

# A FORTRAN 90 numerical library

Alberto Ramos. Madrid, November 2006.

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# Generalities

---

This is the documentation of a total of eleven 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 License (<http://www.gnu.org/copyleft/gpl.html>) 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>

Enjoy programming.

## Installation

To install this library in a Unix/Linux environment, simply edit the Makefile file, and set the F90 and F90OPT variables to whatever your compiler and your favourite optimisation flags are. After running make you should obtain a file called libf90.a, and probably (that depends on 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 contains the definition of Single Precision, and Double Precision data. All the other numerical modules use 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 portable 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.

```
.  
.   
USE NumTypes  
.   
.   
Real (kind=SP) :: A
```

```
Real (kind=DP) :: D
Complex (kind=SPC) :: Ac
Complex (kind=DPC) :: Dc
.
.
```

# Two

---

## MODULE Constants

---

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

### 2.1 Name conventions

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

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

### 2.2 $\pi$ -related constants

#### 2.2.1 Real

The complex  $\pi$ -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	$\pi$
TWOPI_SP	TWOPI_DP	$2\pi$
HALFPI_SP	HALFPI_DP	$\frac{\pi}{2}$

Table 2.1:  $\pi$ -related real constants defined in the `MODULE constants`.

#### 2.2.2 Complex

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

### 2.3 Square roots and log related constants

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

SPC Name	DPC Name	Value
UNITIMAG_SPC	UNITIMAG_DPC	$\iota$
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:  $\pi$ -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  $\gamma$  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

Program Test

USE Error

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

Stop

End Program Test

### 3.2 Routines

#### 3.2.1 Subroutine `perror([routine], msg)`

##### 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.

##### 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.

### Examples

```
Program Test
  USE Error
```

```
  Integer :: N1, N2
```

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

```
  If (N2 == 0) Then
    CALL Perror('Test', 'Division by cero. I will print the product of the two numbers')
    Write(*,*)N1*N2
  Else
    Write(*,*)N1/N2
  End If
```

```
  Stop
End Program Test
```

### 3.2.2 Subroutine abort([routine], msg)

#### 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.

#### 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.

### Examples

```
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 Numerical integration of functions

#### 4.1.1 Function Trapecio(a, b, Func, [Tol])

##### Description

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

##### 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`.

## Output

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

## Examples

```

Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol

  Interface
    Function Fint(X)
      USE NumTypes

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

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

  Stop
End Program Test

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

  USE NumTypes

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

  Fint = X**2

  Return
End Function Fint

```

### 4.1.2 Function Simpson(a, b, Func, [Tol])

#### 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 **Trapeccio**.

#### 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  $Tol = 0.01$ .

#### Output

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

#### Examples

Program Test

```
USE NumTypes
USE Integration
```

```
Real (kind=DP) :: Tol
```

```
Interface
  Function Fint(X)
    USE NumTypes

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

```

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

Stop
End Program Test

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

USE NumTypes

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

Fint = X**2

Return
End Function Fint

```

#### 4.1.3 Function TrapecioAb(a, b, Func, [Tol])

##### Description

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

##### 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`.



## Output

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

## Examples

```

Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol

  Interface
    Function Fint(X)
      USE NumTypes

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

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

  Stop
End Program Test

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

  USE NumTypes

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

  Fint = X**2

  Return
End Function Fint

```

#### 4.1.4 Function SimpsonAb(a, b, Func, [Tol])

##### 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 `TrapeccioAb`

##### 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`.

##### Output

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

##### Examples

Program Test

```
USE NumTypes
USE Integration
```

```
Real (kind=DP) :: Tol
```

```
Interface
  Function Fint(X)
    USE NumTypes

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

```

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

Stop
End Program Test

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

USE NumTypes

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

Fint = X**2

Return
End Function Fint

```

#### 4.1.5 Function SimpsonInfUp(a, Func, [Tol])

##### Description

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

##### 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  $Tol = 0.01$ .

## Output

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

## examples

```

Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol

  Interface
    Function Fint(X)
      USE NumTypes

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

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

  Stop
End Program Test

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

  USE NumTypes

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

  Fint = exp(-X**2)

  Return
End Function Fint

```

### 4.1.6 Function SimpsonInfDw(a, Func, [Tol])

#### 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.

#### 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`.

#### Output

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

#### examples

Program Test

```
USE NumTypes
USE Integration
```

```
Real (kind=DP) :: Tol
```

```
Interface
```

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

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

```
  End Function Fint
End Interface
```

```

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

Stop
End Program Test

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

USE NumTypes

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

Fint = exp(-X**2)

Return
End Function Fint

```

#### 4.1.7 Function SimpsonSingUp(a, b, Func, [Tol], gamma)

##### 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  $0 < \gamma < 1$ .

##### 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  $\text{Tol} = 0.01$ .

**gamma:** The “degree of divergence” of the function in  $x \approx b$ .

## Output

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

## Examples

Program Test

```

    USE NumTypes
    USE Integration

```

```

    Real (kind=DP) :: Tol

```

Interface

```

    Function Fint(X)
        USE NumTypes

```

```

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

```

```

        Real (kind=DP) :: Fint

```

```

    End Function Fint

```

End Interface

```

    Tol = 1.0E-6_DP

```

```

    Write(*,*)'Integral of 1/sqrt(-x) between -1 and 0:'

```

```

    Write(*,*)SimpsonSingUp(-1.0_DP, 0.0_DP, Fint, Tol, 0.5_DP)

```

Stop

End Program Test

```

! *****

```

```

! *

```

```

Function Fint(X)

```

```

! *

```

```

! *****

```

```

    USE NumTypes

```

```

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

```

```

    Real (kind=DP) :: Fint

```

```

    Fint = Sqrt(-X)

    Return
End Function Fint

```

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

##### 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  $0 < \gamma < 1$ .

##### 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  $x \approx a$ .

##### Output

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

##### Examples

```

Program Test
  USE NumTypes
  USE Integration

  Real (kind=DP) :: Tol

```



```

Interface
  Function Fint(X)
    USE NumTypes

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

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

Stop
End Program Test

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

USE NumTypes

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

Fint = Sqrt(X)

Return
End Function Fint

```

## 4.2 Numerical integration of ODE's

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

#### 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:

$$\frac{dy_i(x)}{dx} = f_i(y_j, x)$$

and the initial conditions:

$$y_i(x_0)$$

After the integration we get:

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

So to define a set of first order ODE's we need the value of the derivative of the variable  $i$  in the 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**)

### 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.

### Output

A vector that contains the values of the functions  $y_i$  in the point **Xfin**.

### Examples

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

$$\frac{dy_1(x)}{dx} = y_2(x); \quad \frac{dy_2(x)}{dx} = -y_1(x)$$

And which solution is clearly:

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

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

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

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, these values with the real ones.

```

Program Test
  USE NumTypes
  USE Integration

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

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

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

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

  Stop
End Program Test

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

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

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

  Return
End Function FEuler

```

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

#### 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:

$$\frac{dy_i(x)}{dx} = f_i(y_j, x)$$

and the initial conditions:

$$y_i(x_0)$$

After the integration we get:

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

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

#### 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.

#### Output

A vector that contains the values of the functions  $y_i$  in the point **Xfin**.

**Examples**

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

$$\frac{dy_1(x)}{dx} = y_2(x); \quad \frac{dy_2(x)}{dx} = -y_1(x)$$

And which solution is clearly:

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

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

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

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 Euler, the Runge-Kutta and the exact values.

**Program Test**

```
USE NumTypes
```

```
USE Integration
```

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

**Interface**

```
Function Feuler(X, Y) Result (Func)
```

```
USE NumTypes
```

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

```
Real (kind=DP) :: Func(Size(Y))
```

```
End Function Feuler
```

```
End Interface
```

```
Tol = 1.0E-3_DP
```

```
In(1) = 0.0_DP
```

```
In(2) = 1.0_DP
```

```
Write(*,*)'Values of sin(1) and cos(1): '
```

```
Write(*,*)' Euler: '
```

```
Write(*,*)Euler(In, 0.0_DP, 1.0_DP, Feuler, Tol)
```

```
Write(*,*)' Runge-Kutta: '
```

```
Write(*,*)Rgnkta(In, 0.0_DP, 1.0_DP, Feuler, Tol)
```

```
Write(*,*)' Exact: '
```

```
Write(*,*)Sin(1.0_DP), Cos(1.0_DP)
```

```
Stop
```

```
End Program Test
```

```
! *****
```

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

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

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

  Return
End Function FEuler
```

# Five

---

## 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.

### 5.1 Subroutine `Pivoting(M,Ipiv,Idet)`

#### 5.1.1 Description

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

#### 5.1.2 Arguments

`M(:, :)`: Real 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 vector. 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

#### 5.1.3 Examples

Program `TestLinear`

```
USE NumTypes
USE Linear
```

```
Integer, Parameter :: Nord = 4
```

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

```
Integer :: Ipiv(Nord), Iperm
```

```

! Fill M of random numbers
CALL Random_Number(M)

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

CALL Pivoting (M, Ipiv, Iperm)
Write(*,*)'Permuted M: '
Do I = 1, Nord
  Write(*, '(100ES10.3)')(M(I,J), J = 1, Nord)
End Do

Stop
End Program TestLinear

```

## 5.2 Subroutine LU(M, Ipiv, Idet)

### 5.2.1 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

$$M = LU \quad (5.1)$$

and  $L$  is lower triangular, and  $U$  upper triangular.

$$L = \begin{pmatrix} 1 & 0 & 0 & \dots \\ L_{21} & 1 & 0 & \dots \\ L_{31} & L_{32} & 1 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}; \quad U = \begin{pmatrix} U_{11} & U_{12} & U_{13} & \dots \\ 0 & U_{22} & U_{23} & \dots \\ 0 & 0 & U_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (5.2)$$

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*  $M$ .

### 5.2.2 Arguments

**M(:, :):** Real 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 vector. 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



## 5.2.3 Examples

Program TestLinear

```

USE NumTypes
USE Linear

Integer, Parameter :: Nord = 4

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

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

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

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

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

```

```

M = MatMul(L,U)
Write(*,*)'LU (Same as M with some rows permuted): '
Do I = 1, Nord
  Write(*,'(100ES10.3)')(M(I,J), J = 1, Nord)
End Do

Stop
End Program TestLinear

```

### 5.3 Subroutine LUsolve(M, b)

#### 5.3.1 Description

Solves the linear system of equations

$$\begin{aligned}
 M_{11}x_1 + M_{12}x_2 + M_{13}x_3 + M_{14}x_4 + \dots &= b_1 \\
 M_{21}x_1 + M_{22}x_2 + M_{23}x_3 + M_{24}x_4 + \dots &= b_2 \\
 &\vdots
 \end{aligned}
 \tag{5.3}$$

#### 5.3.2 Arguments

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

**b(:):** Real single or double precision vector. The independent terms before calling the routine, and the solution after calling it. *Note that b is overwritten when calling this routine.*

#### 5.3.3 Examples

Program TestLinear

```

USE NumTypes
USE Linear

Integer, Parameter :: Nord = 10

Real (kind=DP) :: M(Nord,Nord), L(Nord,Nord), U(Nord,Nord), &
  & Mcp(Nord,Nord), b(Nord), bcp(Nord)
Integer :: I piv(Nord), Iperm

! Fill M and b of random numbers, and make a copy of both
CALL Random_Number(M)
CALL Random_Number(b)
Mcp = M
bcp = b

```

```

! Solve the linear system
CALL LUsolve(M,b)

! Check that it is a solution:
b = MatMul(Mcp,b)
Write(*,*)'b: '
Write(*,'(100ES10.3)')(Abs(bcp(I)-b(I)), I = 1, Nord)

Stop
End Program TestLinear

```

## 5.4 Function Det(M)

### 5.4.1 Description

Computes the determinant of the matrix  $M$ .

### 5.4.2 Arguments

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

### 5.4.3 Output

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

### 5.4.4 Examples

Program TestLinear

```

USE NumTypes
USE Linear

Integer, Parameter :: Nord = 10

Real (kind=DP) :: M(Nord,Nord), L(Nord,Nord), U(Nord,Nord), &
    & Mcp(Nord,Nord), b(Nord), bcp(Nord)
Integer :: I piv(Nord), Iperm

! Fill M of randoms numbers
CALL Random_Number(M)

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

```

```
Stop  
End Program TestLinear
```

# Six

---

## 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.

### 6.1 Subroutine Qsort(X,Ipt)

#### 6.1.1 Description

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

#### 6.1.2 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.

#### 6.1.3 Examples

Program TestNN

```
USE NumTypes
USE NonNumeric

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

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

```

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

! 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

```

## 6.2 Function Locate(X, X<sub>0</sub>, Iin)

### 6.2.1 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  $X(:)$

### 6.2.2 Arguments

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

**X<sub>0</sub>**: 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.

### 6.2.3 Output

Integer. The position  $n$  such that

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

### 6.2.4 Examples

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 neighborr
! 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(Idc)
Write(*,'(1A,1ES33.25)')'Next element in the list:      ', X(Idc+1)

Stop
End Program TestNN
```





## Seven

---

# MODULE SpecialFunc

---

This is the documentation of the `MODULE SpecialFunc`, a set of `FORTTRAN 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.

### 7.1 Function GammaLn(X)

#### 7.1.1 Description

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

#### 7.1.2 Arguments

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

#### 7.1.3 Output

A real Double precision (DP).

#### 7.1.4 Examples

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

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

```

## 7.2 Function Theta(i, z, tau, Prec)

### 7.2.1 Description

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

$$\vartheta_i(z|\tau) \tag{7.1}$$

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  $\pi$  and  $\tau\pi$ .

### 7.2.2 Arguments

- i:** Integer. Intent (in). Says 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 ( $\text{Im}(\tau) > 0$ ).
- Prec:** Real, Optional. If **z** is DPC (SPC), **Prec** must be double precision (single precision). An estimation of the desired precision of the result.

### 7.2.3 Output

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

### 7.2.4 Examples

```

Program TestSpecialFunc

USE NumTypes
USE SpecialFunc

Complex (DPC) :: Z, tau

Z = Cmplx(0.546734, 2.76457643, kind=DPC)

```

```

tau = Cmplx(0.0_DP, 3.76387540_DP)

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

Stop
End Program TestSpecialFunc

```

## 7.3 Function ThetaChar(a, b, z, tau, Prec)

### 7.3.1 Description

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

$$\vartheta \left[ \begin{array}{c} a \\ b \end{array} \right] (z|\tau) \quad (7.2)$$

### 7.3.2 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.

### 7.3.3 Output

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

### 7.3.4 Examples

```
Program TestSpecialFunc
```

```

USE NumTypes
USE SpecialFunc

```

```

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

```

```

Integer :: q, s

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

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

Stop
End Program TestSpecialFunc

```

## 7.4 Function Hermite(n,x,Dval)

### 7.4.1 Description

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

### 7.4.2 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.

### 7.4.3 Output

The value of the  $n^{\text{th}}$  Hermite Polynomial in the point  $X$ .

### 7.4.4 Examples

```
Program TestSpecialFunc
```

```

USE NumTypes
USE SpecialFunc

Integer :: q

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

Stop
End Program TestSpecialFunc

```

## 7.5 Function HermiteFunc(n,x,Dval)

### 7.5.1 Description

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

$$\frac{1}{\sqrt{n!2^n}\sqrt{\pi}}e^{-x^2/2}H_n(x) \quad (7.3)$$

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

### 7.5.2 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.

### 7.5.3 Output

The value of the  $n^{\text{th}}$  Hermite function in the point  $X$ .

### 7.5.4 Examples

```

Program TestSpecialFunc

```

```

    USE NumTypes

```

```

USE SpecialFunc

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

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

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

Stop
End Program TestSpecialFunc

```

## 7.6 Function Basis(X1, X2, n, s, q, itau, Prec)

### 7.6.1 Description

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

$$|n, s\rangle = e^{i\frac{f}{2}x_1x_2} \sum_{k \in s+q\mathbb{Z}} e^{-u^2/2} H_n(u) e^{2\pi i k \frac{x_1}{l_1}} \quad n = 0, \dots, \infty; s = 1, \dots, q \quad (7.4)$$

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

### 7.6.2 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:  $\text{itau} = l_2/l_1$ .

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

### 7.6.3 Output

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

## 7.6.4 Examples

Program TestSpecialFunc

```

USE NumTypes
USE SpecialFunc

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

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

Stop
End Program TestSpecialFunc

```





# Eight

---

## 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.

### 8.1 Function Mean(X)

#### 8.1.1 Description

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

#### 8.1.2 Arguments

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

#### 8.1.3 Output

A real double or simple precision (same type as the input).

#### 8.1.4 Examples

Program Tests

```
USE NumTypes
USE Error
USE Statistics
```

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

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

Stop
End Program Tests
```

## 8.2 Function Var(X)

### 8.2.1 Description

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

### 8.2.2 Arguments

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

### 8.2.3 Output

A real double or simple precision (same type as the input).

### 8.2.4 Examples

Program Tests

```
USE NumTypes
USE Error
USE Statistics

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

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

Stop
End Program Tests
```

## 8.3 Function Stddev(X)

### 8.3.1 Description

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

### 8.3.2 Arguments

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

### 8.3.3 Output

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

### 8.3.4 Examples

Program Tests

```
USE NumTypes
USE Error
USE Statistics
```

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

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

```
Stop
End Program Tests
```

## 8.4 Function Moment(X, k)

### 8.4.1 Description

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

### 8.4.2 Arguments

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

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

### 8.4.3 Output

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

### 8.4.4 Examples

Program Tests

```

USE NumTypes
USE Error
USE Statistics

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

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

Stop
End Program Test

```

## 8.5 Subroutine Normal(X, [Rm], [Rsig])

### 8.5.1 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.

### 8.5.2 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.

### 8.5.3 Examples

Program Tests

```

USE NumTypes
USE Error
USE Statistics

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

```

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

```
Stop
End Program Tests
```

## 8.6 Subroutine Histogram(Val, Ndiv, Ntics, Vmin, Vmax, h)

### 8.6.1 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.

### 8.6.2 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.

### 8.6.3 Examples

Program Tests

```
USE NumTypes
USE Error
USE Statistics

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

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

Do I = 1, Ndiv
    Xac = Xmin + (I-1)*h
```

```

        Write(*,'(1ES33.25,1I)')Xac, Ntics(I)
    End Do

    Stop
End Program Tests

```

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

### 8.7.1 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.

### 8.7.2 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 them to some non-zero value.

**Func:** Optional. This routine defines 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.

**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  $\chi^2$  per degree of freedom of the fit.

### 8.7.3 Examples

#### Program Tests

```

USE NumTypes
USE Error
USE Statistics

Integer, Parameter :: Nmax = 200, Npinta = 100, Npar = 4, Ndiv = 100
Real (kind=DP) :: X(Nmax), Y(Nmax), Yerr(Nmax), &
  & Coef(Npar), Cerr(Npar), Corr, Xd(Nmax,2), &
  & Xmin, Xmax, h, Xac
Integer :: Ntics(Ndiv)

Interface
  Function Fd(Xx, i)

    USE NumTypes

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

```

```

      End Function FD
End Interface

CALL Random_Number(Xd)
Xd(:, :) = 10.0_DP*(Xd(:, :) - 0.8_DP)

CALL Normal(Yer, 0.0_DP, 1.0E-3_DP)
Y(:) = 12.34_DP*Xd(:,1)*sin(Xd(:,2)) - 2.23_DP + &
      & 0.67_DP*Xd(:,1)**2*Xd(:,2) + 0.23_DP*Xd(:,1) + Yer(:)

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

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

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

Stop
End Program Tests

! *****
! *
Function Fd(X, i)
! *
! *****

USE NumTypes

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

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

```



---

```
Else If (I==4) Then
    Fd = X(1)
End If

Return
End Function FD
```



# Nine

---

## MODULE Polynomial

---

This is the documentation of the `MODULE Polynomial`, a set of `FORTTRAN 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.

### 9.1 Type `Pol`

#### 9.1.1 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.

#### 9.1.2 Components

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

`dg`: Integer. The degree of the polynomial.

#### 9.1.3 Examples

A small example showing how to define a polynomial.

```
Program TestPoly
```

```
    USE NumTypes
    USE Error
    USE Polynomial
```

```
    Type (Pol) :: P1
```

```
    Stop
End Program TestPoly
```

## 9.2 Assignment

### 9.2.1 Description

You can directly assign one defined polynomial to another, or to an array of real numbers, that are interpreted as the coefficients.

### 9.2.2 Examples

Program TestPoly

```

USE NumTypes
USE Error
USE Polynomial

Integer, Parameter :: Deg = 4
Real (kind=DP) :: Hcoef(Deg+1)
Type (Pol) :: Hermite4

! The fourth Hermite polynomial is  $x^4 - 6x^2 + 3$ , so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(1)   = 3.0_DP
Hcoef(3)   = -6.0_DP
Hcoef(5)   = 1.0_DP

Hermite4 = Hcoef

! Now Show what we have in our data type:
Do I = 0, Hermite4%deg
  Write(*, '(1I5,ES33.25)') I, Hermite4%Coef(I)
End Do

Stop
End Program TestPoly
```

## 9.3 Operator +

### 9.3.1 Description

You can naturally sum Pol data types.

### 9.3.2 Examples

Program TestPoly

```

USE NumTypes
USE Error
```

```

USE Polynomial

Integer, Parameter :: Deg = 4
Real (kind=DP) :: Hcoef(Deg+1)
Type (Pol) :: Hermite4, Hermite3, Sum

! The Third Hermite polynomial is  $x^3 - 3x$ , so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(2)   = -3.0_DP
Hcoef(4)   = 1.0_DP

Hermite3 = Hcoef(1:4)

! The fourth Hermite polynomial is  $x^4 - 6x^2 + 3$ , so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(1)   = 3.0_DP
Hcoef(3)   = -6.0_DP
Hcoef(5)   = 1.0_DP

Hermite4 = Hcoef

! Now Add the two polynomials, and show the result.
Sum = Hermite3 + Hermite4
Do I = 0, Sum%deg
  Write(*,'(1I5,ES33.25)')I, Sum%Coef(I)
End Do

Stop
End Program TestPoly

```

## 9.4 Operator -

### 9.4.1 Description

You can subtract Pol data types.

### 9.4.2 Examples

Program TestPoly

```

USE NumTypes
USE Error
USE Polynomial

```

```

Integer, Parameter :: Deg = 4

```

```

Real (kind=DP) :: Hcoef(Deg+1)
Type (Pol) :: Hermite4, Hermite3, Sum

! The Third Hermite polynomial is  $x^3 - 3x$ , so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(2)   = -3.0_DP
Hcoef(4)   = 1.0_DP

Hermite3 = Hcoef(1:4)

! The fourth Hermite polynomial is  $x^4 - 6x^2 + 3$ , so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(1)   = 3.0_DP
Hcoef(3)   = -6.0_DP
Hcoef(5)   = 1.0_DP

Hermite4 = Hcoef

! Now Subtract the two polynomials, and show the result.
Sum = Hermite3 - Hermite4
Do I = 0, Sum%deg
  Write(*, '(1I5,ES33.25)') I, Sum%Coef(I)
End Do

Stop
End Program TestPoly

```

## 9.5 Operator \*

### 9.5.1 Description

You can naturally multiply Pol data types and Pol data types with double precision real numbers.

### 9.5.2 Examples

```

Program TestPoly

USE NumTypes
USE Error
USE Polynomial

Integer, Parameter :: Deg = 4
Real (kind=DP) :: Hcoef(Deg+1)
Type (Pol) :: Hermite4, Hermite3, Sum

```

```

! The Third Hermite polynomial is  $x^3 - 3x$ , so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(2)   = -3.0_DP
Hcoef(4)   = 1.0_DP

Hermite3 = Hcoef(1:4)

! The fourth Hermite polynomial is  $x^4 - 6x^2 + 3$ , so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(1)   = 3.0_DP
Hcoef(3)   = -6.0_DP
Hcoef(5)   = 1.0_DP

Hermite4 = Hcoef

! Now multiply the two polynomials, and show the result.
Sum = Hermite3 * Hermite4
Do I = 0, Sum%deg
    Write(*,'(1I5,ES33.25)')I, Sum%Coef(I)
End Do

Stop
End Program TestPoly

```

## 9.6 Subroutine Init(P, Dgr)

### 9.6.1 Description

Allocate memory space for the coefficients of a Pol type.

### 9.6.2 Arguments

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

Dgr Integer. The degree of the polynomial.

### 9.6.3 Examples

Program TestPoly

```

USE NumTypes
USE Error
USE Polynomial

```

```

Integer, Parameter :: Deg = 4

```

```

Real (kind=DP) :: Hcoef(Deg+1)
Type (Pol) :: Hermite4, Hermite3, Sum

! An alternative way of setting the third Hermite
! polynomial.
CALL Init(Hermite3, 3)
Hermite3%Coef(0) = 0.0_DP
Hermite3%Coef(1) = -3.0_DP
Hermite3%Coef(2) = 0.0_DP
Hermite3%Coef(3) = 1.0_DP
Hermite3%dg = 3

Stop
End Program TestPoly

```

## 9.7 Function Degree(P)

### 9.7.1 Description

Returns the degree of the polynomial P.

### 9.7.2 Arguments

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

### 9.7.3 Output

Integer. The degree of the polynomial P.

### 9.7.4 Examples

```

Program TestPoly

USE NumTypes
USE Error
USE Polynomial

Integer, Parameter :: Deg = 4
Real (kind=DP) :: Hcoef(Deg+1), X
Type (Pol) :: Hermite4, Hermite3, Sum

! The Third Hermite polynomial is  $x^3 - 3x$ , so
! we first assign the values of the coefficients.
Hcoef = 0.0_DP
Hcoef(2) = -3.0_DP
Hcoef(4) = 1.0_DP

```



```

Hermite3 = Hcoef(1:4)

! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(1)   = 3.0_DP
Hcoef(3)   = -6.0_DP
Hcoef(5)   = 1.0_DP

Hermite4 = Hcoef

! Now Mutiply the two polynomials, and show the result.
Sum = Hermite3 * Hermite4

! Show the degree of the product. It should be 4+3=7.
Write(*,*)Degree(Sum)

Stop
End Program TestPoly

```

## 9.8 Function Value(P, X)

### 9.8.1 Description

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

### 9.8.2 Arguments

P: Type Po1. The polynomial.

X: Real double precision. The point in which you want to compute the value.

### 9.8.3 Output

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

### 9.8.4 Examples

Program TestPoly

```

USE NumTypes
USE Error
USE Polynomial

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

```

```

Type (Pol) :: Hermite4, Hermite3, Sum

! The Third Hermite polynomial is  $x^3 - 3x$ , so
! we first assign the values of the coefficients.
Hcoef    = 0.0_DP
Hcoef(2) = -3.0_DP
Hcoef(4) = 1.0_DP

Hermite3 = Hcoef(1:4)

! The fourth Hermite polynomial is  $x^4 - 6x^2 + 3$ , so
! we first assign the values of the coefficients.
Hcoef    = 0.0_DP
Hcoef(1) = 3.0_DP
Hcoef(3) = -6.0_DP
Hcoef(5) = 1.0_DP

Hermite4 = Hcoef

! Now Mutiply the two polynomials, and show the result.
Sum = Hermite3 * Hermite4

! Compute the valuye of the product in some point in two
! different ways.
X = 9.34564_DP
Write(*, '(ES33.25)') Value(Sum, X)
Write(*, '(ES33.25)') Value(Hermite3, X) * Value(Hermite4, X)

Stop
End Program TestPoly

```

## 9.9 Function Deriv(P)

### 9.9.1 Description

Computes the derivative of the polynomial P.

### 9.9.2 Arguments

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

### 9.9.3 Output

Type Pol. Another polynomial: the derivative of P.

## 9.9.4 Examples

Program TestPoly

```

USE NumTypes
USE Error
USE Polynomial

Integer, Parameter :: Deg = 4
Real (kind=DP) :: Hcoef(Deg+1), X
Type (Pol) :: Hermite4, Hermite3, Res, Sum

! The Third Hermite polynomial is  $x^3 - 3x$ , so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(2) = -3.0_DP
Hcoef(4) = 1.0_DP

Hermite3 = Hcoef(1:4)

! The fourth Hermite polynomial is  $x^4 - 6x^2 + 3$ , so
! we first assign the values of the coefficients.
Hcoef      = 0.0_DP
Hcoef(1) = 3.0_DP
Hcoef(3) = -6.0_DP
Hcoef(5) = 1.0_DP

Hermite4 = Hcoef

! Now compute the derivative of Hermite4
Res = Deriv(Hermite4)

! From the recursion relation of the Hermite polynomials
! we should obtain twice the same number:
X = 7.346582_DP
Write(*, '(ES33.25)') Value(Res, X)
Write(*, '(ES33.25)') 4.0_DP * Value(Hermite3, X)

Stop
End Program TestPoly

```

## 9.10 Function Integra(P, Cte)

### 9.10.1 Description

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

### 9.10.2 Arguments

P: Type Pol. The polynomial whose integral we want to compute.

C: Real single or double precision. Optional. The constant of integration. If not present, the default value is 0.

### 9.10.3 Output

Type Pol. Another polynomial: the integral of P.

### 9.10.4 Examples

Program TestPoly

```

USE NumTypes
USE Error
USE Polynomial

Integer, Parameter :: Deg = 4
Real (kind=DP) :: Hcoef(Deg+1), X
Type (Pol) :: Hermite4, Hermite3, Res, Sum

! The Third Hermite polynomial is x^3 - 3x, so
! we first assign the values of the coefficients.
Hcoef = 0.0_DP
Hcoef(2) = -3.0_DP
Hcoef(4) = 1.0_DP

Hermite3 = Hcoef(1:4)

! The fourth Hermite polynomial is x^4 - 6x^2 + 3, so
! we first assign the values of the coefficients.
Hcoef = 0.0_DP
Hcoef(1) = 3.0_DP
Hcoef(3) = -6.0_DP
Hcoef(5) = 1.0_DP

Hermite4 = Hcoef

! Now compute the derivative of Hermite4
```

```

Res = Integra(Hermite3, 3.0_DP/4.0_DP)

! From the recursion relation of the Hermite polynomials
! we should obtain twice the same number:
X = 7.346582_DP
Write(*,'(ES33.25)')Value(Res, X)
Write(*,'(ES33.25)')0.25_DP*Value(Hermite4, X)

Stop
End Program TestPoly

```

## 9.11 Function InterpolValue(X, Y, Xo)

### 9.11.1 Description

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

### 9.11.2 Arguments

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

Xo: The ppoint at which you want to compute the interpolation polynomial.

### 9.11.3 Output

Real double precision. The value of the interpolation polynomial in Xo.

### 9.11.4 Examples

Program TestPoly

```

USE NumTypes
USE Error
USE Polynomial

Integer, Parameter :: Deg = 4, Np = 7
Real (kind=DP) :: Hcoef(Deg+1), X, Xp(Np), Yp(Np)
Type (Pol) :: Hermite4, Hermite3, Res, Sum

CALL Random_Number(Xp)
Yp = 3.347234_DP*Xp - 2.475875_DP*Xp**3 - 7.23467_DP*Xp**4 + &
    & 1.47854_DP*Xp**6

! Now we compute the value of the interpolation polynomial

```

```

! at X, and compare it with the real value of the Polynomial
X = -1.23899843_DP
Write(*,'(ES33.25)')InterpolValue(Xp, Yp, X)
Write(*,'(ES33.25)')3.347234_DP*X - 2.475875_DP*X**3 - &
    & 7.23467_DP*X**4 + 1.47854_DP*X**6

Stop
End Program TestPoly

```

## 9.12 Function Interpol(X, Y)

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

### 9.12.1 Arguments

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

### 9.12.2 Output

Type Pol. The interpolation polynomial.

### 9.12.3 Examples

Program TestPoly

```

USE NumTypes
USE Error
USE Polynomial

Integer, Parameter :: Deg = 4, Np = 7
Real (kind=DP) :: Hcoef(Deg+1), X, Xp(Np), Yp(Np)
Type (Pol) :: Hermite4, Hermite3, Res, Sum

CALL Random_Number(Xp)
Yp = 3.347234_DP*Xp - 2.475875_DP*Xp**3 - 7.23467_DP*Xp**4 + &
    & 1.47854_DP*Xp**6

! Now we compute the interpolation polynomial
! at X, and compare it with the real value of the Polynomial
X = -1.23899843_DP
Res = Interpol(Xp,Yp)
Write(*,'(ES33.25)')Value(Res, X)
Write(*,'(ES33.25)')3.347234_DP*X - 2.475875_DP*X**3 - &

```

```
& 7.23467_DP*X**4 + 1.47854_DP*X**6
```

```
Stop
End Program TestPoly
```

## 9.13 Subroutine Spline(X, Y, Ypp0, YppN, Pols)

### 9.13.1 Description

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

### 9.13.2 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.

### 9.13.3 Examples

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)
```

```
CALL Random_Number(Xp)
! Order Xp
CALL Qsort(Xp)
Yp = 3.347234_DP*Xp - 2.475875_DP*Xp**3 - 7.23467_DP*Xp**4 + &
& 1.47854_DP*Xp**6
```

```
! Now we compute the interpolation polynomial
! at X, and compare it with the real value of the Polynomial, and
! the value of the spline cubic interpolation polynomial.
X = 0.23899843_DP
Res = Interpol(Xp,Yp)
CALL Spline(Xp, Yp, 0.0_DP, 0.0_DP, Spl)
```

```
Write(*,'(ES33.25)')Value(Res, X)
Write(*,'(ES33.25)')Value(Spl(Locate(Xp, X)), X)
Write(*,'(ES33.25)')3.347234_DP*X - 2.475875_DP*X**3 - &
    & 7.23467_DP*X**4 + 1.47854_DP*X**6

Stop
End Program TestPoly
```



# Ten

---

## MODULE Root

---

This is the documentation of the `MODULE Root`, a set of FORTRAN 90 routines to compute root 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.

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

#### 10.1.1 Description

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

#### 10.1.2 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:

$$\begin{aligned}P(x) &= x^2 + ax + b \\P(x) &= x^3 + ax^2 + bx + c \\P(x) &= x^4 + ax^3 + bx^2 + cx + d\end{aligned}$$

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

#### 10.1.3 Examples

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
```

```

CALL Random_Number(a)
CALL Random_Number(b)
CALL Random_Number(c)
CALL Random_Number(d)
CALL RootPol(a,b,z1,z2)
Write(*,'(3ES20.12)')Z1, Abs(z1**2 + a*z1 + Cmplx(b,kind=DPC))
Write(*,'(3ES20.12)')Z2, Abs(z2**2 + a*z2 + Cmplx(b,kind=DPC))

CALL RootPol(a,b,c, z1,z2, z3)
Write(*,*)
Write(*,'(3ES20.12)')Z1, Abs(z1**3+a*z1**2+b*z1+Cmplx(c,kind=DPC))
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))

ac = Cmplx(a,kind=DPC)
bc = Cmplx(b,a,kind=DPC)
cc = Cmplx(c,kind=DPC)
dc = Cmplx(d,kind=DPC)
CALL RootPol(ac,bc,z1,z2)
Write(*,*)
Write(*,'(3ES20.12)')Z1, Abs(z1**2 + ac*z1 + Cmplx(bc,kind=DPC))
Write(*,'(3ES20.12)')Z2, Abs(z2**2 + ac*z2 + Cmplx(bc,kind=DPC))
CALL RootPol(ac,bc,cc, dc, z1,z2, z3, z4)
Write(*,*)
Write(*,'(3ES20.12)')Z1, Abs(z1**4+ac*z1**3+bc*z1**2+cc*z1+dc)
Write(*,'(3ES20.12)')Z2, Abs(z2**4+ac*z2**3+bc*z2**2+cc*z2+dc)
Write(*,'(3ES20.12)')Z3, Abs(z3**4+ac*z3**3+bc*z3**2+cc*z3+dc)
Write(*,'(3ES20.12)')Z4, Abs(z4**4+ac*z4**3+bc*z4**2+cc*z4+dc)

Stop
End Program TestRoot

```

## 10.2 Function Newton(Xo, Fnew, [Tol])

### 10.2.1 Description

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

### 10.2.2 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.

### 10.2.3 Output

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

### 10.2.4 Examples

Program TestRoot

```

USE NumTypes
USE Error
USE Root

Real (kind=DP) :: a, b, c, d, X
Complex (kind=DPC) :: z1, z2, z3, z4, ac, bc, cc, dc

Interface
  Subroutine FNew(Xo, F, D)

    USE NumTypes

    Real (kind=DP), Intent (in) :: Xo
    Real (kind=DP), Intent (out) :: F, D
  End Subroutine FNew
End Interface

! Compute the value such that cos(x) = x
X = Newton(0.0_DP, Fnew, 1.0E-10_DP)
Write(*, '(1A,ES33.25)') 'Point: ', X
Write(*, '(1A,ES33.25)') 'Value of Cos: ', Cos(X)

```

```

      Stop
End Program TestRoot

! *****
! *
Subroutine FNew(Xo, F, D)
! *
! *****

USE NumTypes

Real (kind=DP), Intent (in) :: Xo
Real (kind=DP), Intent (out) :: F, D

F = Xo - Cos(Xo)
D = 1.0_DP + Sin(Xo)

Return
End Subroutine FNew

```

## 10.3 Function Bisec(a, b, Fbis, [Tol])

### 10.3.1 Description

Compute the root of the function defined by Fbis.

### 10.3.2 Arguments

**a, b:** Real single or double precision. Initial points, such that  $\text{Fbis}(a)\text{Fbis}(b) < 0$ .

**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.

### 10.3.3 Output

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

### 10.3.4 Examples

Program TestRoot

```

USE NumTypes
USE Error
USE Root

Real (kind=DP) :: a, b, c, d, X
Complex (kind=DPC) :: z1, z2, z3, z4, ac, bc, cc, dc

Interface
  Function Fbis(X)

    USE NumTypes

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

! Compute the value such that cos(x) = x
X = Bisec(0.0_DP, 1.1_DP, Fbis, 1.0E-10_DP)
Write(*,'(1A,ES33.25)')'Point:      ', X
Write(*,'(1A,ES33.25)')'Value of Cos: ', Cos(X)

Stop
End Program TestRoot

! *****
! *
Function FBis(X)
! *
! *****

USE NumTypes
```

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

Fbis = X - Cos(X)

Return
End Function FBis
```

# Eleven

---

## 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.

### 11.1 Type `Fourier_Serie`

#### 11.1.1 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.

#### 11.1.2 Components

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

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

#### 11.1.3 Examples

A small example showing how to define a polynomial.

Program `TestFourier`

```
USE NumTypes
USE Constants
USE Fourier
```

```
Type (Fourier_Serie) :: Ff
```

```
Stop
End Program TestPoly
```

## 11.2 Type Fourier\_Serie\_2D

### 11.2.1 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.

### 11.2.2 Components

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

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

### 11.2.3 Examples

A small example showing how to define a polynomial.

Program TestFourier

```
USE NumTypes
USE Constants
USE Fourier
```

```
Type (Fourier_Serie_2D) :: Ff
```

```
Stop
End Program TestPoly
```

## 11.3 Assignment

### 11.3.1 Description

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

### 11.3.2 Examples

This example uses the `Init_Serie` subroutine. For details of the usage of this function look at the section (11.8), page (80).

Program TestFourier

```
USE NumTypes
USE Constants
USE Fourier
```

```
Type (Fourier_Serie) :: FS1, FS2
```

```
CALL Init_Serie(FS1, 20)
CALL Init_Serie(FS2, 20)
```



```

FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

FS2 = FS1

Write(*,'(2ES33.25)')FS2%Coef( 1)
Write(*,'(2ES33.25)')FS2%Coef(-1)

Stop
End Program TestFourier

```

## 11.4 Operator +

### 11.4.1 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.

### 11.4.2 Examples

This example uses the `Init_Serie` subroutine. For details of the usage of this function look at the section (11.8), page (80).

Program TestFourier

```

USE NumTypes
USE Constants
USE Fourier

Type (Fourier_Serie_2D) :: FS1, FS2, FS3
Integer :: Nt

Nt = 4
CALL Init_Serie(FS1, Nt)
CALL Init_Serie(FS2, Nt)

FS1%Coef( 1,1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
FS1%Coef(-1,1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

FS2%Coef( 1,1) = Cmplx(-1.0_DP, 4.5_DP, kind=DPC)
FS2%Coef(-1,1) = Cmplx(-1.0_DP, -6.78745_DP, kind=DPC)

FS3 = FS1 + FS2
Write(*,'(2ES33.25)')FS3%Coef( 1,1)
Write(*,'(2ES33.25)')FS3%Coef(-1,1)

```

```

    Stop
End Program TestFourier

```

## 11.5 Operator -

### 11.5.1 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.

### 11.5.2 Examples

```

Program TestFourier

```

```

    USE NumTypes
    USE Constants
    USE Fourier

```

```

    Type (Fourier_Serie) :: FS1, FS2, FS3
    Integer :: Nt

```

```

    Nt = 4
    CALL Init_Serie(FS1, Nt)

```

```

    FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
    FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

```

```

    FS2 = FS1

```

```

    FS3 = FS1 - FS2
    Write(*,'(2ES33.25)')FS3%Coef( 1)
    Write(*,'(2ES33.25)')FS3%Coef(-1)

```

```

    Stop
End Program TestFourier

```

## 11.6 Operator \*

### 11.6.1 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.

### 11.6.2 Examples

```

Program TestFourier

```

```

USE NumTypes
USE Constants
USE Fourier

Type (Fourier_Serie) :: FS1, FS2, FS3
Integer :: Nt

Nt = 4
CALL Init_Serie(FS1, Nt)

FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

FS2 = FS1

FS3 = FS1 * FS2
Write(*,'(2ES33.25)')FS3%Coef( 0)

Stop
End Program TestFourier

```

## 11.7 Operator \*\*

### 11.7.1 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.

### 11.7.2 Examples

Program TestFourier

```

USE NumTypes
USE Constants
USE Fourier

Type (Fourier_Serie) :: FS1, FS2, FS3
Integer :: Nt

Nt = 4
CALL Init_Serie(FS1, Nt)
CALL Init_Serie(FS2, Nt)
CALL Init_Serie(FS3, Nt)

FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)

```

```

FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

FS3%Coef(0) = Cmplx(1.0_DP, 0.0_DP, kind=DPC)

FS2 = FS1**8
Do I = 1, 8
    FS3 = FS3 * FS1
End Do

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

Stop
End Program TestFourier

```

## 11.8 Subroutine Init\_Serie(FS,Ns)

### 11.8.1 Description

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

### 11.8.2 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.

### 11.8.3 Examples

Any of the examples of some of the previous sections are also good examples of the use of the `Init_Serie` subroutine. Here we simply repeat one of them.

Program TestFourier

```

USE NumTypes
USE Constants
USE Fourier

Type (Fourier_Serie) :: FS1, FS2, FS3
Integer :: Nt

Nt = 4
CALL Init_Serie(FS1, Nt)

FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

```

```

FS2 = FS1

FS3 = FS1 * FS2
Write(*,'(2ES33.25)')FS3%Coef( 0)

Stop
End Program TestFourier

```

## 11.9 Function Eval\_Serie(FS, X, [Y], Tx, [Ty])

### 11.9.1 Description

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

### 11.9.2 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.

### 11.9.3 Output

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

### 11.9.4 Examples

Program TestFourier

```

USE NumTypes
USE Constants
USE Fourier

Type (Fourier_Serie) :: FS1, FS2, FS3
Integer :: Nt

Nt = 4
CALL Init_Serie(FS1, Nt)
CALL Init_Serie(FS2, Nt)
CALL Init_Serie(FS3, Nt)

FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)

```

```

    FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

    FS2 = FS1**2

    FS3 = FS1*FS2

    Write(*,'(2ES33.25)')Eval_Serie(FS1,0.12_DP,1.0_DP) * &
        & Eval_Serie(FS2,0.12_DP,1.0_DP)
    Write(*,'(2ES33.25)')Eval_Serie(FS3,0.12_DP,1.0_DP)

    Stop
End Program TestFourier

```

## 11.10 Function Unit(FS, Ns)

### 11.10.1 Description

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

### 11.10.2 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.

### 11.10.3 Examples

Program TestFourier

```

    USE NumTypes
    USE Constants
    USE Fourier

    Type (Fourier_Serie) :: FS1, FS2, FS3
    Integer :: Nt

    Nt = 4
    CALL Init_Serie(FS1, Nt)
    CALL Init_Serie(FS2, Nt)
    CALL Init_Serie(FS3, Nt)

    FS1%Coef( 1) = Cmplx(1.0_DP, 0.5_DP, kind=DPC)
    FS1%Coef(-1) = Cmplx(1.0_DP, 0.7_DP, kind=DPC)

    CALL Unit(FS2, Nt)

```

```

FS3 = FS1*FS2

Write(*,'(2ES33.25)')Eval_Serie(FS1,0.12_DP,1.0_DP)
Write(*,'(2ES33.25)')Eval_Serie(FS3,0.12_DP,1.0_DP)

Stop
End Program TestFourier

```

## 11.11 Function DFT(Data, Is)

### 11.11.1 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

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

the inverse one is defined as

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

### 11.11.2 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.

### 11.11.3 Output

Type **Fourier\_Serie** if **Data(:)** is one dimensional, and type **Fourier\_Serie\_2D** if **Data(:, :)** is two dimensional.

### 11.11.4 Examples

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

```

Program TestFourier

```

```

USE NumTypes
USE Constants
USE Fourier

```

```

Integer, Parameter :: Nmax=20

```

```

Type (Fourier_Serie) :: FS1, FS2, FS3
Complex (kind=DPC) :: Data(Nmax), X
Integer :: Nt

Do I = 1, Nmax
    X = Cmplx(TWOPI_DP*I/Nmax)
    Data(I) = Sin(X)
End Do

FS1 = DFT(Data)

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

```

## 11.12 Function Conjg(FS)

### 11.12.1 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  $\tilde{f}(-k)$ .

### 11.12.2 Arguments

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

### 11.12.3 Output

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

### 11.12.4 Examples

Program TestFourier

```

USE NumTypes
USE Constants
USE Fourier

Integer, Parameter :: Nmax=20
Type (Fourier_Serie) :: FS1, FS2, FS3
Complex (kind=DPC) :: Data(Nmax), X
Integer :: Nt

```



```

Do I = 1, Nmax
  X = Cmplx(TWOPI_DP*I/Nmax,kind=DPC)
  Data(I) = Sin(X) + Cmplx(0.0_DP,I*2.0_DP,kind=DPC)
End Do

FS1 = DFT(Data)

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)

Stop
End Program TestFourier

```

## 11.13 Subroutine Save\_Serie(FS, File)

### 11.13.1 Description

Write the Fourier series FS to the file File.

### 11.13.2 Arguments

**FS:** Type `Fourier_Serie` or type `Fourier_Serie_2D`. The Fourier series that you want to store in a file.

**File:** Character (len=\*). The name of the file in which you want to save FS.

### 11.13.3 Examples

Program TestFourier

```

USE NumTypes
USE Constants
USE Fourier

Integer, Parameter :: Nmax=20
Type (Fourier_Serie) :: FS1, FS2, FS3
Complex (kind=DPC) :: Data(Nmax), X
Integer :: Nt

Do I = 1, Nmax
  X = Cmplx(TWOPI_DP*I/Nmax,kind=DPC)
  Data(I) = Sin(X) + Cmplx(0.0_DP,I*2.0_DP,kind=DPC)
End Do

FS1 = DFT(Data)

CALL Save(FS1,'datamodes.dat')

```

```

    Stop
End Program TestFourier

```

## 11.14 Subroutine Read\_Serie(FS, File)

### 11.14.1 Description

Reads the Fourier series FS stored in the file File.

### 11.14.2 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 (len=\*). The name of the file in which the saved series is.

### 11.14.3 Examples

```

Program TestFourier

```

```

    USE NumTypes
    USE Constants
    USE Fourier

```

```

    Integer, Parameter :: Nmax=20
    Type (Fourier_Serie) :: FS1, FS2, FS3
    Complex (kind=DPC) :: Data(Nmax), X
    Integer :: Nt

```

```

    Do I = 1, Nmax
        X = Cmplx(TWOPI_DP*I/Nmax,kind=DPC)
        Data(I) = Sin(X) + Cmplx(0.0_DP,I*2.0_DP,kind=DPC)
    End Do

```

```

    FS1 = DFT(Data)

```

```

    CALL Save_Serie(FS1,'datamodes.dat')
    CALL Read_Serie(FS2,'datamodes.dat')

```

```

    Write(*, '(ES33.25)') Sum(Abs(FS1%Coef(:) - FS2%Coef(:)))

```

```

    Stop
End Program TestFourier

```

---

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