

NAG Fortran Library Routine Document

D02NSF

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

D02NSF is a setup routine which must be called by the user, prior to an integrator in Chapter D02M/N, if full matrix linear algebra is required.

2 Specification

```
SUBROUTINE D02NSF (NEQ, NEQMAX, JCEVAL, NWKJAC, RWORK, IFAIL)
INTEGER          NEQ, NEQMAX, NWKJAC, IFAIL
real           RWORK(50 + 4 * NEQMAX)
CHARACTER*1     JCEVAL
```

3 Description

This routine defines the linear algebra to be used as full matrix linear algebra, permits the user to specify the method for calculating the Jacobian and checks the validity of certain input values.

4 References

None.

5 Parameters

1: NEQ – INTEGER *Input*

On entry: the number of differential equations.

Constraint: $1 \leq \text{NEQ} \leq \text{NEQMAX}$.

2: NEQMAX – INTEGER *Input*

On entry: a bound on the maximum number of differential equations to be solved during the integration.

Constraint: $\text{NEQMAX} \geq \text{NEQ}$.

3: JCEVAL – CHARACTER*1 *Input*

On entry: specifies the technique to be used to compute the Jacobian, as follows:

JCEVAL = 'N'

The Jacobian is to be evaluated numerically by the integrator. If this option is used, then the actual argument corresponding to JAC in the call to D02NBF or D02NGF must be either D02NBZ or D02NGZ respectively.

JCEVAL = 'A'

The user will supply a subroutine to evaluate the Jacobian on a call to the integrator.

JCEVAL = 'D'

The default choice is to be made. In this case 'D' is interpreted as 'N'.

Only the first character of the actual argument JCEVAL is passed to D02NSF; hence it is permissible for the actual argument to be more descriptive 'Numerical', 'Analytical' or 'Default' on a call to D02NSF.

Constraint: JCEVAL = 'N', 'A' or 'D'.

4: NWKJAC – INTEGER

Input

On entry: the size of the workspace array WKJAC, which the user is supplying to the integrator, as declared in the (sub)program from which D02NSF is called.

Constraint: $NWKJAC \geq NEQMAX \times (NEQMAX + 1)$.

5: 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 setup routine to the integrator and therefore the contents of this array must not be changed before calling the integrator.

6: 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 NEQ > NEQMAX,
or $NWKJAC < NEQMAX \times (NEQMAX + 1)$,
or JCEVAL \neq 'N', 'A' or 'D'.

7 Accuracy

Not applicable.

8 Further Comments

This routine must be called as a setup routine before a call to either D02NBF or D02NGF and may be called as the linear algebra setup routine before a call to either D02NMF or D02NNF.

9 Example

See Section 9 of the documents for D02NBF, D02NGF and D02NMF.