A FORTRAN 90 numerical library

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Generalities

This is the documentation of a total of thirteen FORTRAN 90 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 License¹ 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 90, this means that it should run on any machine and with any compiler. In particular the code of all these modules has been compiled using GNU gfortran, INTEL ifort and DIGITAL f90 for PC.

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The source code of all the modules as well as the last version of this document should always be available (in it's last version) at:

http://lattice.ft.uam.es/perpag/alberto/codigo_en.php

there is also a sourceforge.net project, where the last version of both the source code and the documentation should be available:

http://sourceforge.net/projects/afnl

Enjoy programming.

Installation

To install this library in a Unix/Linux environment, simply edit the Makefile file, and set the F90 and F900PT variables to whatever your compiler and your favourite optimisation flags are. After running make you should obtain a file called libf90.a, and probably (that depends on

¹http://www.gnu.org/copyleft/gpl.html

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the particular compiler) some .mod files. Copy the libf90.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 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.

```
Program Types_of_Data
USE NumTypes

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

```
Complex (kind=SPC) :: Ac
Complex (kind=DPC) :: Dc

Write(*,*)Kind(A), Kind(Aa)

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 precision 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)

4 MODULE Constants

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: $\pi\text{-related}$ 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	$\gamma (=0.5772\dots)$

 $Table\ 2.4$: 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.

```
Program Test
USE Error

Write(stderr,*)''This is printed in standard error.''

Stop
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 occurred. It is an optional argument.

6 MODULE Error

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.

```
Program Test
      USE Error
3
      Integer :: N1, N2
5
      Write(*,*)'Two integer numbers:'
7
      \mathtt{Read}(*,*)N1,N2
      If (N2 == 0) Then
9
        CALL Perror ('Test', 'Division by cero. See the product: ')
        Write (*,*) N1*N2
11
         \texttt{Write}\,(*\,,*)\,\mathrm{N}1/\mathrm{N}2
13
      End If
15
      Stop
   End Program Test
17
```

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 occurred. 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.

```
Program Test
USE Error

Integer :: N1, N2

Write(*,*)'Two integer numbers:'
Read(*,*)N1,N2

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
2
     USE Integration
4
     Real (kind=DP) :: Tol
6
     Interface
        Function Fint(X)
8
           USE NumTypes
10
           Real (kind=DP), Intent (in) :: X
           Real (kind=DP) :: Fint
12
         End Function Fint
     End Interface
14
     Tol = 1.0E-6_DP
16
     Write(*,*)'Integral of x**2 between 0 and 1:'
     Write (*,*) Trapecio (0.0\_DP, 1.0\_DP, Fint, Tol)
18
20
     Stop
   End Program Test
22
24
   Function Fint(X)
26
     *************
28
     USE NumTypes
30
     \texttt{Real} \ (\texttt{kind=\!DP}) \;, \ \texttt{Intent} \ (\texttt{in}) \; :: \; X
     Real (kind=DP) :: Fint
32
     Fint = X{**}2
34
     Return
36
   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.

```
Program Test
     USE NumTypes
     USE Integration
3
     Real (kind=DP) :: Tol
5
7
     Interface
        Function Fint(X)
          USE NumTypes
9
          Real (kind=DP), Intent (in) :: X
11
          Real (kind=DP) :: Fint
        End Function Fint
13
```

```
End Interface
15
      Tol = 1.0E-6-DP
      Write(*,*)'Integral of x**2 between 0 and 1:'
17
      Write(*,*)Simpson(0.0\_DP, 1.0\_DP, Fint, Tol)
19
      Stop
   End Program Test
21
23
   Function Fint(X)
25
27
      USE NumTypes
29
      Real (kind=DP), Intent (in) :: X
31
      {\tt Real} \ ({\tt kind}\!\!=\!\!\! DP) \ :: \ {\tt Fint}
33
      Fint = X**2
35
      Return
37
   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
1
     USE NumTypes
     USE Integration
3
     Real (kind=DP) :: Tol
5
     Interface
7
        Function Fint(X)
           USE NumTypes
9
           \texttt{Real} \ (\texttt{kind=}DP) \,, \ \texttt{Intent} \ (\texttt{in}) \ :: \ X
11
           {\tt Real} \ ({\tt kind}\!\!=\!\!\!DP) \ :: \ {\tt Fint}
        End Function Fint
13
     End Interface
15
     Tol = 1.0E-6DP
     Write(*,*)'Integral of x**2 between 0 and 1:'
17
     Write (*,*) Trapecio Ab (0.0 DP, 1.0 DP, Fint, Tol)
19
     Stop
   End Program Test
21
   ! **************
23
   Function Fint(X)
^{25}
     *************
27
     USE NumTypes
29
     Real (kind=DP), Intent (in) :: X
31
     Real (kind=DP) :: Fint
33
     Fint = X**2
35
     Return
37
   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.

```
Program Test
     USE NumTypes
     USE Integration
3
     Real (kind=DP) :: Tol
5
7
     Interface
        Function Fint(X)
          USE NumTypes
9
          Real (kind=DP), Intent (in) :: X
11
          Real (kind=DP) :: Fint
        End Function Fint
13
```

```
End Interface
15
    Tol = 1.0E-6DP
17
    Write(*,*)'Integral of x**2 between 0 and 1:'
    Write(*,*)SimpsonAb(0.0\_DP, 1.0\_DP, Fint, Tol)
19
    Stop
  End Program Test
21
   **************
23
  Function Fint(X)
25
27
    ****************
    USE NumTypes
29
    Real (kind=DP), Intent (in) :: X
31
    Real (kind=DP) :: Fint
33
    Fint = X**2
35
    Return
  End Function Fint
37
```

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.

4.5.3Output

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

4.5.4examples

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

```
{\tt Program}\ {\rm Test}
      USE NumTypes
      USE Integration
3
      Real (kind=DP) :: Tol
5
7
      Interface
         Function Fint(X)
           USE NumTypes
9
           Real (kind=DP), Intent (in) :: X
11
            Real (kind=DP) :: Fint
         End Function Fint
13
      End Interface
15
      Tol = 1.0E-6DP
      Write (*,*) 'Integral of e**(-x**2) between 0 and infinity:'
17
      Write (*,*) SimpsonInfUp (0.0 DP, Fint, Tol)
19
      Stop
   End Program Test
21
23
   Function Fint(X)
25
27
      USE NumTypes
29
      \texttt{Real (kind=}DP)\,,\;\;\texttt{Intent (in)}\;::\;\;X
31
      Real (kind=DP) :: Fint
33
      Fint = \exp(-X * * 2)
35
      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.

```
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
13
     End Interface
15
     Tol = 1.0E-6_DP
     Write (*,*) 'Integral of e**(-x**2) between -infinity and 0:'
17
     Write (*,*) SimpsonInfDw (0.0_DP, Fint, Tol)
19
     Stop
   End Program Test
21
23
25
   Function Fint(X)
27
     USE NumTypes
29
     Real (kind=DP), Intent (in) :: X
31
     Real (kind=DP) :: Fint
33
     Fint = exp(-X**2)
35
     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
3
     Real (kind=DP) :: Tol
5
     Interface
7
        Function Fint(X)
           USE NumTypes
9
           Real (kind=DP), Intent (in) :: X
11
           Real (kind=DP) :: Fint
         End Function Fint
13
     End Interface
15
     Tol = 1.0E-6_DP
     Write (*,*) 'Integral of 1/\operatorname{sqrt}(-x) between -1 and 0:'
17
     Write (*,*) SimpsonSingUp (-1.0 \text{-DP}, 0.0 \text{-DP}, \text{Fint}, \text{Tol}, 0.5 \text{-DP})
19
     Stop
   End Program Test
21
   ! ***************
23
   \textbf{Function} \ \operatorname{Fint}\left(X\right)
^{25}
     *************
     USE NumTypes
29
     Real (kind=DP), Intent (in) :: X
31
     Real (kind=DP) :: Fint
33
```

```
Fint = Sqrt(-X)

Return
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
3
     Real (kind=DP) :: Tol
5
     Interface
7
        Function Fint(X)
          USE NumTypes
9
           \texttt{Real} \ (\texttt{kind=\!DP}) \,, \ \texttt{Intent} \ (\texttt{in}) \ :: \ X 
11
          Real (kind=DP) :: Fint
13
        End Function Fint
     End Interface
15
     Tol = 1.0E-6_DP
     Write (*,*) 'Integral of 1/sqrt(x) between 0 and 1:'
17
     Write(*,*)SimpsonSingDw(0.0\_DP, 1.0\_DP, Fint, Tol, 0.5\_DP)
19
     Stop
   End Program Test
21
23
   ! **************
   Function Fint(X)
25
    ******************
27
     USE NumTypes
29
     Real (kind=DP), Intent (in) :: X
31
     Real (kind=DP) :: Fint
33
     Fint = Sqrt(X)
35
     Return
   End Function Fint
37
```

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:

$$\frac{\mathrm{d}y_i(x)}{\mathrm{d}x} = f_i(y_j, x)$$

and the initial conditions:

$$y_i(x_0)$$

After the integration we get:

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

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:

$$\frac{\mathrm{d}y_1(x)}{\mathrm{d}x} = y_2(x); \qquad \frac{\mathrm{d}y_2(x)}{\mathrm{d}x} = -y_1(x)$$

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:

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

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
1
     USE NumTypes
     USE Integration
3
     Real (kind=DP) :: Tol, In(2)
5
     Interface
7
       Function Feuler (X, Y) Result (Func)
9
         USE NumTypes
         Real (kind=DP), Intent (in) :: X, Y(:)
11
         Real (kind=DP) :: Func(Size(Y))
       End Function Feuler
13
     End Interface
15
     Tol = 1.0E-2DP
17
     In(1) = 0.0 DP
     In(2) = 1.0 DP
19
     Write (*,*) 'Values of \sin(1) and \cos(1): '
     Write (*,*) Euler (In, 0.0 DP, 1.0 DP, Feuler, Tol)
21
     Write (*,*) Sin (1.0 DP), Cos (1.0 DP)
23
   End Program Test
25
27
   ! **************
    Function FEuler(X, Y) Result (Func)
29
     ************
31
       Real (kind=8), Intent (in) :: X, Y(:)
33
       Real (kind=8) :: Func(Size(Y))
35
       Func(1) = Y(2)
       \operatorname{Func}(2) = -Y(1)
37
       Return
39
     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:

$$\frac{\mathrm{d}y_i(x)}{\mathrm{d}x} = f_i(y_j, x)$$

and the initial conditions:

$$y_i(x_0)$$

After the integration we get:

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

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:

$$\frac{\mathrm{d}y_1(x)}{\mathrm{d}x} = y_2(x); \qquad \frac{\mathrm{d}y_2(x)}{\mathrm{d}x} = -y_1(x)$$

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:

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

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
2
     USE Integration
4
     Real (kind=DP) :: Tol, In(2)
6
     Interface
       Function Feuler(X, Y) Result (Func)
8
          USE NumTypes
10
           \texttt{Real} \ (\texttt{kind=}DP) \,, \ \texttt{Intent} \ (\texttt{in}) \ :: \ X, \ Y(:) 
          Real (kind=DP) :: Func(Size(Y))
12
       End Function Feuler
     End Interface
14
16
     Tol = 1.0E-3_DP
     In(1) = 0.0 DP
18
     In(2) = 1.0 DP
     Write (*,*) 'Values of \sin(1) and \cos(1): '
20
     Write(*,*)' Euler:
     Write(*,*) Euler(In, 0.0_DP, 1.0_DP, Feuler, Tol)
22
     Write (*,*) 'Runge-Kutta:
     Write (*,*) Rgnkta (In, 0.0 DP, 1.0 DP, Feuler, Tol)
24
     Write(*,*)' Exact:
     Write (*,*) Sin (1.0 DP), Cos (1.0 DP)
^{26}
     Stop
28
   End Program Test
30
     *************
32
     Function FEuler(X, Y) Result (Func)
36
```

```
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
```

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 (conjugate gradient, simplex, etc...).

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

5.1.1 Description

The function Step(X, FStep, Tol) returns the position of the minimum of the Function Fstep with an optional precision Tol.

5.1.2 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} .

5.1.3 Output

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

5.1.4 Example

Listing 5.1: Minimising a function.

```
Program TestMin
     USE NumTypes
     USE Optimization
4
     Integer, Parameter :: Ndim = 4
6
     Real (kind=DP) :: XoM(Ndim), Xmin(Ndim)
8
     Interface
10
        Function FstepM(Xo)
          USE NumTypes
12
          Real (kind=DP), Intent (in) :: Xo(:)
          Real (kind=DP) :: FstepM
14
        End Function FstepM
     End Interface
16
18
     ! Initial guess of the position of the minimum
     XoM(1) = 1.373 DP
20
     XoM(2) = 1.373 DP
     XoM(3) = 1.373 DP
22
     XoM(4) = 1.373 DP
24
     Write(*,*)'Initial Position: '
26
     Do I = 1, Ndim
        Write (*, '(1A,1I4,1A,1ES33.25)')' Variable ', I, ": ", XoM(I)
28
     End Do
30
     Xmin = Step (XoM, FstepM, 1.0E-7_DP)
     Write(*,*)
32
     Write (*,*) 'Position of the minimum: '
     Do I = 1, Ndim
34
        Write (*, '(1A,1I4,1A,1ES33.25)') 'Variable', I, ": ", Xmin(I)
```

```
End Do
36
38
     Stop
   End Program TestMin
40
     **********
42
   Function FstepM(Xo)
44
46
     USE NumTypes
48
     Real (kind=DP), Intent (in) :: Xo(:)
     Real (kind=DP) :: FstepM
50
52
     FstepM = (Xo(1) - 1.0 DP) **2 + &
          & (Xo(2)-2.0DP)**2 + &
54
          & (Xo(3)+3.0DP)**4 + &
          & (Xo(4) - 4.0 DP) **8
56
58
     Return
   End Function FstepM
60
```

5.2 Function MaxPosition(FVal, IpX, IpY)

5.2.1 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(:).

5.2.2 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.

5.2.3 Output

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

5.2.4 Example

Listing 5.2: Example of the usage of the routine MaxPosition.

```
Program MaxLoc
2
     USE NumTypes
4
     USE Constants
     USE Optimization
     USE Error
6
      IMPLICIT NONE
8
     10
     Character (len=200) :: Filename
     Real (kind=DP) :: DnullX, DnullY
12
      \texttt{Real (kind=}DP) \,, \,\, \texttt{Allocatable} \,\, :: \,\, F\,(:\,,:) \\
     Integer :: IpX(10), IpY(10)
14
     Write(stderr,*) "SizeX, SizeY, Filename"
16
     Read(*,*)IsX, IsY, Filename
18
     Allocate(F(IsX, IsY))
      Open (Unit=666, File=Trim(Filename), Action="READ")
20
     \quad \text{Do} \ I \, = \, 1 \, , \ \mathrm{IsX}
         Do J = 1, IsY
^{22}
            Read(666,*) DnullX, DnullY, F(I,J)
            Write (stderr,*) DnullX, DnullY, F(I,J)
24
         End Do
     End Do
26
     Close (666)
28
     Nmax = MaxPosition(F, IpX, IpY)
     Write(*,*)"# Number of maxima: ", Nmax
30
     Write (*,*) "# Positions of the maxima: "
     Do I = 1, Nmax
32
         Write(*,*)IpX(I), IpY(I)
     End Do
34
     Stop
36
   End Program MaxLoc
```

Six

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.

6.1 Subroutine Pivoting(M, Ipiv, Idet)

6.1.1 Description

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

6.1.2 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

6.1.3 Examples

Listing 6.1: 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
```

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```
! Fill M of random numbers
      CALL Random_Number (M)
15
      Write(*,*)'Original M:'
      Do I = 1, Nord
17
         Write (*, '(100 \text{ ES} 10.3)') (M(I, J), J = 1, Nord)
19
      CALL Pivoting (M, Ipiv, Iperm)
21
      Write (*,*) 'Permuted M:
      Do I = 1, Nord
23
         Write (*, '(100 \text{ ES}10.3)') (M(I, J), J = 1, Nord)
25
      Stop
27
   End Program TestLinear
```

6.2 Subroutine LU(M, Ipiv, Idet)

6.2.1 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

$$M = LU (6.1)$$

where L is lower triangular, and U upper triangular.

$$L = \begin{pmatrix} 1 & 0 & 0 & \dots \\ L_{21} & 1 & 0 & \dots \\ L_{31} & L_{32} & 1 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}; \quad U = \begin{pmatrix} U_{11} & U_{12} & U_{13} & \dots \\ 0 & U_{22} & U_{23} & \dots \\ 0 & 0 & U_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$
(6.2)

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.

6.2.2 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

6.2.3 Examples

Listing 6.2: Making the LU decomposition.

```
Program TestLinear
2
     USE NumTypes
     USE Linear
4
     Integer, Parameter :: Nord = 4
6
     Real (kind=DP) :: M(Nord, Nord), L(Nord, Nord), U(Nord, Nord), &
          & Mcp(Nord, Nord)
     Integer :: Ipiv(Nord), Iperm
10
12
     ! Fill M of random numbers, and make a copy
     CALL Random_Number (M)
14
     Mcp = M
     L = 0.0 DP
16
     U = 0.0 DP
18
     ! Make the LU decomposition and fill the matrices
     ! L and U
20
     CALL Lu(M, Ipiv, Iperm)
     22
        L(I,I) = 1.0 DP
        U(I,I) = M(I,I)
24
        Do J = I+1, Nord
           L(J,I) = M(J,I)
^{26}
           U(I,J) = M(I,J)
28
        End Do
     End Do
30
     ! Now Make the product and see that it is the original matrix with
     ! some rows permuted
32
     Write(*,*)'M: '
     Do I = 1, Nord
34
        Write (*, '(100 \text{ ES}10.3)') (\text{Mcp}(I, J), J = 1, \text{Nord})
     End Do
36
     Write (*,*)'L: '
38
     Do I = 1, Nord
        Write (*, '(100 ES10.3)')(L(I,J), J = 1, Nord)
40
     End Do
     Write(*,*)'U: '
42
     Do I = 1, Nord
        Write (*, '(100 ES10.3)')(U(I, J), J = 1, Nord)
44
     End Do
46
     M = MatMul(L, U)
     Write(*,*)'LU (Same as M with some rows permuted): '
48
     Do I = 1, Nord
```

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```
50 | Write(*,'(100ES10.3)')(M(I,J), J = 1, Nord)
End Do

52 | Stop
End Program TestLinear
```

6.3 Subroutine LUsolve(M, b)

6.3.1 Description

Solves the linear system of equations

$$M_{11}x_1 + M_{12}x_2 + M_{13}x_3 + M_{14}x_4 + \dots = b_1$$

$$M_{21}x_1 + M_{22}x_2 + M_{23}x_3 + M_{24}x_4 + \dots = b_2$$

$$\vdots$$

$$(6.3)$$

6.3.2 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.

6.3.3 Examples

Listing 6.3: Solving systems of linear equations.

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

6.4. Function Det(M)

```
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  Stop
End Program TestLinear
```

6.4 Function Det(M)

6.4.1 Description

Computes the determinant of the matrix M.

6.4.2 Arguments

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

6.4.3 Output

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

6.4.4 Examples

Listing 6.4: Computing the determinant of a matrix.

```
Program TestLinear
2
     USE NumTypes
     USE Linear
4
     Integer, Parameter :: Nord = 10
6
     Real (kind=DP) :: M(Nord, Nord), L(Nord, Nord), U(Nord, Nord), &
8
          & Mcp(Nord, Nord), b(Nord), bcp(Nord)
     Integer :: Ipiv(Nord), Iperm
10
12
     ! Fill M of randoms numbers
     CALL Random_Number (M)
14
     ! Now compute the determinant.
16
     Write (*, '(ES15.8)') Det (M)
18
     Stop
20
   End Program TestLinear
```

Seven

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.

7.1 Subroutine Swap(X, Ind1, Ind2)

7.1.1 Description

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

7.1.2 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.

7.1.3 Examples

Listing 7.1: Sorting data.

```
Program TestNN
     USE NumTypes
3
     USE NonNumeric
5
     Integer, Parameter :: Nmax = 10
     Integer :: Ima(Nmax), I
7
9
     ! Fill Ima(:)
     Forall (I=1:Nmax) Ima(I) = I
11
     ! Plot the numbers
13
     Do I = 1, Nmax
        Write(*,'(1000I10)')Ima(I)
15
```

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```
End Do

! Swap first and last elemeths 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
```

7.2 Subroutine Insrt(X[, Ipt])

7.2.1 Description

Sort the elements of X(:) in ascendant order¹.

7.2.2 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.

7.2.3 Examples

Listing 7.2: Sorting data.

```
Program TestNN
     USE NumTypes
3
     USE NonNumeric
5
     Integer, Parameter :: Nmax = 10
     Integer :: Ima(Nmax)
7
     Real (kind=DP) :: X(Nmax), Y(Nmax)
9
     ! Fill X(:) with random data, and define Y(:)
11
     CALL Random_Number(X)
     Y = Sin(12.34 DP*(X-0.5 DP))
13
     ! Plot an unsorted data table
15
     Do I = 1, Nmax
17
        Write (*, '(1000 ES13.5)')X(I), Y(I)
```

¹This 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
```

7.3 Subroutine Qsort(X[, Ipt])

7.3.1 Description

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

7.3.2 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.

7.3.3 Examples

Listing 7.3: Sorting data.

```
Program TestNN
2
     USE NumTypes
     USE NonNumeric
4
     Integer, Parameter :: Nmax = 10
6
     Integer :: Ima(Nmax)
     Real (kind=DP) :: X(Nmax), Y(Nmax)
10
     ! Fill X(:) with random data, and define Y(:)
     CALL Random_Number(X)
12
     Y = Sin(12.34 DP*(X-0.5 DP))
14
     ! Plot an unsorted data table
     Do I = 1, Nmax
16
        Write (*, '(1000 ES13.5)')X(I), Y(I)
     End Do
18
```

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```
! Sort them, and plot the table again. Same points, but this time ! sorted  

CALL Qsort(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
```

7.4 Function Locate(X, X₀[, Iin])

7.4.1 Description

Given a sorted vector of elements X(:), and a point X_0 , Locate returns the position n such that $X(n) < X_0 < X(n+1)$. If 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(:)

7.4.2 Arguments

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

 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.

7.4.3 Output

Integer. The position n such that

$$X(n) < X_0 < X(n+1)$$

7.4.4 Examples

Listing 7.4: Searching data position in an ordered list.

```
Program TestNN

USE NumTypes
USE NonNumeric

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

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

Eight

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.

8.1 Function GammaLn(X)

8.1.1 Description

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

8.1.2 Arguments

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

8.1.3 Output

A real Double precision (DP).

8.1.4 Examples

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

Listing 8.1: 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)))

End Do

Stop
End Program TestSpecialFunc
```

8.2 Function Theta(i, z, tau[, Prec])

8.2.1 Description

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

$$\vartheta_i(z|\tau) \tag{8.1}$$

For a definition and properties of these functions take a look [1], here we will only say that following the conventions of the cited reference, our Theta functions have quasi-periods π and $\tau\pi$.

8.2.2 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}

8.2.3 Output

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

8.2.4 Examples

Listing 8.2: 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)
10
12
       Check the quasi-periodicity of the Third
       Jacobi Theta function.
     Write(*,*)Theta(3, Z)
                                       tau)
14
     Write(*,*)Theta(3, Z+Cmplx(PI_DP), tau)
     Write(*,*)Theta(3, Z+PLDP*tau, tau) * &
16
          &exp(PLIMAG_DPC*tau + 2.0_DP*UNITIMAG_DPC*Z)
18
     Stop
20
   End Program TestSpecialFunc
```

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

8.3.1 Description

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

$$\vartheta \left[\begin{array}{c} a \\ b \end{array} \right] (z|\tau) \tag{8.2}$$

8.3.2 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 $(\text{Im}(\tau) > 0)$.

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

8.3.3 Output

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

8.3.4 Examples

Listing 8.3: 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
9
     Z = Cmplx(0.546734, 2.76457643, kind=DPC)
11
     tau = Cmplx(0.0 DP, 3.76387540 DP)
13
     Write(*,*)'Theta 1:'
15
     Write (*,*) Theta (1, Z, tau)
     Write(*,*) - ThetaChar(0.5 DP, 0.5 DP, Z, tau)
17
     Write (*,*) 'Theta 2:'
     Write (*,*) Theta (2, Z, tau)
19
     Write (*,*) ThetaChar (0.5 DP, 0.0 DP, Z, tau)
     Write(*,*)'Theta 3:
21
     Write (*,*) Theta (3, Z, tau)
     Write (*,*) ThetaChar (0.0\_DP, 0.0\_DP, Z, tau)
23
     Write (*,*) 'Theta 4:'
     Write(*,*)Theta(4, Z, tau)
25
     Write (*,*) ThetaChar (0.0 \text{-DP}, 0.5 \text{-DP}, Z, tau)
27
     Stop
29
   End Program TestSpecialFunc
```

8.4 Function Hermite(n,x[, Dval])

8.4.1 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.

8.4.2 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.

8.4.3 Output

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

8.4.4 Examples

Listing 8.4: Computing the first 31 Hermite numbers.

```
Program TestSpecialFunc
```

```
2
     USE NumTypes
     USE SpecialFunc
     Integer :: q
6
8
     Write(*,*)'The first 31 Hermite Numbers'
     Write (*,*) 'http://www.research.att.com/~njas/sequences/A067994'
10
     Do q = 1, 31
        Write(*,'(1I4,1ES33.25)')q, Hermite(q, 0.0_DP)
12
14
     Stop
   End Program TestSpecialFunc
16
```

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

8.5.1 Description

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

$$\frac{1}{\sqrt{n!2^n\sqrt{\pi}}}e^{-x^2/2}H_n(x)$$
 (8.3)

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.

8.5.2 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.

8.5.3 Output

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

8.5.4 Examples

Listing 8.5: Compute the Hermite functions.

```
Program TestSpecialFunc

USE NumTypes
USE SpecialFunc
```

```
Real(kind=DP) :: Deriv, X1, X2, Sum
     Complex (DPC) :: Wmas, Wmenos, Z, tau
8
     Integer :: q, s
10
     Write(*,*)'A (really bad) proof of orthonormality:'
12
     X1 = -10.0 \text{-DP}
     Sum = 0.0 DP
     pole q = -1000, 1000
14
        Sum = Sum + HermiteFunc(6,X1)**2
        X1 = X1 + 0.01 DP
16
     End Do
18
     Write (*, '(1ES33.25)') Sum *0.01_DP
20
     Stop
   End Program TestSpecialFunc
22
```

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

8.6.1 Description

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

$$|n,s\rangle = e^{i\frac{f}{2}x_1x_2} \sum_{k \in s+q\mathbb{Z}} e^{-u^2/2} H_n(u) e^{2\pi i k \frac{x_1}{l_1}} \qquad n = 0, \dots \infty; s = 1, \dots, q$$
 (8.4)

defined in the appendix of [2] (look there for more details and properties).

8.6.2 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.

8.6.3 Output

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

8.6.4 Examples

Listing 8.6: Computing the bassi of a special Hilbert space (details in [2]).

```
Program TestSpecialFunc
```

```
USE NumTypes
    USE SpecialFunc
4
6
    \texttt{Real}(\texttt{kind}\!\!=\!\!\!DP) \ :: \ X1\,, \ X2
    Complex (DPC) :: Wmas, Wmenos,
    Integer :: I, q, s
8
10
    Write (*,*) 'Looking at the quasi-periodicity properties:'
    X1 = 0.97834D0
12
    X2 = 0.873873D0
    q = 4
14
    s = 3
16
    Do I = 0, 8
       Wmas
            = Basis(X1, X2+1.0DP, I, s, q, 1.0DP, 1.0D-15) * &
            & \exp(PI\_IMAG\_DPC*X1*q)
18
       Wmenos = Basis(X1+1.0DP, X2, I, s, q, 1.0DP, 1.0D-15) * &
            & exp(-PLIMAG_DPC*X2*q)
20
       22
    End Do
24
26
    Stop
  End Program TestSpecialFunc
```

Nine

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.

9.1 Function Mean(X)

9.1.1 Description

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

9.1.2 Arguments

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

9.1.3 Output

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

9.1.4 Examples

Listing 9.1: Computing the Mean of a vector of numbers.

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

Stop
End Program Tests
```

9.2 Function Var(X)

9.2.1 Description

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

9.2.2 Arguments

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

9.2.3 Output

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

9.2.4 Examples

Listing 9.2: Computing the Variance of a set of numbers.

```
Program Tests
     USE NumTypes
3
     USE Error
     USE Statistics
5
     Integer, Parameter :: Nmax = 100, Npinta = 100, Npar = 4
7
     Real (kind=DP) :: X(Nmax), Y(Nmax), Yer(Nmax), &
9
          & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax,2)
11
     CALL Random_Number(X)
     Write (*, '(ES33.25)') Var(X)
13
15
     Stop
   End Program Tests
```

9.3 Function Stddev(X)

9.3.1 Description

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

9.3.2 Arguments

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

9.3.3 Output

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

9.3.4 Examples

Listing 9.3: Compputing the standard deviation.

```
Program Tests
     USE NumTypes
3
     USE Error
     USE Statistics
5
     Integer, Parameter :: Nmax = 100, Npinta = 100, Npar = 4
7
     Real (kind=DP) :: X(Nmax), Y(Nmax), Yer(Nmax), &
          & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax,2)
9
11
     CALL Random_Number(X)
     Write (*, '(ES33.25)') Stddev(X)
13
15
     Stop
   End Program Tests
17
```

9.4 Function Moment(X, k)

9.4.1 Description

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

9.4.2 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.

9.4.3 Output

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

MODULE Statistics

9.4.4 Examples

Listing 9.4: Computing the k^{th} moment of a data set.

```
Program Tests
     USE NumTypes
3
     USE Error
     USE Statistics
5
     Integer, Parameter :: Nmax = 100, Npinta = 100, Npar = 4
7
     Real (kind=DP) :: X(Nmax), Y(Nmax), Yer(Nmax), &
          & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax,2)
9
11
     CALL Random_Number(X)
     Write (*,*) 'We should obtain the same numbers twice: '
13
     Write (*, '(ES33.25)') Moment (X, 2), Var(X)
15
     Stop
   End Program Test
17
```

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

9.5.1 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.

9.5.2 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.

9.5.3 Examples

Listing 9.5: Obtaining numbers with a normal distribution.

```
Program Tests

USE NumTypes
USE Error
USE Statistics
```

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

9.6.1 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.

9.6.2 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.

9.6.3 Examples

Listing 9.6: Making Histograms.

```
Program Tests

USE NumTypes
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)
```

MODULE Statistics

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

9.7.1 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.

9.7.2 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 dimensional array. The errors of the points. If you don't have them, you should put all of hem to some non-zero value.

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.

9.7.3 Examples

Listing 9.7: Doing linear regressions.

```
Program Tests
2
     USE NumTypes
     USE Error
4
     USE Statistics
6
     Integer, Parameter :: Nmax = 200, Npinta = 100, Npar = 4, Ndiv = 100
     Real (kind=DP) :: X(Nmax), Y(Nmax), Yer(Nmax), &
8
          & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax, 2), &
          & Xmin, Xmax, h, Xac
10
     Integer :: Ntics(Ndiv)
12
     Interface
        Function Fd(Xx, i)
14
          USE NumTypes
16
```

MODULE Statistics

```
Real (kind=DP), Intent (in) :: Xx(:)
18
           {\tt Integer}\,,\ {\tt Intent}\ ({\tt in})\ ::\ i
20
           Real (kind=DP) :: Fd
         End Function FD
22
     End Interface
24
     CALL Random_Number(Xd)
26
     Xd(:,:) = 10.0 DP*(Xd(:,:) - 0.8 DP)
28
     CALL Normal (Yer, 0.0 \text{-DP}, 1.0 \text{E}-3 \text{-DP})
     Y(:) = 12.34 DP*Xd(:,1)*sin(Xd(:,2)) - 2.23 DP + &
30
           & 0.67 \text{_DP*Xd}(:,1)**2*Xd(:,2) + 0.23 \text{_DP*Xd}(:,1) + Yer(:)
32
     CALL LinearReg (Xd, Y, Yer, Fd, Coef, Cerr, Corr)
34
      ! This should print the adjusted parameters,
36
     ! that have values: 12.34, -2.23, 0.67, 0.23
     Do I = 1, Npar
38
         Write (*, '(2ES33.25)') Coef(I), Cerr(I)
     End Do
40
     ! This prints the ChiSqr, that should be very
42
     ! close to 1.
     Write (*, '(1A,1ES33.25)') 'ChiSqr of the Fit: ', Corr
44
46
   End Program Tests
48
   ! ***********
50
   Function Fd(X, i)
52
   ! **********
54
     USE NumTypes
56
      \texttt{Real (kind=}DP) \;,\;\; \texttt{Intent (in)} \;::\; X(:) \\
58
      Integer, Intent (in) :: i
     Real (kind=DP) :: Fd
60
     If (I==1) Then
62
         Fd = 1.0 DP
     Else If (I==2) Then
64
         \mathrm{Fd}\,=\,X(\,1\,)*\sin\left(X(\,2\,)\,\right)
     Else If (I==3) Then
66
         Fd = X(1) **2 *X(2)
     Else If (I == 4) Then
68
         Fd = X(1)
     End If
70
```

Return
End Function FD

Ten

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.

10.1 Type Pol

10.1.1 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.

10.1.2 Components

Coef(:): Real double precision one dimensional array.

dg: Integer. The degree of the polynomial.

10.1.3 Examples

A small example showing how to define a polynomial.

Listing 10.1: Defining a polynomial.

```
Program TestPoly

USE NumTypes
USE Error
USE Polynomial

Type (Pol) :: P1

Stop
End Program TestPoly
```

10.2 Type CmplxPol

10.2.1 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.

10.2.2 Components

Coef(:): Complex double precision one dimensional array.

dg: Integer. The degree of the polynomial.

10.2.3 Examples

A small example showing how to define a polynomial of complex coefficients.

Listing 10.2: Defining a polynomial.

```
Program TestPoly

USE NumTypes
USE Error
USE Polynomial

Type (CmplxPol) :: P1

Stop
End Program TestPoly
```

10.3 Assignment

10.3.1 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.

10.3.2 Examples

Listing 10.3: Assigning polynomials.

```
Program TestPoly

USE NumTypes
USE Error
USE Polynomial

Integer, Parameter :: Deg = 4
Real (kind=DP) :: Hcoef(Deg+1)
```

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```
Type (Pol) :: Hermite4
10
     ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
12
     ! we first assign the values of the coefficients.
     Hcoef
             = 0.0 \text{ DP}
     Hcoef(1) = 3.0 DP
14
     Hcoef(3) = -6.0 DP
     Hcoef(5) = 1.0 DP
16
     Hermite4 = Hcoef
18
     ! Now Show what we have in our data type:
20
     Do I = 0, Hermite 4\% dg
        Write (*, '(1 I5, ES33.25)') I, Hermite 4% Coef(I)
22
     End Do
24
     Stop
   End Program TestPoly
```

10.4 Operator +

10.4.1 Description

You can naturally sum Pol or CmplxPol data types.

10.4.2 Examples

Listing 10.4: Adding polynomials.

```
Program TestPoly
2
     USE NumTypes
     USE Error
4
     USE Polynomial
6
     Integer, Parameter :: Deg = 4
     Real (kind=DP) :: Hcoef(Deg+1)
     Type (Pol) :: Hermite4, Hermite3, Sum
10
     ! The Third Hermite polynomial is x^3 - 3x, so
12
     ! we first assign the values of the coefficients.
     Hcoef
              = 0.0 \, DP
     Hcoef(2) = -3.0 DP
14
     Hcoef(4) = 1.0 DP
16
     Hermite3 = Hcoef(1:4)
18
     ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
     ! we first assign the values of the coefficients.
20
              = 0.0 \, DP
     Hcoef(1) = 3.0 DP
^{22}
```

```
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(*,'(115,ES33.25)')I, Sum%Coef(I)

End Do

Stop
End Program TestPoly
```

10.5 Operator -

10.5.1 Description

You can subtract Pol or CmplxPol data types.

10.5.2 Examples

Listing 10.5: Substracting polynomials.

```
Program TestPoly
     USE NumTypes
3
     USE Error
     USE Polynomial
5
     Integer, Parameter :: Deg = 4
7
     Real (kind=DP) :: Hcoef(Deg+1)
     Type (Pol) :: Hermite4, Hermite3, Sum
9
     ! The Third Hermite polynomial is x^3 - 3x, so
11
     ! we first assign the values of the coefficients.
     Hcoef
              = 0.0 \, DP
13
     Hcoef(2) = -3.0 DP
     Hcoef(4) = 1.0 DP
15
     Hermite3 = Hcoef(1:4)
17
     ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
19
     ! we first assign the values of the coefficients.
     Hcoef
             = 0.0 \, DP
21
     Hcoef(1) =
                 3.0_DP
     Hcoef(3) = -6.0 DP
23
     Hcoef(5) = 1.0 DP
^{25}
     Hermite4 = Hcoef
27
```

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```
! 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
```

10.6 Operator *

10.6.1 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.

10.6.2 Examples

Listing 10.6: Computing the product of two polynomials.

```
Program TestPoly
     USE NumTypes
3
     USE Error
     USE Polynomial
5
     Integer, Parameter :: Deg = 4
7
     Real (kind=DP) :: Hcoef(Deg+1)
     Type (Pol) :: Hermite4, Hermite3, Sum
9
     ! The Third Hermite polynomial is x^3 - 3x, so
11
     ! we first assign the values of the coefficients.
     Hcoef
              = 0.0 \, DP
13
     Hcoef(2) = -3.0 DP
     Hcoef(4) = 1.0 DP
15
     Hermite3 = Hcoef(1:4)
17
     ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
19
     ! we first assign the values of the coefficients.
     Hcoef
                  0.0 \, DP
21
     Hcoef(1) =
                  3.0 \, \mathrm{DP}
     Hcoef(3) = -6.0 DP
23
     Hcoef(5) = 1.0 DP
^{25}
     Hermite4 = Hcoef
27
     ! Now multiply the two polynomials, and show the result.
     Sum = Hermite3 * Hermite4
29
     Do I = 0, Sum%dg
        Write(*,'(1I5,ES33.25)')I, Sum%Coef(I)
31
```

```
End Do

Stop
End Program TestPoly
```

10.7 Subroutine Init(P, Dgr)

10.7.1 Description

Allocate memory space for the coefficients of a Pol or a CmplxPol type.

10.7.2 Arguments

P: Type Pol or CmplxPol. The polynomial that you want to allocate space for.

Dgr: Integer. The degree of the polynomial.

10.7.3 Examples

Listing 10.7: Initialising a polynomial data type.

```
Program TestPoly
     USE NumTypes
3
     USE Error
     USE Polynomial
5
     Integer, Parameter :: Deg = 4
7
     Real (kind=DP) :: Hcoef(Deg+1)
     Type (Pol) :: Hermite4, Hermite3, Sum
9
11
     ! An alternative way of setting the third Hermite
     ! polynomial.
13
     CALL Init (Hermite3, 3)
     Hermite3\%Coef(0) =
                            0.0 \, \mathrm{DP}
15
     Hermite3\%Coef(1) = -3.0\_DP
     Hermite3\%Coef(2) =
                            0.0 \, \mathrm{DP}
17
     Hermite3\%Coef(3) = 1.0 DP
     Hermite3\%dg = 3
19
21
     Stop
   End Program TestPoly
23
```

10.8 Function Degree(P)

10.8.1 Description

Returns the degree of the polynomial P.

10.8.2 Arguments

P: Type Pol or CmplxPol. The polynomial whose degree we want to know.

10.8.3 Output

Integer. The degree of the polynomial P.

10.8.4 Examples

Listing 10.8: Returns the degree of a polynomial.

```
Program TestPoly
     USE NumTypes
3
     USE Error
     USE Polynomial
5
7
     Integer, Parameter :: Deg = 4
     Real (kind=DP) :: Hcoef(Deg+1), X
     Type (Pol) :: Hermite4, Hermite3, Sum
9
     ! The Third Hermite polynomial is x^3 - 3x, so
11
     ! we first assign the values of the coefficients.
     Hcoef
              = 0.0 \, DP
13
     Hcoef(2) = -3.0 DP
     Hcoef(4) = 1.0 DP
15
     Hermite3 = Hcoef(1:4)
17
     ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
19
     ! we first assign the values of the coefficients.
     Hcoef
                 0.0 \, \mathrm{DP}
              =
21
     Hcoef(1) = 3.0 DP
     Hcoef(3) = -6.0 DP
23
     Hcoef(5) = 1.0 DP
^{25}
     Hermite4 = Hcoef
27
     ! Now Mutiply the two polynomials, and show the result.
     Sum = Hermite3 * Hermite4
29
     ! Show the degree of the product. It should be 4+3=7.
31
     Write(*,*) Degree(Sum)
33
     Stop
35
   End Program TestPoly
```

10.9 Function Value(P, X)

10.9.1 Description

Computes the value of the polynomial P in the point X.

10.9.2 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.

10.9.3 Output

Real double precision. The value of the polynomial P in the point X.

10.9.4 Examples

Listing 10.9: Computes the values of a polynomial at some points.

```
Program TestPoly
2
     USE NumTypes
     USE Error
4
     USE Polynomial
6
     Integer, Parameter :: Deg = 4
     Real (kind=DP) :: Hcoef(Deg+1), X
8
     Type (Pol) :: Hermite4, Hermite3, Sum
10
     ! The Third Hermite polynomial is x^3 - 3x, so
     ! we first assign the values of the coefficients.
12
              = 0.0 \, DP
     Hcoef
     Hcoef(2) = -3.0 DP
14
     Hcoef(4) = 1.0 DP
16
     Hermite3 = Hcoef(1:4)
18
     ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
     ! we first assign the values of the coefficients.
20
                  0.0_DP
     Hcoef
     Hcoef(1) =
                 3.0 \, \mathrm{DP}
22
     Hcoef(3) = -6.0 DP
     Hcoef(5) = 1.0 DP
^{24}
     Hermite4 = Hcoef
26
     ! Now Mutiply the two polynomials, and show the result.
28
     Sum = Hermite3 * Hermite4
30
     ! 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
```

10.10 Function Deriv(P)

10.10.1 Description

Computes the derivative of the polynomial P.

10.10.2 Arguments

P: Type Pol or CmplxPol. The polynomial whose derivative we want to compute.

10.10.3 Output

Type Pol. Another polynomial: the derivative of P.

10.10.4 Examples

Listing 10.10: Computing the derivative of a polynomial.

```
Program TestPoly
3
     USE NumTypes
     USE Error
     USE Polynomial
5
     Integer, Parameter :: Deg = 4
7
     Real (kind=DP) :: Hcoef(Deg+1), X
     Type (Pol) :: Hermite4, Hermite3, Res, Sum
9
     ! The Third Hermite polynomial is x^3 - 3x, so
11
     ! we first assign the values of the coefficients.
     Hcoef
              = 0.0 \, DP
13
     Hcoef(2) = -3.0 DP
     Hcoef(4) = 1.0 DP
15
     Hermite3 = Hcoef(1:4)
17
     ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
19
     ! we first assign the values of the coefficients.
     Hcoef
              = 0.0 \, DP
21
     Hcoef(1) = 3.0 DP
     Hcoef(3) = -6.0 DP
23
     Hcoef(5) = 1.0 DP
```

```
25
     Hermite4 = Hcoef
27
     ! Now compute the derivative of Hermite4
     Res = Deriv (Hermite4)
29
     ! From the recursion relation of the Hermite polynomials
31
     ! we should obtain twwice the same number:
     X = 7.346582 DP
33
     Write(*,'(ES33.25)') Value(Res, X)
     Write (*, '(ES33.25)')4.0 DP*Value (Hermite3, X)
35
37
     Stop
   End Program TestPoly
```

10.11 Function Integra(P[, Cte])

10.11.1 Description

Computes the integral of the polynomial P. If Cte is present then it is used as *integration* constant.

10.11.2 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.

10.11.3 Output

Type Pol. Another polynomial: the integral of P.

10.11.4 Examples

Listing 10.11: Computing the integral of a polynomial.

```
Program TestPoly
     USE NumTypes
3
     USE Error
     USE Polynomial
5
     Integer, Parameter :: Deg = 4
7
     Real (kind=DP) :: Hcoef(Deg+1), X
     Type (Pol) :: Hermite4, Hermite3, Res, Sum
9
     ! The Third Hermite polynomial is x^3 - 3x, so
11
     ! we first assign the values of the coefficients.
     Hcoef
              = 0.0 \, DP
13
```

```
Hcoef(2) = -3.0 DP
     Hcoef(4) = 1.0 DP
15
17
     Hermite3 = Hcoef(1:4)
     ! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
19
     ! we first assign the values of the coefficients.
                  0.0 \, \mathrm{DP}
21
     Hcoef(1) =
                  3.0_DP
     Hcoef(3) = -6.0 DP
23
     Hcoef(5) =
                  1.0_DP
25
     Hermite4 = Hcoef
27
     ! Now compute the derivative of Hermite4
     Res = Integra (Hermite3, 3.0 DP/4.0 DP)
29
     ! From the recursion relation of the Hermite polynomials
31
     ! we should obtain twwice the same number:
     X = 7.346582 DP
33
     Write (*, '(ES33.25)') Value (Res, X)
     Write (*, '(ES33.25)')0.25_DP*Value (Hermite4, X)
35
37
     Stop
   End Program TestPoly
```

10.12 Function InterpolValue(X, Y, Xo)

10.12.1 Description

Computes the value of the interpolation polynomial that pass trough (X(:), Y(:)) in the point Xo.

10.12.2 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.

10.12.3 Output

Real double precision if input is real and complex double precision if input is complex. The value of the interpolation polynomial in Xo.

10.12.4 Examples

Listing 10.12: Compute values of the Interpolation polynomial.

```
Program TestPoly
     USE NumTypes
3
     USE Error
     USE Polynomial
5
     Integer, Parameter :: Deg = 4, Np = 7
7
     Real (kind=DP) :: Hcoef(Deg+1), X, Xp(Np), Yp(Np)
     Type (Pol) :: Hermite4, Hermite3, Res, Sum
9
11
     CALL Random_Number(Xp)
     Yp = 3.347234 DP*Xp - 2.475875 DP*Xp**3 - 7.23467 DP*Xp**4 + &
13
          & 1.47854_DP*Xp**6
15
     ! Now we compute the value of the interpolation polynomial
     ! at X, and compare it with the real value of the Polynomial
17
     X = -1.23899843 DP
     Write (*, '(ES33.25)') InterpolValue (Xp, Yp, X)
19
     Write (*, '(ES33.25)')3.347234 DP*X -2.475875 DP*X**3 -\&
          & 7.23467 DP*X**4 + 1.47854 DP*X**6
21
23
     Stop
   End Program TestPoly
25
```

10.13 Function Interpol(X, Y)

Computes the interpolation polynomial that pass trough (X(:), Y(:)). Note that using this function can be very unstable.

10.13.1 Arguments

X(:), Y(:): Real double precision or Complex double precision one dimensional arrays. Specify the points at which the interpolation polynomial should pass.

10.13.2 Output

Type Pol if input is real, and CmplxPol if input is complex. The interpolation polynomial.

10.13.3 Examples

Listing 10.13: 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)
9
     Type (Pol) :: Hermite4, Hermite3, Res, Sum
11
     CALL Random_Number(Xp)
     Yp = 3.347234 DP*Xp - 2.475875 DP*Xp**3 - 7.23467 DP*Xp**4 + &
13
          & 1.47854 DP*Xp**6
15
     ! Now we compute the interpolation polynomial
     ! at X, and compare it with the real value of the Polynomial
17
     X = -1.23899843 DP
19
     Res = Interpol(Xp, Yp)
     Write (*, '(ES33.25)') Value (Res, X)
     Write (*, '(ES33.25)')3.347234_DP*X - 2.475875_DP*X**3 - &
21
          & 7.23467 DP*X**4 + 1.47854 DP*X**6
23
     Stop
25
   End Program TestPoly
```

10.14 Subroutine Spline(X, Y, Ypp0, YppN, Pols)

10.14.1 Description

Compute the cubic spline interpolation polynomial that pass trough (X(:), Y(:)).

10.14.2 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.

10.14.3 Examples

Listing 10.14: 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)
```

```
Type (Pol) :: Hermite4, Hermite3, Res, Sum, Spl(Np-1)
10
12
     CALL Random_Number(Xp)
     ! Order Xp
14
     CALL Qsort(Xp)
     Yp = 3.347234 DP*Xp - 2.475875 DP*Xp**3 - 7.23467 DP*Xp**4 + &
16
          & 1.47854_DP*Xp**6
18
     ! Now we compute the interpolation polynomial
     ! at X, and compare it with the real value of the Polynomial, and
20
     ! the value of the spline cubic interpolation polynomial.
     X = 0.23899843 DP
22
     Res = Interpol(Xp, Yp)
     CALL Spline (Xp, Yp, 0.0 DP, 0.0 DP, Spl)
24
     Write (*, '(ES33.25)') Value (Res, X)
     Write (*, '(ES33.25)') Value (Spl(Locate(Xp, X)), X)
^{26}
     Write(*,'(ES33.25)')3.347234_DP*X - 2.475875_DP*X**3 - &
          & 7.23467 DP*X**4 + 1.47854 DP*X**6
28
30
     Stop
   End Program TestPoly
```

Eleven

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.

11.1 Subroutine RootPol(a, b, [c, d], z1, z2, [z3, z4])

11.1.1 Description

Returns the complex roots of a polynomial of degree 2, 3 or 4.

11.1.2 Arguments

a, b, c, d: The coefficients of the polynomial. The meaning of the coefficieents a, b, c, d depends on the degree of the polynomial:

$$P(x) = x^{2} + ax + b$$

 $P(x) = x^{3} + ax^{2} + bx + c$
 $P(x) = x^{4} + ax^{3} + bx^{2} + cx + d$

z1,z2,z3,z4: Complex simple or double precision. The roots of the polynomial.

11.1.3 Examples

Listing 11.1: 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
```

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```
10
     CALL Random_Number(a)
12
     CALL Random_Number(b)
     CALL Random_Number(c)
     CALL Random_Number(d)
14
     CALL RootPol(a,b,z1,z2)
     Write (*, '(3ES20.12)') Z1, Abs (z1**2 + a*z1 + Cmplx(b, kind=DPC))
16
     Write(*,'(3ES20.12)')Z2, Abs(z2**2 + a*z2 + Cmplx(b,kind=DPC))
18
     CALL RootPol(a,b,c, z1,z2, z3)
     Write(*,*)
20
     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)
     bc = Cmplx(b,a,kind=DPC)
26
     cc = Cmplx(c, kind=DPC)
     dc = Cmplx(d, kind=DPC)
28
     CALL RootPol(ac, bc, z1, z2)
     Write(*,*)
30
     Write (*, '(3 \times 20.12)') \times 1, Abs(z1**2 + ac*z1 + Cmplx(bc, kind=DPC))
     Write(*,'(3ES20.12)')Z2, Abs(z2**2 + ac*z2 + Cmplx(bc,kind=DPC))
32
     CALL RootPol(ac, bc, cc, dc, z1, z2, z3, z4)
     Write (*, '(3ES20.12)') Z1, Abs(z1**4+ac*z1**3+bc*z1**2+cc*z1+dc)
     Write (*, '(3 \times 20.12)') \times 2, Abs (z2**4+ac*z2**3+bc*z2**2+cc*z2+dc)
36
     Write (*, '(3 \times 20.12)') \times 23, Abs (z3**4+ac*z3**3+bc*z3**2+cc*z3+dc)
     Write(*,'(3ES20.12)')Z4, Abs(z4**4+ac*z4**3+bc*z4**2+cc*z4+dc)
38
40
     Stop
   End Program TestRoot
```

11.2 Function Newton(Xo, Fnew, [Tol])

11.2.1 Description

Compute a root of the function defined by the routine Fnew.

11.2.2 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.

11.2.3 Output

Real single or double precision. The position of the root.

11.2.4 Examples

Listing 11.2: Computing roots of non-linear functions with the Newton method.

```
Program TestRoot
2
     USE NumTypes
     USE Error
4
     USE Root
6
     Real (kind=DP) :: a, b, c, d, X
     Complex (kind=DPC) :: z1, z2, z3, z4, ac, bc, cc, dc
8
10
     Interface
        Subroutine FNew(Xo, F, D)
12
          USE NumTypes
14
          Real (kind=DP), Intent (in) :: Xo
16
          Real (kind=DP), Intent (out) :: F, D
        End Subroutine FNew
18
     End Interface
20
     ! Compute the value such that cos(x) = x
22
     X = Newton(0.0 DP, Fnew, 1.0E-10DP)
     Write (*, '(1A, ES33.25)') 'Point:
24
     Write(*,'(1A,ES33.25)')' Value of Cos: ', Cos(X)
26
     Stop
28
```

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```
End Program TestRoot
30
                     ******
32
   Subroutine FNew(Xo, F, D)
34
     **********
36
     USE NumTypes
38
     Real (kind=DP), Intent (in) :: Xo
     Real (kind=DP), Intent (out) :: F, D
40
42
     F = Xo - Cos(Xo)
    D = 1.0 \text{-DP} + \text{Sin}(X_0)
44
46
     Return
   End Subroutine FNew
```

11.3 Function Bisec(a, b, Fbis, [Tol])

11.3.1 Description

Compute the root of the function defined by Fbis.

11.3.2 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.

11.3.3 Output

Real single or double precision. The position of the root of Fbis.

11.3.4 Examples

Listing 11.3: Computing roots with the bisection method.

```
Program TestRoot
     USE NumTypes
3
     USE Error
     USE Root
5
     \texttt{Real} \ (\texttt{kind=}DP) \ :: \ a \,, \ b \,, \ c \,, \ d \,, \ X
7
     9
     Interface
        Function Fbis(X)
11
          USE NumTypes
13
          Real (kind=DP), Intent (in) :: X
15
          Real (kind=DP) :: Fbis
        End Function Fbis
17
     End Interface
19
     ! Compute the value such that cos(x) = x
    X = Bisec(0.0 DP, 1.1 DP, Fbis, 1.0E-10 DP)
21
     Write (*, '(1A, ES33.25)') 'Point:
     Write (*, '(1A, ES33.25)') 'Value of Cos: ', Cos(X)
23
25
     Stop
   End Program TestRoot
27
29
   ! **********
   Function FBis(X)
31
   ! **********
33
     USE NumTypes
35
     \texttt{Real (kind=}DP)\,,\;\;\texttt{Intent (in)}\;::\;\;X
37
     Real (kind=DP) :: Fbis
39
     Fbis = X - Cos(X)
41
     Return
43
   End Function FBis
```

Twelve

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.

12.1 Type Fourier_Serie

12.1.1 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.

12.1.2 Components

Coef(:): Complex double precision one dimensional array. The modes.

Nterm: Integer. The number of terms of the Fourier series.

12.1.3 Examples

A small example showing how to define a Fourier serie.

Listing 12.1: Defining a Fourier serie.

```
Program TestFourier

USE NumTypes
USE Constants
USE Fourier

Type (Fourier_Serie) :: Ff

Stop
End Program TestPoly
```

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12.2 Type Fourier_Serie_2D

12.2.1 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.

12.2.2 Components

Coef(:,:): Complex double precision two dimensional array. The modes.

Nterm: Integer. The number of terms of the Fourier series.

12.2.3 Examples

A small example showing how to define a polynomial.

Listing 12.2: Defining a two-dimensional Fourier serie.

```
Program TestFourier

USE NumTypes
USE Constants
USE Fourier

Type (Fourier_Serie_2D) :: Ff

Stop
End Program TestPoly
```

12.3 Assignment

12.3.1 Description

You can directly assign one defined Fourier series (one or two dimensional) to another.

12.3.2 Examples

This example uses the Init_Serie subroutine. For details of the usage of this function look at the section (12.8), page (86).

Listing 12.3: 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)
```

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```
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
```

12.4 Operator +

12.4.1 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.

12.4.2 Examples

This example uses the Init_Serie subroutine. For details of the usage of this function look at the section (12.8), page (86).

Listing 12.4: Adding Fourier series.

```
Program TestFourier
     USE NumTypes
3
     USE Constants
     USE Fourier
5
7
     Type (Fourier_Serie_2D) :: FS1, FS2, FS3
     Integer :: Nt
9
     Nt = 4
     CALL Init_Serie (FS1, Nt)
11
     CALL Init_Serie (FS2, Nt)
13
     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)
15
     FS2\%Coef(1,1) = Cmplx(-1.0 DP, 4.5 DP, kind=DPC)
17
     FS2\%Coef(-1,1) = Cmplx(-1.0 DP, -6.78745 DP, kind=DPC)
19
     FS3 = FS1 + FS2
21
     Write (*, '(2ES33.25)')FS3%Coef(1,1)
23
     Write (*, '(2ES33.25)')FS3\%Coef(-1,1)
     Stop
25
   End Program TestFourier
```

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12.5 Operator -

12.5.1 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.

12.5.2 Examples

Listing 12.5: Subtracting Fourier series

```
Program TestFourier
2
     USE NumTypes
     USE Constants
4
     USE Fourier
6
     Type (Fourier_Serie) :: FS1, FS2, FS3
     {\tt Integer} \; :: \; \, Nt
8
     Nt = 4
10
     CALL Init_Serie (FS1, Nt)
12
     FS1\%Coef(1) = Cmplx(1.0 DP, 0.5 DP, kind=DPC)
     FS1\%Coef(-1) = Cmplx(1.0\_DP, 0.7\_DP, kind=DPC)
14
     FS2 = FS1
16
     FS3 = FS1 - FS2
18
     Write (*, '(2ES33.25)')FS3%Coef(1)
     Write (*, '(2ES33.25)') FS3%Coef (-1)
20
22
     Stop
   End Program TestFourier
```

12.6 Operator *

12.6.1 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.

12.6.2 Examples

Listing 12.6: Computing the convolution of Fourier series.

```
Program TestFourier

USE NumTypes
USE Constants
```

```
USE Fourier
5
     Type (Fourier_Serie) :: FS1, FS2, FS3
7
     Integer :: Nt
9
     Nt = 4
     CALL Init_Serie (FS1, Nt)
11
     FS1\%Coef(1) = Cmplx(1.0 DP, 0.5 DP, kind=DPC)
13
     FS1\%Coef(-1) = Cmplx(1.0 DP, 0.7 DP, kind=DPC)
15
     FS2 = FS1
17
     FS3 = FS1 * FS2
     Write (*, '(2ES33.25)')FS3%Coef(0)
19
     Stop
21
   End Program TestFourier
```

12.7 Operator **

12.7.1 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.

12.7.2 Examples

Listing 12.7: "Exponentiating" Fourier series.

```
Program TestFourier
2
     USE NumTypes
     USE Constants
4
     USE Fourier
6
     Type (Fourier_Serie) :: FS1, FS2, FS3
     {\tt Integer} \; :: \; \, Nt
8
     Nt = 4
10
     CALL Init_Serie (FS1, Nt)
     CALL Init_Serie (FS2, Nt)
12
     CALL Init_Serie (FS3, Nt)
14
     FS1\%Coef(1) = Cmplx(1.0DP, 0.5DP, kind=DPC)
     FS1\%Coef(-1) = Cmplx(1.0 DP, 0.7 DP, kind=DPC)
16
     FS3\%Coef(0) = Cmplx(1.0 DP, 0.0 DP, kind=DPC)
18
     FS2 = FS1**8
20
```

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```
Do I = 1, 8
    FS3 = FS3 * FS1
    End Do

Write(*,'(2ES33.25)')FS2%Coef( 0)
Write(*,'(2ES33.25)')FS3%Coef( 0)

Stop
End Program TestFourier
```

12.8 Subroutine Init_Serie(FS,Ns)

12.8.1 Description

Allocate memory space for the modes of a one or two dimensional Fourier series.

12.8.2 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.

12.8.3 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 12.8: Initialising a Fourier series.

```
Program TestFourier
1
     USE NumTypes
3
     USE Constants
     USE Fourier
5
     Type (Fourier_Serie) :: FS1, FS2, FS3
7
     Integer :: Nt
9
     Nt = 4
     CALL Init_Serie (FS1, Nt)
11
     FS1\%Coef(1) = Cmplx(1.0 DP, 0.5 DP, kind=DPC)
13
     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)
     Stop
21
   End Program TestFourier
```

12.9 Function Eval_Serie(FS, X, [Y], Tx, [Ty])

12.9.1 Description

Compute the value of the Fourier series FS with periods Tx, Ty at the point X, Y.

12.9.2 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.

12.9.3 Output

Real double precision. The value of the function defined by the modes in FS at the point (X[,Y]).

12.9.4 Examples

Listing 12.9: Evaluating a Fourier series at a point.

```
Program TestFourier
2
     USE NumTypes
     USE Constants
4
     USE Fourier
6
     Type (Fourier_Serie) :: FS1, FS2, FS3
     Integer :: Nt
8
     Nt = 4
10
     CALL Init_Serie (FS1, Nt)
     CALL Init_Serie (FS2, Nt)
12
     CALL Init_Serie (FS3, Nt)
14
     FS1\%Coef(1) = Cmplx(1.0 DP, 0.5 DP, kind=DPC)
16
     FS1\%Coef(-1) = Cmplx(1.0 DP, 0.7 DP, kind=DPC)
18
     FS2 = FS1**2
20
     FS3 = FS1*FS2
^{22}
     Write (*, '(2ES33.25)') Eval_Serie (FS1,0.12_DP,1.0_DP) * &
                          & Eval_Serie (FS2, 0.12_DP, 1.0_DP)
24
     Write (*, '(2ES33.25)') Eval_Serie (FS3,0.12_DP,1.0_DP)
26
```

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```
Stop
28 End Program TestFourier
```

12.10 Function Unit(FS, Ns)

12.10.1 Description

Allocate memory space for the modes of a one or two dimensional Fourier series and sets the zero mode equal to 1.

12.10.2 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.

12.10.3 Examples

Listing 12.10: Obtaining a constant Fourier series.

```
Program TestFourier
     USE NumTypes
     USE Constants
4
     USE Fourier
6
     Type (Fourier_Serie) :: FS1, FS2, FS3
     Integer :: Nt
8
     Nt = 4
10
     CALL Init_Serie (FS1, Nt)
     CALL Init_Serie (FS2, Nt)
12
     CALL Init_Serie (FS3, Nt)
14
     FS1\%Coef(1) = Cmplx(1.0 DP, 0.5 DP, kind=DPC)
16
     FS1\%Coef(-1) = Cmplx(1.0 DP, 0.7 DP, kind=DPC)
18
     CALL Unit (FS2, Nt)
20
     FS3 = FS1*FS2
22
     Write (*, '(2ES33.25)') Eval_Serie (FS1,0.12_DP,1.0_DP)
     Write (*, '(2ES33.25)') Eval_Serie (FS3,0.12_DP,1.0_DP)
24
26
     Stop
   End Program TestFourier
```

12.11 Function DFT(Data, Is)

12.11.1 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

$$\tilde{f}(k) = \sum_{n=0}^{N} f_n e^{\frac{2\pi i n}{N}} \qquad \forall k \in \left[-\frac{N}{2}, \frac{N}{2} \right]$$

the inverse one is defined as

$$\tilde{f}(k) = \frac{1}{N} \sum_{n=0}^{N} f_n e^{\frac{-2\pi i n}{N}} \qquad \forall k \in \left[-\frac{N}{2}, \frac{N}{2} \right]$$

12.11.2 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.

12.11.3 Output

Type Fourier_Serie if Data(:) is one dimensional, and type Fourier_Serie_2D if Data(:,:) is two dimensional.

12.11.4 Examples

This example compute the discrete Fourier transform of $f(x_i) = \sin(x_i)$.

Listing 12.11: Computing the Discrete Fourier Transform.

```
Program TestFourier
     USE NumTypes
3
     USE Constants
     USE Fourier
5
     Integer, Parameter :: Nmax=20
7
     Type (Fourier_Serie) :: FS1, FS2, FS3
     Complex (kind=DPC) :: Data(Nmax), X
9
     Integer :: Nt
11
     Do I = 1, Nmax
        X = Cmplx(TWOPLDP*I/Nmax)
13
        Data(I) = Sin(X)
     End Do
15
     FS1 = DFT(Data)
17
```

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```
Write(*,'(1A,2ES33.25)')'Mode k= 1: ', FS1%Coef( 1)
Write(*,'(1A,2ES33.25)')'Mode k=-1: ', FS1%Coef(-1)
Write(*,'(ES33.25)')Sum(Abs(FS1%Coef(:)))

Stop
End Program TestFourier
```

12.12 Function Conjg(FS)

12.12.1 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 $\tilde{f}(-k)$.

12.12.2 Arguments

FS: Type Fourier_Serie or type Fourier_Serie_2D. The Fourier series whose conjugate you want to compute.

12.12.3 Output

Type Fourier_Serie if FS is of type Fourier_Serie, and type Fourier_Serie_2D if FS is of Type Fourier_Serie_2D.

12.12.4 Examples

Listing 12.12: Computing the Conjugate Fourier Series.

```
Program TestFourier
2
     USE NumTypes
     USE Constants
4
     USE Fourier
6
     Integer, Parameter :: Nmax=20
     Type (Fourier_Serie) :: FS1, FS2, FS3
8
     Integer :: Nt
10
     Do I = 1, Nmax
12
       X = Cmplx(TWOPLDP*I/Nmax, kind=DPC)
       Data(I) = Sin(X) + Cmplx(0.0 DP, I*2.0 DP, kind=DPC)
14
     End Do
16
     FS1 = DFT(Data)
18
     Write (*, '(2ES33.25)') Eval_Serie (FS1,0.23_DP,1.0_DP)
     Write (*, '(2ES33.25)') Eval_Serie (Conjg (FS1), 0.23_DP, 1.0_DP)
20
```

```
Stop
24 End Program TestFourier
```

12.13 Subroutine Save_Serie(FS, File)

12.13.1 Description

Write the Fourier series FS to the file File.

12.13.2 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.

12.13.3 Examples

Listing 12.13: Saving a Fourier Serie in a file.

```
Program TestFourier
2
      USE NumTypes
4
      USE Constants
      USE Fourier
6
      Integer, Parameter :: Nmax=20
      Type (Fourier_Serie) :: FS1, FS2, FS3
8
      \begin{array}{lll} {\tt Complex} & ({\tt kind}\!\!=\!\!\!DPC) & :: & {\tt Data}(Nmax)\,, \ X \end{array}
      Integer :: Nt
10
      Do I = 1, Nmax
12
         X = Cmplx(TWOPLDP*I/Nmax, kind=DPC)
          Data(I) = Sin(X) + Cmplx(0.0 DP, I*2.0 DP, kind=DPC)
14
      End Do
16
      FS1 = DFT(Data)
18
      CALL Save (FS1, 'datamodes.dat')
20
      Stop
   End Program TestFourier
```

12.14 Subroutine Read_Serie(FS, File)

12.14.1 Description

Reads the Fourier series FS stored in the file File.

92 MODULE Fourier

12.14.2 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.

12.14.3 Examples

Listing 12.14: Reading a Fourier serie from a file.

```
Program TestFourier
2
     USE NumTypes
     USE Constants
4
     USE Fourier
6
     Integer, Parameter :: Nmax=20
     Type (Fourier_Serie) :: FS1, FS2, FS3
8
     Complex (kind=DPC) :: Data(Nmax), X
     Integer :: Nt
10
     Do I = 1, Nmax
12
        X = Cmplx(TWOPLDP*I/Nmax, kind=DPC)
        Data(I) = Sin(X) + Cmplx(0.0 DP, I*2.0 DP, kind=DPC)
14
     End Do
16
     FS1 = DFT(Data)
18
     CALL Save_Serie (FS1, 'datamodes.dat')
     CALL Read_Serie (FS2, 'datamodes.dat')
20
     Write(*,'(ES33.25)')Sum(Abs(FS1%Coef(:) - FS2%Coef(:)))
22
24
   End Program TestFourier
26
```

Thirteen

MODULE Time

Th MODULE Time is a module to provide access to date and time properties.

13.1 Type tm

13.1.1 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...

13.1.2 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].
```

13.1.3 Example

A small example defining a tm data type.

Listing 13.1: Defining a Time data type.

```
Program Test

USE NumTypes
USE Time
```

```
Type (tm) :: Oneday

OneDay%hour = 12
OneDay%min = 0
OneDay%sec = 0
OneDay%mday = 10
OneDay%mon = 0
OneDay%year = 2007
OneDay%wday = 3

Stop
End Program Test
```

13.2 Function gettime()

13.2.1 Description

The function gettime() returns the current time and date in a type tm data type.

13.2.2 Arguments

This function has no arguments.

13.2.3 Output

Type tm, containing all the information about the date and time.

13.2.4 Example

A small program that prints the current year.

Listing 13.2: Obtaining the current date and time.

```
Program Test

USE NumTypes
USE Time

Type (tm) :: Oneday

Oneday = gettime()

Write(*,*)'Current year: ', Oneday%year

Stop
End Program Test
```

13.3 Function isleap(Nyr)

13.3.1 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* 1582¹.

13.3.2 Arguments

Nyr: Integer. The year.

13.3.3 Output

Logical. .true. if Nyr is a leap year, and .false. otherwise.

13.3.4 Example

A small program that tell us if the current year is leap.

Listing 13.3: Are we in a leap year?.

```
Program Test
     USE NumTypes
3
     USE Time
5
     Type (tm) :: Oneday
7
     Oneday = gettime()
9
     If (isleap(Oneday%year)) Then
       Write(*,*)'We are in a leap year.'
11
       Write(*,*)'We are not in a leap year.'
13
     End If
15
     Stop
   End Program Test
```

13.4 Function asctime(t)

13.4.1 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:

¹For more details, take a look at

Wed Jan 10 19:15:49 2007

13.4.2 Arguments

t: Type tm. A Type tm data type containing the date and time.

13.4.3 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.

13.4.4 Example

A small program that prints the current time.

Listing 13.4: Printing current date/time.

```
Program Test

USE NumTypes
USE Time

Write(*,'(1A)') asctime(gettime())

Stop
End Program Test
```

13.5 Function Day_of_Week(Day, Month, Year)

13.5.1 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.

13.5.2 Arguments

Day: Integer. The day of the month [1-31].

Month: Integer. The month of the year [0-11].

Year: Integer. The year.

13.5.3 Output

Integer. The day of the week since sunday, thus a number between 0 and 6, with 0 corresponding to sunday.

13.5.4 Example

A small program that prints the date and time of the first of january of 1900.

Listing 13.5: Day of week of the first of January 1900.

```
Program Test
     USE NumTypes
3
     USE Time
5
     Type (tm) :: Oneday
7
     Oneday%hour = 12
     Oneday%min = 0
9
     OneDay\%sec = 0
     OneDay%mday = 1
11
     OneDaymon = 0
     OneDay\%year = 1900
13
     OneDay\%wday = Day_of_Week(Oneday\%mday, Oneday\%mon, Oneday\%year)
15
     Write(*,*) asctime(Oneday)
17
     Stop
19
   End Program Test
```

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