NAG Fortran Library Routine Document

D02NYF

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

D02NYF is a diagnostic routine which the user may call either after any user-specified exit or after a mid-integration error exit from any of the integrators in Chapter D02M/N.

2 Specification

```
 SUBROUTINE D02NYF(NEQ, NEQMAX, HU, H, TCUR, TOLSF, RWORK, NST, NRE, NJE,
1                  NQU, NQ, NITER, IMXER, ALGEQU, INFORM, IFAIL)
 INTEGER           NEQ, NEQMAX, NST, NRE, NJE, NQU, NQ, NITER, IMXER,
1                  INFORM(23), IFAIL
 real              HU, H, TCUR, TOLSF, RWORK(50+4*NEQMAX)
 LOGICAL           ALGEQU(NEQ)
```

3 Description

This routine permits the user to inspect statistics produced by any integrator in this sub-chapter. These statistics concern the integration only.

4 References

None.

5 Parameters

1: NEQ – INTEGER *Input*

On entry: the value used for the parameter NEQ when calling the integrator.

Constraint: NEQ $\geq$ 1.

2: NEQMAX – INTEGER *Input*

On entry: the value used for the parameter NEQMAX when calling the integrator.

Constraint: NEQMAX $\geq$ NEQ.

3: HU – ***real*** *Output*

On exit: the last successful step size.

4: H – ***real*** *Output*

On exit: the proposed next step size for continuing the integration.

5: TCUR – ***real*** *Output*

On exit: the value of the independent variable, t, which the integrator has actually reached. TCUR will always be at least as far as the output value of the argument t in the direction of integration, but may be further (if overshooting and interpolation at TOUT was specified).

6: TOLSF – ***real*** *Output*

On exit: a tolerance scale factor, TOLSF ≥ 1.0, which is computed when a request for too much accuracy is detected by the integrator (indicated by a return with IFAIL $= 3$ or IFAIL $= 14$). If ITOL is left unaltered but RTOL and ATOL are uniformly scaled up by a factor of TOLSF the next call to the integrator is deemed likely to succeed.

7: RWORK(50+4∗NEQMAX) – ***real*** array *Workspace*

This must be the same workspace array as the array RWORK supplied to the integrator. It is used to pass information from the integrator to D02NYF and therefore the contents of this array must not be changed before calling D02NYF.

8: NST – INTEGER *Output*

On exit: the number of steps taken in the integration so far.

9: NRE – INTEGER *Output*

On exit: the number of function or residual evaluations (FCN or RESID calls) used in the integration so far.

10: NJE – INTEGER *Output*

On exit: the number of Jacobian evaluations used in the integration so far. This equals the number of matrix LU decompositions.

11: NQU – INTEGER *Output*

On exit: the order of the method last used (successfully) in the integration.

12: NQ – INTEGER *Output*

On exit: the proposed order of the method for continuing the integration.

13: NITER – INTEGER *Output*

On exit: the number of iterations performed in the integration so far by the nonlinear equation solver.

14: IMXER – INTEGER *Output*

On exit: the index of the component of largest magnitude in the weighted local error vector (e_i/w_i), for $i = 1, 2, \ldots, \text{NEQ}$.

15: ALGEQU(NEQ) – LOGICAL array *Output*

On exit: ALGEQU(i) = .TRUE. if the ith equation integrated was detected to be algebraic, otherwise ALGEQU(i) = .FALSE.. Note that when the integrators for explicit equations are being used, then ALGEQU(i) = .FALSE., for $i = 1, 2, \ldots, \text{NEQ}$.

16: INFORM(23) – INTEGER array *Workspace*

This must be the same array as the array INFORM supplied to the integrator. It is used to pass information from the integrator to D02NYF and therefore its contents must not be changed before calling D02NYF.

17: 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, NEQ < 1,
or NEQMAX < 1,
or NEQ $>$ NEQMAX.

7 Accuracy

Not applicable.

8 Further Comments

Statistics for sparse matrix linear algebra calls (if appropriate) may be determined by a call to D02NXF.

9 Example

See Section 9 of the document for D02NBF.