NAG 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

D03PYF 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, RSAVE, LRSAVE, IFAIL)
 INTEGER           NPDE, NBKPTS, NPOLY, NPTS, INTPTS, ITYPE, LRSAVE,
1                  IFAIL
 double precision  U(NPDE,NPTS), XBKPTS(NBKPTS), XP(INTPTS),
1                  UP(NPDE,INTPTS,ITYPE), RSAVE(LRSAVE)
```

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, RSAVE and LRSAVE 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) – ***double precision*** 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) – ***double precision*** array *Input*

On entry: XBKPTS(i), for $i = 1, 2, \ldots, \text{NBKPTS}$, must contain the break points as used by D03PDF/D03PDA or D03PJF/D03PJA.

Constraint: $\text{XBKPTS}(1) < \text{XBKPTS}(2) < \cdots < \text{XBKPTS}(\text{NBKPTS})$.

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) – ***double precision*** array *Input*

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

Constraint: $\text{XBKPTS}(1) \leq \text{XP}(1) < \text{XP}(2) < \cdots < \text{XP}(\text{INTPTS}) \leq \text{XBKPTS}(\text{NBKPTS})$.

When ITYPE $= 2$, $\text{XP}(i) \neq \text{XBKPTS}(j)$, for $i = 1, 2, \ldots, \text{INTPTS}$ and $j = 2, 3, \ldots, \text{NBKPTS} - 1$

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.

ITYPE $= 1$
The solution at the interpolation points are computed.

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) – ***double precision*** array *Output*

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

If ITYPE $= 2$, UP($i, j, 1$) contains $U_i\left(x_j, t_{\text{out}}\right)$ and UP($i, j, 2$) contains $\dfrac{\partial U_i}{\partial x}$ at these points.

11: RSAVE(LRSAVE) – ***double precision*** array *Communication Array*

The array RSAVE contains information required by D03PYF as returned by D03PDF/D03PDA or D03PJF/D03PJA. The contents of RSAVE must not be changed from the call to D03PDF/D03PDA or D03PJF/D03PJA. Some elements of this array are overwritten on exit.

12: LRSAVE – INTEGER *Input*

On entry: the size of the workspace RSAVE, as in D03PDF/D03PDA or D03PJF/D03PJA.

13: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction 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, if you are 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 $i = 1, 2, \ldots,$ NBKPTS, are not ordered.

IFAIL $= 2$

On entry, the interpolation points XP(i), for $i = 1, 2, \ldots,$ 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 $= 3$

You are 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 in D03PDF/D03PDA.