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 $i = 1, 2, \ldots,$ 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/D03PDA or D03PJF/D03PJA.

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/D03PDA or D03PJF/D03PJA.

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/D03PDA or D03PJF/D03PJA.

Constraint: XBKPTS(1) $<$ XBKPTS(2) $< \ldots <$ XBKPTS(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: $1 \leq$ NPOLY ≤ 49.

6: NPTS – INTEGER *Input*

On entry: the number of mesh points as used by D03PDF/D03PDA or D03PJF/D03PJA.

Constraint: NPTS $=$ (NBKPTS $- 1) \times$ 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) $< \ldots <$ 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 $U_i(x_j, t_{\text{out}})$, 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 $U_i(x_j, t_{\text{out}})$ 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 $i = 1, \ldots,$ 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/D03PDA or D03PJF/D03PJA.

8 Further Comments

None.

9 Example

See Section 9 of the document for D03PDF/D03PDA.