

NAG Fortran Library Routine Document

D02XKF

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

D02XKF interpolates components of the solution of a system of first-order ordinary differential equations from information provided by the integrators in Chapter D02M/N. It provides C^1 interpolation suitable for general use.

2 Specification

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SUBROUTINE D02XKF(XSOL, SOL, M, YSAVE, NEQMAX, NY2DIM, ACOR, NEQ, X,
1              NQU, HU, H, IFAIL)
  INTEGER      M, NEQMAX, NY2DIM, NEQ, NQU, IFAIL
  real        XSOL, SOL(M), YSAVE(NEQMAX,NY2DIM), ACOR(NEQMAX), X,
1              HU, H

```

3 Description

D02XKF evaluates the first m components of the solution of a system of ordinary differential equations at any point using C^1 polynomial interpolation based on information generated by the integrator. This information must be passed unchanged to D02XKF. D02XKF should not normally be used to extrapolate outside the range of values obtained from the above routines.

It may be used with the D02N routines only when the BDF integration method is being employed (setup routine D02NVF), provided the Petzold error test was not selected.

4 References

None.

5 Parameters

- | | | |
|----|--|---------------|
| 1: | XSOL – <i>real</i> | <i>Input</i> |
| | <i>On entry:</i> the point at which the first m components of the solution are to be evaluated. XSOL should not be an extrapolation point, that is XSOL should satisfy $(XSOL - X) \times HU \leq 0.0$. Extrapolation is permitted but not recommended. | |
| 2: | SOL(M) – <i>real</i> array | <i>Output</i> |
| | <i>On exit:</i> the calculated value of the i th component of the solution at XSOL, for $i = 1, 2, \dots, m$. | |
| 3: | M – INTEGER | <i>Input</i> |
| | <i>On entry:</i> the number of components of the solution whose values at XSOL are required. The first m components are evaluated. | |
| | <i>Constraint:</i> $1 \leq M \leq NEQ$. | |
| 4: | YSAVE(NEQMAX,NY2DIM) – <i>real</i> array | <i>Input</i> |
| | <i>On entry:</i> the values provided in the parameter YSAVE on return from the integrator. | |

- 5: NEQMAX – INTEGER *Input*
On entry: the value used for the parameter NEQMAX when calling the integrator.
Constraint: $\text{NEQMAX} \geq 1$.
- 6: NY2DIM – INTEGER *Input*
On entry: the value used for the parameter NY2DIM when calling the integrator.
Constraint: $\text{NY2DIM} \geq \text{NQU} + 1$.
- 7: ACOR(NEQMAX) – *real* array *Input*
On entry: the value returned in position $(\text{NEQMAX} + 50 + i)$, for $i = 1, 2, \dots, \text{NEQ}$, of the parameter RWORK returned by the integrator. If one of the forward communication D02N routines is being employed and D02XKF is to be used in the user-supplied MONITR routine, then ACOR(i) must contain the value given in position $(i, 2)$ of the MONITR argument ACOR, for $i = 1, 2, \dots, \text{NEQ}$.
- 8: NEQ – INTEGER *Input*
On entry: the value used for the parameter NEQ when calling the integrator.
Constraint: $1 \leq \text{NEQ} \leq \text{NEQMAX}$.
- 9: X – *real* *Input*
On entry: the latest value at which the solution has been computed, as provided in the parameter TCURR on return from the optional output D02NYF.
- 10: NQU – INTEGER *Input*
On entry: the order of the method used up to the latest value at which the solution has been computed, as provided in the parameter NQU on return from the optional output D02NYF.
Constraint: $\text{NQU} \geq 1$.
- 11: HU – *real* *Input*
On entry: the last successful step used, that is the step used in the integration to get to X, as provided in the parameter HU on return from the optional output D02NYF.
- 12: H – *real* *Input*
On entry: the next step size to be attempted in the integration, as provided in the parameter H on return from the optional output D02NYF.
- 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: $\text{IFAIL} = 0$ 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.**
If D02XKF is to be used for extrapolation, IFAIL must be set to 1 before entry. It is then essential to test the value of IFAIL on exit for $\text{IFAIL} = 1$ or 2.

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, $M < 1$,
 or $NEQ < 1$,
 or $NEQMAX < 1$,
 or $NEQ > NEQMAX$,
 or $M > NEQ$,
 or $NQU < 1$,
 or $NY2DIM < NQU + 1$,
 or the BDF integrator was not previously used,
 or the Petzold error test, if applicable, was used.

$IFAIL = 2$

On entry, $HU = 0.0$ or $H = 0.0$. This error can only occur if H and HU have been changed by the user or possibly if the integrator has failed before calling $D02XKF$.

$IFAIL = 3$

$D02XKF$ has been called for extrapolation. Before returning with this error exit, the value of the solution at $XSOL$ is calculated and placed in SOL .

7 Accuracy

The solution values returned will be of a similar accuracy to those computed by the integrator.

8 Further Comments

$D02XKF$ provides a C^1 interpolant and as such is ideal for most applications, for example for tabulation and root-finding. In general $D02XKF$ should be preferred to $D02XJF$ for interpolation as the latter provides only a C^0 interpolant. $D02XJF$ is the natural interpolant employed by the BDF method and it is supplied only to permit the user to reproduce the internal values used by the integrator.

9 Example

See Section 9 of the documents for $D02NDF$ and $D02NMF$.
