 = FS1**2

  FS3 = FS1*FS2

  Write(*,'(2ES33.25)') Eval_Serie(FS1,0.12_DP,1.0_DP) * &
                      & Eval_Serie(FS2,0.12_DP,1.0_DP)
  Write(*,'(2ES33.25)') Eval_Serie(FS3,0.12_DP,1.0_DP)

```

```
  Stop
End Program TestFourier
```

14.10 Function Unit(FS, Ns)

14.10.1 Description

Allocate memory space for the modes of a one or two dimensional Fourier series and sets the zero mode equal to 1.

14.10.2 Arguments

FS: Type Fourier_Serie or type Fourier_Serie_2D. The Fourier series that you want to allocate space for.

Ns: Integer. The number of modes.

14.10.3 Examples

Listing 14.10: Obtaining a constant Fourier series.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Type (Fourier_Serie) :: FS1, FS2, FS3
  Integer :: Nt

  Nt = 4
  CALL Init_Serie(FS1, Nt)
  CALL Init_Serie(FS2, Nt)
  CALL Init_Serie(FS3, Nt)


  FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
  FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

  CALL Unit(FS2, Nt)

  FS3 = FS1*FS2

  Write(*,'(2ES33.25)')Eval_Serie(FS1,0.12_DP,1.0_DP)
  Write(*,'(2ES33.25)')Eval_Serie(FS3,0.12_DP,1.0_DP)

  Stop
End Program TestFourier
```

14.11 Function DFT(Data, Is)

14.11.1 Description

Compute the Discrete Fourier Transform of the values stored in the complex array `Data`. If `Is` is present and is set to -1, the inverse Discrete Fourier Transform is performed. The direct Fourier transform is defined as

$$\tilde{f}(k) = \sum_{n=0}^{N} f_n e^{\frac{2\pi\imath n}{N}} \qquad \forall k \in \left[-\frac{N}{2}, \frac{N}{2}\right]$$

the inverse one is defined as

$$\tilde{f}(k) = \frac{1}{N}\sum_{n=0}^{N} f_n e^{\frac{-2\pi\imath n}{N}} \qquad \forall k \in \left[-\frac{N}{2}, \frac{N}{2}\right]$$

14.11.2 Arguments

`Data(:[,:])`: One or two dimensional double precision complex array. The data whose Discrete Fourier Transform we want to compute.

`Is`: Integer. Optional. A flag to tell if we want to compute the direct or the inverse Fourier transform.

14.11.3 Output

Type `Fourier_Serie` if `Data(:)` is one dimensional, and type `Fourier_Serie_2D` if `Data(:,:)` is two dimensional.

14.11.4 Examples

This example compute the discrete Fourier transform of $f(x_i) = \sin(x_i)$.

Listing 14.11: Computing the Discrete Fourier Transform.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Integer, Parameter :: Nmax=20
  Type (Fourier_Serie) :: FS1, FS2, FS3
  Complex (kind=DPC) :: Data(Nmax), X
  Integer :: Nt

  Do I = 1, Nmax
     X = Cmplx(TWOPI_DP*I/Nmax)
     Data(I) = Sin(X)
  End Do

  FS1 = DFT(Data)
```

```
19    Write(*,'(1A,2ES33.25)') 'Mode k= 1: ', FS1%Coef( 1)
      Write(*,'(1A,2ES33.25)') 'Mode k=-1: ', FS1%Coef(-1)
21    Write(*,'(ES33.25)' )Sum(Abs(FS1%Coef(:)))

23    Stop
End Program TestFourier
```

14.12 Function Conjg(FS)

14.12.1 Description

Computes the Fourier modes that correspond to the conjugate function. This means: If the modes of FS are $\tilde{f}(k)$, this function returns a Fourier series with modes $\tilde{f}(-k)$.

14.12.2 Arguments

FS: Type Fourier_Serie or type Fourier_Serie_2D. The Fourier series whose conjugate you want to compute.

14.12.3 Output

Type Fourier_Serie if FS is of type Fourier_Serie, and type Fourier_Serie_2D if FS is of Type Fourier_Serie_2D.

14.12.4 Examples

Listing 14.12: Computing the Conjugate Fourier Series.

```
Program TestFourier
2
  USE NumTypes
4 USE Constants
  USE Fourier
6
  Integer, Parameter :: Nmax=20
8 Type (Fourier_Serie) :: FS1, FS2, FS3
  Complex (kind=DPC) :: Data(Nmax), X
10 Integer :: Nt

12 Do I = 1, Nmax
     X = Cmplx(TWOPI_DP*I/Nmax, kind=DPC)
14   Data(I) = Sin(X) + Cmplx(0.0_DP, I*2.0_DP, kind=DPC)
   End Do
16
   FS1 = DFT(Data)
18
   Write(*,'(2ES33.25)')Eval_Serie(FS1,0.23_DP,1.0_DP)
20 Write(*,'(2ES33.25)')Eval_Serie(Conjg(FS1),0.23_DP,1.0_DP)
```

```
22
  Stop
24 End Program TestFourier
```

14.13 Subroutine Save_Serie(FS, File)

14.13.1 Description

Write the Fourier series `FS` to the file `File`.

14.13.2 Arguments

`FS`: Type `Fourier_Serie` or type `Fourier_Serie_2D`. The Fourier series that you want to store in a file.

`File`: Character string of arbitrary length. The name of the file in which you want to save `FS`.

14.13.3 Examples

Listing 14.13: Saving a Fourier Serie in a file.

```
Program TestFourier
2
  USE NumTypes
4 USE Constants
  USE Fourier
6
  Integer, Parameter :: Nmax=20
8 Type (Fourier_Serie) :: FS1, FS2, FS3
  Complex (kind=DPC) :: Data(Nmax), X
10 Integer :: Nt

12 Do I = 1, Nmax
     X = Cmplx(TWOPI_DP*I/Nmax, kind=DPC)
14   Data(I) = Sin(X) + Cmplx(0.0_DP, I*2.0_DP, kind=DPC)
  End Do
16
  FS1 = DFT(Data)
18
  CALL Save(FS1, 'datamodes.dat')
20
  Stop
22 End Program TestFourier
```

14.14 Subroutine Read_Serie(FS, File)

14.14.1 Description

Reads the Fourier series `FS` stored in the file `File`.

14.14.2 Arguments

FS: Type `Fourier_Serie` or type `Fourier_Serie_2D`. The name of the Fourier series data type in which you want to store that data.

File: Character Character string of arbitrary length. The name of the file in which the saved series is.

14.14.3 Examples

Listing 14.14: Reading a Fourier serie from a file.

```
Program TestFourier

  USE NumTypes
  USE Constants
  USE Fourier

  Integer, Parameter :: Nmax=20
  Type (Fourier_Serie) :: FS1, FS2, FS3
  Complex (kind=DPC) :: Data(Nmax), X
  Integer :: Nt

  Do I = 1, Nmax
     X = Cmplx(TWOPI_DP*I/Nmax, kind=DPC)
     Data(I) = Sin(X) + Cmplx(0.0_DP, I*2.0_DP, kind=DPC)
  End Do

  FS1 = DFT(Data)

  CALL Save_Serie(FS1, 'datamodes.dat')
  CALL Read_Serie(FS2, 'datamodes.dat')

  Write(*, '(ES33.25)')Sum(Abs(FS1%Coef(:) - FS2%Coef(:)))


  Stop
End Program TestFourier
```

Fifteen

MODULE Time

Th MODULE Time is a module to provide access to date and time properties.

15.1 Type tm

15.1.1 Description

A new data type, called tm is defined. It has some properties common with the same derived type defined in the C standard library. The components of the type specify a time: Day, year, month, hour, etc...

15.1.2 Components

hour: Integer. Hour of the day [0-23].

min: Integer, Minutes after the hour [0-59].

sec: Integer. Seconds after the minute [0-59].

msec: Integer. Miliseconds after the second [0-999].

year: Integer. Year.

month: Integer. Month of the year [0-11].

mday: Integer. Day of the month [1-31].

wday: Integer. Day of the week since Sunday [0-6].

15.1.3 Example

A small example defining a tm data type.

Listing 15.1: Defining a Time data type.

```
Program Test

  USE NumTypes
  USE Time
```

```
6   Type (tm) :: Oneday

8   OneDay%hour = 12
    OneDay%min  = 0
10  OneDay%sec  = 0
    OneDay%mday = 10
12  OneDay%mon  = 0
    OneDay%year = 2007
14  OneDay%wday = 3

16  Stop
End Program Test
```

15.2 Function `gettime()`

15.2.1 Description

The function `gettime()` returns the current time and date in a `type tm` data type.

15.2.2 Arguments

This function has no arguments.

15.2.3 Output

`Type tm`, containing all the information about the date and time.

15.2.4 Example

A small program that prints the current year.

Listing 15.2: Obtaining the current date and time.

```
1  Program Test

3  USE NumTypes
   USE Time
5
   Type (tm) :: Oneday
7
   Oneday = gettime()
9
   Write(*,*) 'Current year: ', Oneday%year
11
   Stop
13 End Program Test
```

15.3 Function `isleap(Nyr)`

15.3.1 Description

The function `isleap(Nyr)` returns `.true.` if `Nyr` is a leap year, and `.false.` otherwise. Note that the leap years are different in the Julian and Gregorian calendars. In this code the Gregorian calendar is supposed valid *after* 1582[1].

15.3.2 Arguments

`Nyr`: Integer. The year.

15.3.3 Output

Logical. `.true.` if `Nyr` is a leap year, and `.false.` otherwise.

15.3.4 Example

A small program that tell us if the current year is leap.

Listing 15.3: Are we in a leap year?.

```
1  Program Test
2
3    USE NumTypes
4    USE Time
5
6    Type (tm) :: Oneday
7
8    Oneday = gettime()
9
10   If (isleap(Oneday%year)) Then
11     Write(*,*) 'We are in a leap year.'
12   Else
13     Write(*,*) 'We are not in a leap year.'
14   End If
15
16   Stop
17 End Program Test
```

15.4 Function `asctime(t)`

15.4.1 Description

The function `asctime`, returns a 24 length character string from a type `tm` data type, containing the date and time, in a similar way that the function `asctime` of the `C` standard library, for example:

[1] For more details, take a look at

`http://en.wikipedia.org/wiki/Gregorian_calendar`

```
Wed Jan 10 19:15:49 2007
```

15.4.2 Arguments

t: Type tm. A Type tm data type containing the date and time.

15.4.3 Output

Character (len=24). A 24 length character string with the format Www Mmm dd hh:mm:ss yyyy, where Www is the weekday, Mmm the month in letters, dd the day of the month, hh:mm:ss the time, and yyyy the year.

15.4.4 Example

A small program that prints the current time.

Listing 15.4: Printing current date/time.

```
1  Program Test

3    USE NumTypes
     USE Time
5

7    Write(*,'(1A)')asctime(gettime())

9

     Stop
11 End Program Test
```

15.5 Function Day_of_Week(Day, Month, Year)

15.5.1 Description

The function Day_of_Week(Day, Month, Year), returns the day of the week since sunday (sunday is 0), of the date that correspond to the input Day, Month, Year.

15.5.2 Arguments

Day: Integer. The day of the month [1-31].

Month: Integer. The month of the year [0-11].

Year: Integer. The year.

15.5.3 Output

Integer. The day of the week since sunday, thus a number between 0 and 6, with 0 corresponding to sunday.

15.5.4 Example

A small program that prints the date and time of the first of january of 1900.

Listing 15.5: Day of week of the first of January 1900.

```
1  Program Test
2
3    USE NumTypes
4    USE Time
5
6    Type (tm) :: Oneday
7
8    Oneday%hour = 12
9    Oneday%min  = 0
10   OneDay%sec  = 0
11   OneDay%mday = 1
12   OneDay%mon  = 0
13   OneDay%year = 1900
14
15   OneDay%wday = Day_of_Week(Oneday%mday, Oneday%mon, Oneday%year)
16
17   Write(*,*) asctime(Oneday)
18
19   Stop
20 End Program Test
```

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