

# NAG Fortran Library Routine Document

## D03PYF

**Note:** before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details.

### 1 Purpose

This routine may be used in conjunction with either D03PDF/D03PDA or D03PJF/D03PJA. It computes the solution and its first derivative at user-specified points in the spatial co-ordinate.

### 2 Specification

```

SUBROUTINE D03PYF(NPDE, U, NBKPTS, XBKPTS, NPOLY, NPTS, XP, INTPTS,
1          ITYPE, UP, W, NW, IFAIL)
  INTEGER      NPDE, NBKPTS, NPOLY, NPTS, INTPTS, ITYPE, NW, IFAIL
  real       U(NPDE,NPTS), XBKPTS(NBKPTS), XP(INTPTS),
1          UP(NPDE,INTPTS,ITYPE), W(NW)

```

### 3 Description

D03PYF is an interpolation routine for evaluating the solution of a system of partial differential equations (PDEs), or the PDE components of a system of PDEs with coupled ordinary differential equations (ODEs), at a set of user-specified points. The solution of a system of equations can be computed using D03PDF/D03PDA or D03PJF/D03PJA on a set of mesh points; D03PYF can then be employed to compute the solution at a set of points other than those originally used in D03PDF/D03PDA or D03PJF/D03PJA. It can also evaluate the first derivative of the solution. Polynomial interpolation is used between each of the break-points  $XBKPTS(i)$ , for  $i = 1, 2, \dots, NBKPTS$ . When the derivative is needed ( $ITYPE = 2$ ), the array  $XP(INTPTS)$  must not contain any of the break-points, as the method, and consequently the interpolation scheme, assumes that only the solution is continuous at these points.

### 4 References

None.

### 5 Parameters

**Note:** the parameters U, NPTS, NPDE, XBKPTS, NBKPTS, W and NW must be supplied unchanged from either D03PDF/D03PDA or D03PJF/D03PJA.

- 1: NPDE – INTEGER *Input*  
*On entry:* the number of PDEs.  
*Constraint:*  $NPDE \geq 1$ .
- 2: U(NPDE,NPTS) – **real** array *Input*  
*On entry:* the PDE part of the original solution returned in the parameter U by the routine D03PDF/D03PDA or D03PJF/D03PJA.
- 3: NBKPTS – INTEGER *Input*  
*On entry:* the number of break-points.  
*Constraint:*  $NBKPTS \geq 2$ .

- 4: XBKPTS(NBKPTS) – *real* array *Input*  
*On entry:* XBKPTS( $i$ ), for  $i = 1, 2, \dots, \text{NBKPTS}$ , must contain the break-points as used by D03PDF/D03PDA or D03PJF/D03PJA.  
*Constraint:*  $\text{XBKPTS}(1) < \text{XBKPTS}(2) < \dots < \text{XBKPTS}(\text{NBKPTS})$ .
- 5: NPOLY – INTEGER *Input*  
*On entry:* the degree of the Chebyshev polynomial used for approximation as used by D03PDF/D03PDA or D03PJF/D03PJA.  
*Constraint:*  $1 \leq \text{NPOLY} \leq 49$ .
- 6: NPTS – INTEGER *Input*  
*On entry:* the number of mesh points as used by D03PDF/D03PDA or D03PJF/D03PJA.  
*Constraint:*  $\text{NPTS} = (\text{NBKPTS} - 1) \times \text{NPOLY} + 1$ .
- 7: XP(INTPTS) – *real* array *Input*  
*On entry:* XP( $i$ ), for  $i = 1, 2, \dots, \text{INTPTS}$ , must contain the spatial interpolation points.  
*Constraint:*  $\text{XBKPTS}(1) \leq \text{XP}(1) < \text{XP}(2) < \dots < \text{XP}(\text{INTPTS}) \leq \text{XBKPTS}(\text{NBKPTS})$ .  
When  $\text{ITYPE} = 2$ ,  $\text{XP}(i) \neq \text{XBKPTS}(j)$ , for  $i = 1, 2, \dots, \text{INTPTS}$ ;  $j = 2, 3, \dots, \text{NBKPTS} - 1$ .
- 8: INTPTS – INTEGER *Input*  
*On entry:* the number of interpolation points.  
*Constraint:*  $\text{INTPTS} \geq 1$ .
- 9: ITYPE – INTEGER *Input*  
*On entry:* specifies the interpolation to be performed.  
If  $\text{ITYPE} = 1$ , the solution at the interpolation points are computed. If  $\text{ITYPE} = 2$ , both the solution and the first derivative at the interpolation points are computed.  
*Constraint:*  $\text{ITYPE} = 1$  or  $2$ .
- 10: UP(NPDE,INTPTS,ITYPE) – *real* array *Output*  
*On exit:* if  $\text{ITYPE} = 1$ , UP( $i, j, 1$ ), contains the value of the solution  $U_i(x_j, t_{\text{out}})$ , at the interpolation points  $x_j = \text{XP}(j)$ , for  $j = 1, 2, \dots, \text{INTPTS}$ ;  $i = 1, 2, \dots, \text{NPDE}$ .  
If  $\text{ITYPE} = 2$ , UP( $i, j, 1$ ) contains  $U_i(x_j, t_{\text{out}})$  and UP( $i, j, 2$ ) contains  $\frac{\partial U_i}{\partial x}$  at these points.
- 11: W(NW) – *real* array *Input*  
*On entry:* the array W as returned by D03PDF/D03PDA or D03PJF/D03PJA. The contents of W must not be changed from the call to D03PDF/D03PDA or D03PJF/D03PJA.
- 12: NW – INTEGER *Input*  
*On entry:* the size of the workspace W, as in D03PDF/D03PDA or D03PJF/D03PJA.
- 13: IFAIL – INTEGER *Input/Output*  
*On entry:* IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.  
*On exit:* IFAIL = 0 unless the routine detects an error (see Section 6).  
For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the

value 1 is recommended. Otherwise, for users not familiar with this parameter the recommended value is 0. **When the value  $-1$  or  $1$  is used it is essential to test the value of IFAIL on exit.**

## 6 Error Indicators and Warnings

If on entry  $IFAIL = 0$  or  $-1$ , explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

$IFAIL = 1$

On entry,  $ITYPE \neq 1$  or  $2$ ,  
 or  $NPOLY < 1$ ,  
 or  $NPDE < 1$ ,  
 or  $NBKPTS < 2$ ,  
 or  $INTPTS < 1$ ,  
 or  $NPTS \neq (NBKPTS - 1) \times NPOLY + 1$ ,  
 or  $XBKPTS(i)$ , for  $i = 1, \dots, NBKPTS$ , are not ordered.

$IFAIL = 2$

On entry, the interpolation points  $XP(i)$ , for  $i = 1, \dots, INTPTS$ , are not in strictly increasing order, or when  $ITYPE = 2$ , at least one of the interpolation points stored in  $XP$  is equal to one of the break-points stored in  $XBKPTS$ .

$IFAIL = 3$

The user is attempting extrapolation, that is, one of the interpolation points  $XP(i)$ , for some  $i$ , lies outside the interval  $[XBKPTS(1), XBKPTS(NBKPTS)]$ . Extrapolation is not permitted.

## 7 Accuracy

See the documents for D03PDF/D03PDA or D03PJF/D03PJA.

## 8 Further Comments

None.

## 9 Example

See Section 9 of the document for D03PDF/D03PDA.