

NAG Fortran Library Routine Document

D02LXF

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

D02LXF is a setup routine which must be called by the user prior to the first call of the integrator D02LAF and may be called prior to any further call to D02LAF.

2 Specification

```

SUBROUTINE D02LXF(NEQ, H, TOL, THRES, THRESP, MAXSTP, START, ONESTEP,
1              HIGH, RWORK, LRWORK, IFAIL)
  INTEGER      NEQ, MAXSTP, LRWORK, IFAIL
  real       H, TOL, THRES(NEQ), THRESP(NEQ), RWORK(LRWORK)
  LOGICAL     START, ONESTEP, HIGH

```

3 Description

This routine permits the user to set optional inputs prior to any call of D02LAF. It must be called before the first call of routine D02LAF and it may be called before any continuation call of routine D02LAF.

4 References

None.

5 Parameters

- 1: NEQ – INTEGER *Input*
On entry: the number of second-order ordinary differential equations to be solved by D02LAF.
Constraint: $NEQ \geq 1$.
- 2: H – *real* *Input*
On entry: if START = .TRUE., H may specify an initial step size to be attempted in D02LAF.
 If START = .FALSE., then H may specify a step size to override the choice of next step attempted made internally to D02LAF.
 The sign of H is not important, as the absolute value of H is chosen and the appropriate sign is selected by D02LAF.
 If this option is not required then the user must set $H = 0.0$.
- 3: TOL – *real* *Input*
On entry: TOL must be set to a relative tolerance for controlling the error in the integration by D02LAF. D02LAF has been designed so that, for most problems, a reduction in TOL leads to an approximately proportional reduction in the error in the solution. However the actual relation between TOL and the accuracy of the solution cannot be guaranteed. The user is strongly recommended to repeat the integration with a smaller value of TOL and compare the results. See the description of THRES and THRESP for further details of how TOL is used.
Constraint: $10 \times \epsilon \leq TOL \leq 1.0$ (ϵ is the *machine precision*, see X02AJF).

- 4: THRES(NEQ) – *real* array *Input*
 5: THRESP(NEQ) – *real* array *Input*

On entry: THRES and THRESP may be set to thresholds for use in the error control of D02LAF. At each step in the numerical integration estimates of the local errors $E1(i)$ and $E2(i)$ in the solution, y_i , and its derivative, y'_i , respectively are computed, for $i = 1, 2, \dots, \text{NEQ}$. For the step to be accepted conditions of the following type must be satisfied:

$$\max_{1 \leq i \leq \text{NEQ}} \left(\frac{E1(i)}{\max(\text{THRES}(i), |y_i|)} \right) \leq \text{TOL},$$

$$\max_{1 \leq i \leq \text{NEQ}} \left(\frac{E2(i)}{\max(\text{THRESP}(i), |y'_i|)} \right) \leq \text{TOL}.$$

If one or both of these is not satisfied then the step size is reduced and the solution is recomputed.

If $\text{THRES}(1) \leq 0.0$ on entry, then a value of $50.0 \times \epsilon$ is used for $\text{THRES}(i)$, for $i = 1, 2, \dots, \text{NEQ}$, where ϵ is *machine precision*. Similarly for THRESP.

Constraints:

$$\begin{aligned} \text{THRES}(1) &\leq 0.0 \text{ or } \text{THRES}(i) > 0.0, \text{ for } i = 1, 2, \dots, \text{NEQ}, \\ \text{THRESP}(1) &\leq 0.0 \text{ or } \text{THRESP}(i) > 0.0, \text{ for } i = 1, 2, \dots, \text{NEQ}. \end{aligned}$$

- 6: MAXSTP – INTEGER *Input*

On entry: a bound on the number of steps attempted in any one call of D02LAF.

If $\text{MAXSTP} \leq 0$ on entry, a value of 1000 is used.

- 7: START – LOGICAL *Input/Output*

On entry: specifies whether or not the call of D02LAF is for a new problem. $\text{START} = \text{.TRUE.}$ indicates that a new problem is to be solved. $\text{START} = \text{.FALSE.}$ indicates the call of D02LXF is prior to a continuation call of D02LAF.

On exit: $\text{START} = \text{.FALSE.}$.

- 8: ONESTP – LOGICAL *Input*

On entry: the mode of operation for D02LAF. If $\text{ONESTP} = \text{.TRUE.}$, D02LAF will operate in one-step mode, that is it will return after each successful step. If $\text{ONESTP} = \text{.FALSE.}$, D02LAF will operate in interval mode, that is it will return at the end of the integration interval.

- 9: HIGH – LOGICAL *Input*

On entry: if $\text{HIGH} = \text{.TRUE.}$, a high-order method will be used, whereas if $\text{HIGH} = \text{.FALSE.}$, a low-order method will be used. (See the specification of D02LAF for further details.)

- 10: RWORK(LRWORK) – *real* array *Workspace*

This **must** be the same parameter RWORK supplied to D02LAF. It is used to pass information to D02LAF and therefore the contents of this array **must not** be changed before calling D02LAF.

- 11: LRWORK – INTEGER *Input*

On entry: the dimension of the array RWORK as declared in the (sub)program from which D02LXF is called.

Constraints:

$$\begin{aligned} \text{LRWORK} &\geq 16 + 20 \times \text{NEQ} \text{ if } \text{HIGH} = \text{.TRUE.}, \\ \text{LRWORK} &\geq 16 + 11 \times \text{NEQ} \text{ if } \text{HIGH} = \text{.FALSE.}. \end{aligned}$$

12: 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

THRES(1) > 0.0 and for some i THRES(i) ≤ 0.0, $1 \leq i \leq$ NEQ, and/or, THRESP(1) > 0.0 and for some i THRESP(i) ≤ 0.0, $1 \leq i \leq$ NEQ.

IFAIL = 2

LRWORK is too small.

IFAIL = 3

TOL does not satisfy $10 \times \epsilon \leq \text{TOL} \leq 1.0$ (ϵ is the *machine precision*, see X02AJF)

7 Accuracy

Not applicable.

8 Further Comments

Prior to a continuation call of D02LAF, the user may reset **any** of the optional parameters by calling D02LXF with START = .FALSE..

The user may reset:

H to override the internal step size selection;

TOL, THRES, THRESP to change the error requirements;

MAXSTP to increase or decrease the number of steps attempted before an error exit is returned;

ONESTP to change the mode of operation of D02LAF;

HIGH to change the order of the method being used.

9 Example

See Section 9 of the document for D02LAF.