D03PYF – NAG Fortran Library Routine Document

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 or D03PJF. 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,
1                  INTPTS, ITYPE, UP, W, NW, IFAIL)
 INTEGER           NPDE, NBKPTS, NPOLY, NPTS, INTPTS, ITYPE, NW,
1                  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 or D03PJF 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 or D03PJF. It can also evaluate the first derivative of the solution. Polynomial interpolation is used between each of the break-points XBKPTS(i), for $i = 1, 2, \ldots,$ 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 or D03PJF.

1: NPDE — INTEGER *Input*

On entry: the number of PDEs.

Constraint: NPDE ≥ 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 or D03PJF.

3: NBKPTS — INTEGER *Input*

On entry: the number of break-points.

Constraint: NBKPTS ≥ 2.

4: XBKPTS(NBKPTS) — ***real*** array *Input*

On entry: XBKPTS(i), for $i = 1, 2, \ldots,$ NBKPTS, must contain the break-points as used by D03PDF or D03PJF.

Constraint: XBKPTS(1) < XBKPTS(2) < ... < XBKPTS(NBKPTS).

5: NPOLY — INTEGER *Input*

On entry: the degree of the Chebyshev polynomial used for approximation as used by D03PDF or D03PJF.

Constraint: $1 \leq$ NPOLY ≤ 49.

6: NPTS — INTEGER *Input*

On entry: the number of mesh points as used by D03PDF or D03PJF.

Constraint: NPTS = (NBKPTS − 1) × NPOLY + 1.

7: XP(INTPTS) — ***real*** array *Input*

On entry: XP(i), for $i = 1, 2, \ldots,$ INTPTS, must contain the spatial interpolation points.

Constraint: XBKPTS(1) $\leq$ XP(1) < XP(2) < ... < XP(INTPTS) $\leq$ XBKPTS(NBKPTS).

When ITYPE = 2, XP(i) $\neq$ XBKPTS(j), for $i = 1, 2, \ldots,$ INTPTS; $j = 2, 3, \ldots,$ NBKPTS − 1.

8: INTPTS — INTEGER *Input*

On entry: the number of interpolation points.

Constraint: INTPTS ≥ 1.

9: ITYPE — INTEGER *Input*

On entry: specifies the interpolation to be performed.

If ITYPE = 1, the solution at the interpolation points are computed. If ITYPE = 2, both the solution and the first derivative at the interpolation points are computed.

Constraint: ITYPE = 1 or 2.

10: UP(NPDE,INTPTS,ITYPE) — ***real*** array *Output*

On exit: if ITYPE = 1, UP($i, j, 1$), contains the value of the solution $U_i(x_j, t_{out})$, at the interpolation points x_j = XP(j), for $j = 1, 2, \ldots,$ INTPTS; $i = 1, 2, \ldots,$ NPDE.

If ITYPE = 2, UP($i, j, 1$) contains $U_i(x_j, t_{out})$ 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 or D03PJF. The contents of W must not be changed from the call to D03PDF or D03PJF.

12: NW — INTEGER *Input*

On entry: the size of the workspace W, as in D03PDF or D03PJF.

13: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors 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 $i = 1, \ldots,$ NBKPTS, are not ordered.

IFAIL = 2

On entry, the interpolation points XP(i), for $i = 1, \ldots,$ 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 or D03PJF.

8 Further Comments

None.

9 Example

See the example for Section 9 of the document for D03PDF.