

# NAG Library Routine Document

## D02TZF

**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

D02TZF returns information about the solution of a general two-point boundary value problem computed by D02TLF.

### 2 Specification

```

SUBROUTINE D02TZF (MXMESH, NMESH, MESH, IPMESH, ERMX, IERMX, IJERMX,      &
                  RCOMM, ICOMM, IFAIL)
INTEGER              MXMESH, NMESH, IPMESH(MXMESH), IERMX, IJERMX,      &
                  ICOMM(*), IFAIL
REAL (KIND=nag_wp) MESH(MXMESH), ERMX, RCOMM(*)

```

### 3 Description

D02TZF and its associated routines (D02TLF, D02TVF, D02TXF and D02TYF) solve the two-point boundary value problem for a nonlinear mixed order system of ordinary differential equations

$$\begin{aligned}
 y_1^{(m_1)}(x) &= f_1(x, y_1, y_1^{(1)}, \dots, y_1^{(m_1-1)}, y_2, \dots, y_n^{(m_n-1)}) \\
 y_2^{(m_2)}(x) &= f_2(x, y_1, y_1^{(1)}, \dots, y_1^{(m_1-1)}, y_2, \dots, y_n^{(m_n-1)}) \\
 &\vdots \\
 y_n^{(m_n)}(x) &= f_n(x, y_1, y_1^{(1)}, \dots, y_1^{(m_1-1)}, y_2, \dots, y_n^{(m_n-1)})
 \end{aligned}$$

over an interval  $[a, b]$  subject to  $p$  ( $> 0$ ) nonlinear boundary conditions at  $a$  and  $q$  ( $> 0$ ) nonlinear boundary conditions at  $b$ , where  $p + q = \sum_{i=1}^n m_i$ . Note that  $y_i^{(m)}(x)$  is the  $m$ th derivative of the  $i$ th solution component. Hence  $y_i^{(0)}(x) = y_i(x)$ . The left boundary conditions at  $a$  are defined as

$$g_i(z(y(a))) = 0, \quad i = 1, 2, \dots, p,$$

and the right boundary conditions at  $b$  as

$$\bar{g}_j(z(y(b))) = 0, \quad j = 1, 2, \dots, q,$$

where  $y = (y_1, y_2, \dots, y_n)$  and

$$z(y(x)) = (y_1(x), y_1^{(1)}(x), \dots, y_1^{(m_1-1)}(x), y_2(x), \dots, y_n^{(m_n-1)}(x)).$$

First, D02TVF must be called to specify the initial mesh, error requirements and other details. Then, D02TLF can be used to solve the boundary value problem. After successful computation, D02TZF can be used to ascertain details about the final mesh. D02TYF can be used to compute the approximate solution anywhere on the interval  $[a, b]$  using interpolation.

The routines are based on modified versions of the codes COLSYS and COLNEW (see Ascher *et al.* (1979) and Ascher and Bader (1987)). A comprehensive treatment of the numerical solution of boundary value problems can be found in Ascher *et al.* (1988) and Keller (1992).

## 4 References

Ascher U M and Bader G (1987) A new basis implementation for a mixed order boundary value ODE solver *SIAM J. Sci. Stat. Comput.* **8** 483–500

Ascher U M, Christiansen J and Russell R D (1979) A collocation solver for mixed order systems of boundary value problems *Math. Comput.* **33** 659–679

Ascher U M, Mattheij R M M and Russell R D (1988) *Numerical Solution of Boundary Value Problems for Ordinary Differential Equations* Prentice–Hall

Cole J D (1968) *Perturbation Methods in Applied Mathematics* Blaisdell, Waltham, Mass.

Keller H B (1992) *Numerical Methods for Two-point Boundary-value Problems* Dover, New York

## 5 Arguments

1: MXMESH – INTEGER *Input*

*On entry:* the maximum number of points allowed in the mesh.

*Constraint:* this must be identical to the value supplied for the argument MXMESH in the prior call to D02TVF.

2: NMESH – INTEGER *Output*

*On exit:* the number of points in the mesh last used by D02TLF.

3: MESH(MXMESH) – REAL (KIND=nag\_wp) array *Output*

*On exit:* MESH(*i*) contains the *i*th point of the mesh last used by D02TLF, for  $i = 1, 2, \dots, NMESH$ . MESH(1) will contain *a* and MESH(NMESH) will contain *b*. The remaining elements of MESH are not initialized.

4: IPMESH(MXMESH) – INTEGER array *Output*

*On exit:* IPMESH(*i*) specifies the nature of the point MESH(*i*), for  $i = 1, 2, \dots, NMESH$ , in the final mesh computed by D02TLF.

IPMESH(*i*) = 1

Indicates that the *i*th point is a fixed point and was used by the solver before an extrapolation-like error test.

IPMESH(*i*) = 2

Indicates that the *i*th point was used by the solver before an extrapolation-like error test.

IPMESH(*i*) = 3

Indicates that the *i*th point was used by the solver only as part of an extrapolation-like error test.

The remaining elements of IPMESH are initialized to  $-1$ .

See Section 9 for advice on how these values may be used in conjunction with a continuation process.

5: ERMX – REAL (KIND=nag\_wp) *Output*

*On exit:* an estimate of the maximum error in the solution computed by D02TLF, that is

$$ERMX = \max \frac{\|y_i - v_i\|}{(1.0 + \|v_i\|)}$$

where  $v_i$  is the approximate solution for the *i*th solution component. If D02TLF returned successfully with IFAIL = 0, then ERMX will be less than TOLS(IJERMX) where TOLS contains the error requirements as specified in Sections 3 and 5 in D02TVF.

If D02TLF returned with IFAIL = 5, then ERMX will be greater than TOLS(IJERMX).

If D02TLF returned any other value for IFAIL then an error estimate is not available and ERMX is initialized to 0.0.

6: IERMX – INTEGER *Output*

*On exit:* indicates the mesh sub-interval where the value of ERMX has been computed, that is  $[\text{MESH}(\text{IERMX}), \text{MESH}(\text{IERMX} + 1)]$ .

If an estimate of the error is not available then IERMX is initialized to 0.

7: IJERMX – INTEGER *Output*

*On exit:* indicates the component  $i$  ( $= \text{IJERMX}$ ) of the solution for which ERMX has been computed, that is the approximation of  $y_i$  on  $[\text{MESH}(\text{IERMX}), \text{MESH}(\text{IERMX} + 1)]$  is estimated to have the largest error of all components  $y_i$  over mesh sub-intervals defined by MESH.

If an estimate of the error is not available then IJERMX is initialized to 0.

8: RCOMM(\*) – REAL (KIND=nag\_wp) array *Communication Array*

**Note:** the dimension of this array is dictated by the requirements of associated functions that must have been previously called. This array **must** be the same array passed as argument RCOMM in the previous call to D02TLF.

*On entry:* this must be the same array as supplied to D02TLF and **must** remain unchanged between calls.

*On exit:* contains information about the solution for use on subsequent calls to associated routines.

9: ICOMM(\*) – INTEGER array *Communication Array*

**Note:** the dimension of this array is dictated by the requirements of associated functions that must have been previously called. This array **must** be the same array passed as argument ICOMM in the previous call to D02TLF.

*On entry:* this must be the same array as supplied to D02TLF and **must** remain unchanged between calls.

*On exit:* contains information about the solution for use on subsequent calls to associated routines.

10: IFAIL – INTEGER *Input/Output*

*On entry:* IFAIL must be set to 0,  $-1$  or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation for details.

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, because for this routine the values of the output arguments may be useful even if  $\text{IFAIL} \neq 0$  on exit, the recommended value is  $-1$ . **When the value  $-1$  or 1 is used it is essential to test the value of IFAIL on exit.**

*On exit:*  $\text{IFAIL} = 0$  unless the routine detects an error or a warning has been flagged (see Section 6).

## 6 Error Indicators and Warnings

If on entry  $\text{IFAIL} = 0$  or  $-1$ , explanatory error messages are output on the current error message unit (as defined by X04AAF).

**Note:** D02TZF may return useful information for one or more of the following detected errors or warnings.

Errors or warnings detected by the routine:

IFAIL = 1

On entry, an illegal value for MXMESH was specified, or an invalid call to D02TZF was made, for example without a previous call to the solver routine D02TLF.

IFAIL = 2

The solver routine D02TLF did not converge to a solution or did not satisfy the error requirements. The last mesh computed by D02TLF has been returned by D02TZF. This mesh should be treated with extreme caution as nothing can be said regarding its quality or suitability for any subsequent computation.

IFAIL = -99

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -399

Your licence key may have expired or may not have been installed correctly.

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -999

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

## 7 Accuracy

Not applicable.

## 8 Parallelism and Performance

D02TZF is not threaded in any implementation.

## 9 Further Comments

Note that:

if D02TLF returned IFAIL = 0, 4 or 5 then it will always be the case that  $IPMESH(1) = IPMESH(NMESH) = 1$ ;

if D02TLF returned IFAIL = 0 or 5 then it will always be the case that  $IPMESH(i) = 3$ , for  $i = 2, 4, \dots, NMESH - 1$  (even  $i$ ) and  $IPMESH(i) = 1$  or 2, for  $i = 3, 5, \dots, NMESH - 2$  (odd  $i$ );

if D02TLF returned IFAIL = 4 then it will always be the case that  $IPMESH(i) = 1$  or 2, for  $i = 2, 3, \dots, NMESH - 1$ .

If D02TZF returns IFAIL = 0, then examination of the mesh may provide assistance in determining a suitable starting mesh for D02TVF in any subsequent attempts to solve similar problems.

If the problem being treated by D02TLF is one of a series of related problems (for example, as part of a continuation process), then the values of IPMESH and MESH may be suitable as input arguments to D02TXF. Using the mesh points not involved in the extrapolation error test is usually appropriate. IPMESH and MESH should be passed unchanged to D02TXF but NMESH should be replaced by  $(NMESH + 1)/2$ .

If D02TZF returns IFAIL = 2, nothing can be said regarding the quality of the mesh returned. However, it may be a useful starting mesh for D02TVF in any subsequent attempts to solve the same problem.

If D02TLF returns `IFAIL = 5`, this corresponds to the solver requiring more than `MXMESH` mesh points to satisfy the error requirements. If `MXMESH` can be increased and the preceding call to D02TLF was not part, or was the first part, of a continuation process then the values in `MESH` may provide a suitable mesh with which to initialize a subsequent attempt to solve the same problem. If it is not possible to provide more mesh points then relaxing the error requirements by setting `TOLS(IJERMX)` to `ERMX` might lead to a successful solution. It may be necessary to reset the other components of `TOLS`. Note that resetting the tolerances can lead to a different sequence of meshes being computed and hence to a different solution being computed.

## 10 Example

The following example is used to illustrate the use of fixed mesh points, simple continuation and numerical approximation of a Jacobian. See also D02TLF, D02TVF, D02TXF and D02TYF, for the illustration of other facilities.

Consider the Lagerstrom–Cole equation

$$y'' = (y - yy')/\epsilon$$

with the boundary conditions

$$y(0) = \alpha \quad y(1) = \beta, \tag{1}$$

where  $\epsilon$  is small and positive. The nature of the solution depends markedly on the values of  $\alpha, \beta$ . See Cole (1968).

We choose  $\alpha = -\frac{1}{3}, \beta = \frac{1}{3}$  for which the solution is known to have corner layers at  $x = \frac{1}{3}, \frac{2}{3}$ . We choose an initial mesh of seven points  $[0.0, 0.15, 0.3, 0.5, 0.7, 0.85, 1.0]$  and ensure that the points  $x = 0.3, 0.7$  near the corner layers are fixed, that is the corresponding elements of the array `IPMESH` are set to 1. First we compute the solution for  $\epsilon = 1.0\text{E-}4$  using in `GUESS` the initial approximation  $y(x) = \alpha + (\beta - \alpha)x$  which satisfies the boundary conditions. Then we use simple continuation to compute the solution for  $\epsilon = 1.0\text{E-}5$ . We use the suggested values for `NMESH`, `IPMESH` and `MESH` in the call to D02TXF prior to the continuation call, that is only every second point of the preceding mesh is used and the fixed mesh points are retained.

Although the analytic Jacobian for this system is easy to evaluate, for illustration the procedure `FJAC` uses central differences and calls to `FFUN` to compute a numerical approximation to the Jacobian.

### 10.1 Program Text

```
! D02TZF Example Program Text
! Mark 26 Release. NAG Copyright 2016.

Module d02tzfe_mod

! D02TZF Example Program Module:
! Parameters and User-defined Routines

! .. Use Statements ..
Use nag_library, Only: nag_wp
! .. Implicit None Statement ..
Implicit None
! .. Accessibility Statements ..
Private
Public                                :: ffun, fjac, gafun, gajac, gbfun,      &
                                       gbjac, guess

! .. Parameters ..
Integer, Parameter, Public            :: mmax = 2, neq = 1, nin = 5,          &
                                       nlbc = 1, nout = 6, nrbc = 1

! .. Local Scalars ..
Real (Kind=nag_wp), Public, Save     :: alpha, beta, eps

! .. Local Arrays ..
Integer, Public, Save                 :: m(1) = (/2/)

Contains
Subroutine ffun(x,y,neq,m,f,iuser,ruser)
```

```

!      .. Scalar Arguments ..
      Real (Kind=nag_wp), Intent (In) :: x
      Integer, Intent (In)           :: neq
!      .. Array Arguments ..
      Real (Kind=nag_wp), Intent (Out) :: f(neq)
      Real (Kind=nag_wp), Intent (Inout) :: ruser(*)
      Real (Kind=nag_wp), Intent (In) :: y(neq,0:*)
      Integer, Intent (Inout)       :: iuser(*)
      Integer, Intent (In)          :: m(neq)
!      .. Executable Statements ..
      f(1) = (y(1,0)-y(1,0)*y(1,1))/eps
      Return
End Subroutine ffun
Subroutine fjac(x,y,neq,m,dfdy,iuser,ruser)

!      .. Use Statements ..
      Use nag_library, Only: x02ajf
!      .. Scalar Arguments ..
      Real (Kind=nag_wp), Intent (In) :: x
      Integer, Intent (In)           :: neq
!      .. Array Arguments ..
      Real (Kind=nag_wp), Intent (Inout) :: dfdy(neq,neq,0:*), ruser(*)
      Real (Kind=nag_wp), Intent (In) :: y(neq,0:*)
      Integer, Intent (Inout)       :: iuser(*)
      Integer, Intent (In)          :: m(neq)
!      .. Local Scalars ..
      Real (Kind=nag_wp)             :: epsh, fac, ptrb
      Integer                        :: i, j, k
!      .. Local Arrays ..
      Real (Kind=nag_wp)             :: f1(1), f2(1), yp(1,0:3)
!      .. Intrinsic Procedures ..
      Intrinsic                      :: abs, max, sqrt
!      .. Executable Statements ..
      epsh = 100.0_nag_wp*x02ajf()
      fac = sqrt(x02ajf())
      Do i = 1, neq
        Do j = 0, m(i) - 1
          yp(i,j) = y(i,j)
        End Do
      End Do
      Do i = 1, neq
        Do j = 0, m(i) - 1
          ptrb = max(epsh,fac*abs(y(i,j)))
          yp(i,j) = y(i,j) + ptrb
          Call ffun(x,yp,neq,m,f1,iuser,ruser)
          yp(i,j) = y(i,j) - ptrb
          Call ffun(x,yp,neq,m,f2,iuser,ruser)
          Do k = 1, neq
            dfdy(k,i,j) = 0.5_nag_wp*(f1(k)-f2(k))/ptrb
          End Do
          yp(i,j) = y(i,j)
        End Do
      End Do
      Return
End Subroutine fjac
Subroutine gafun(ya,neq,m,nlbc,ga,iuser,ruser)

!      .. Scalar Arguments ..
      Integer, Intent (In)           :: neq, nlbc
!      .. Array Arguments ..
      Real (Kind=nag_wp), Intent (Out) :: ga(nlbc)
      Real (Kind=nag_wp), Intent (Inout) :: ruser(*)
      Real (Kind=nag_wp), Intent (In) :: ya(neq,0:*)
      Integer, Intent (Inout)       :: iuser(*)
      Integer, Intent (In)          :: m(neq)
!      .. Executable Statements ..
      ga(1) = ya(1,0) - alpha
      Return
End Subroutine gafun
Subroutine gbfun(yb,neq,m,nrbc,gb,iuser,ruser)

```

```

!      .. Scalar Arguments ..
      Integer, Intent (In)          :: neq, nrbc
!      .. Array Arguments ..
      Real (Kind=nag_wp), Intent (Out) :: gb(nrbc)
      Real (Kind=nag_wp), Intent (Inout) :: ruser(*)
      Real (Kind=nag_wp), Intent (In) :: yb(neq,0:*)
      Integer, Intent (Inout)        :: iuser(*)
      Integer, Intent (In)           :: m(neq)
!      .. Executable Statements ..
      gb(1) = yb(1,0) - beta
      Return
End Subroutine gbfun
Subroutine gajac(ya,neq,m,nlbc,dgady,iuser,ruser)

!      .. Parameters ..
      Real (Kind=nag_wp), Parameter :: one = 1.0_nag_wp
!      .. Scalar Arguments ..
      Integer, Intent (In)          :: neq, nlbc
!      .. Array Arguments ..
      Real (Kind=nag_wp), Intent (Inout) :: dgady(nlbc,neq,0:*), ruser(*)
      Real (Kind=nag_wp), Intent (In) :: ya(neq,0:*)
      Integer, Intent (Inout)        :: iuser(*)
      Integer, Intent (In)           :: m(neq)
!      .. Executable Statements ..
      dgady(1,1,0) = one
      Return
End Subroutine gajac
Subroutine gbjac(yb,neq,m,nrbc,dgbdy,iuser,ruser)

!      .. Parameters ..
      Real (Kind=nag_wp), Parameter :: one = 1.0_nag_wp
!      .. Scalar Arguments ..
      Integer, Intent (In)          :: neq, nrbc
!      .. Array Arguments ..
      Real (Kind=nag_wp), Intent (Inout) :: dgbdy(nrbc,neq,0:*), ruser(*)
      Real (Kind=nag_wp), Intent (In) :: yb(neq,0:*)
      Integer, Intent (Inout)        :: iuser(*)
      Integer, Intent (In)           :: m(neq)
!      .. Executable Statements ..
      dgbdy(1,1,0) = one
      Return
End Subroutine gbjac
Subroutine guess(x,neq,m,y,dym,iuser,ruser)

!      .. Scalar Arguments ..
      Real (Kind=nag_wp), Intent (In) :: x
      Integer, Intent (In)          :: neq
!      .. Array Arguments ..
      Real (Kind=nag_wp), Intent (Out) :: dym(neq)
      Real (Kind=nag_wp), Intent (Inout) :: ruser(*), y(neq,0:*)
      Integer, Intent (Inout)        :: iuser(*)
      Integer, Intent (In)           :: m(neq)
!      .. Executable Statements ..
      y(1,0) = alpha + (beta-alpha)*x
      y(1,1) = (beta-alpha)
      dym(1) = 0.0_nag_wp
      Return
End Subroutine guess
End Module d02tzfe_mod
Program d02tzfe

!      D02TZF Example Main Program

!      .. Use Statements ..
      Use nag_library, Only: d02tlf, d02tvf, d02txf, d02tyf, d02tzf, nag_wp
      Use d02tzfe_mod, Only: alpha, beta, eps, ffun, fjac, gafun, gajac,      &
                           gbfun, gbjac, guess, m, mmax, neq, nin, nlbc,    &
                           nout, nrbc
!      .. Implicit None Statement ..
      Implicit None
!      .. Local Scalars ..

```

```

Real (Kind=nag_wp)          :: ermx
Integer                     :: i, iermx, ifail, ijermx, j, licomm, &
                           lrcomm, mxmesh, ncol, nmesh
Logical                     :: failed
! .. Local Arrays ..
Real (Kind=nag_wp), Allocatable :: mesh(:), rcomm(:), tol(:), y(:, :)
Real (Kind=nag_wp)          :: ruser(1)
Integer, Allocatable        :: icomm(:), ipmesh(:)
Integer                     :: iuser(2)
! .. Executable Statements ..
Write (nout,*) 'D02TZF Example Program Results'
Write (nout,*)
! Skip heading in data file
Read (nin,*)
Read (nin,*) ncol, nmesh, mxmesh
Allocate (mesh(mxmesh),tol(neq),y(neq,0:mmax-1),ipmesh(mxmesh))

Read (nin,*) alpha, beta, eps
Read (nin,*) mesh(1:nmesh)
Read (nin,*) ipmesh(1:nmesh)
Read (nin,*) tol(1:neq)

! Workspace query to get size of rcomm and icomm
ifail = 0
Call d02tvf(neq,m,nlbc,nrbc,ncol,tol,mxmesh,nmesh,mesh,ipmesh,ruser,0, &
            iuser,2,ifail)
lrcomm = iuser(1)
licomm = iuser(2)
Allocate (rcomm(lrcomm),icomm(licomm))

! Initialize
ifail = 0
Call d02tvf(neq,m,nlbc,nrbc,ncol,tol,mxmesh,nmesh,mesh,ipmesh,rcomm, &
            lrcomm,icomm,licomm,ifail)

eps = 0.1_nag_wp*eps
contn: Do j = 1, 2
    Write (nout,99997) tol(1), eps

! Solve
    ifail = -1
    Call d02tlf(ffun,fjac,gafun,gbfun,gajac,gbjac,guess,rcomm,icomm,iuser, &
               ruser,ifail)
    failed = ifail /= 0

! Extract mesh.
    ifail = -1
    Call d02tzf(mxmesh,nmesh,mesh,ipmesh,ermx,iermx,ijermx,rcomm,icomm, &
               ifail)

! Print mesh statistics.
    Write (nout,99996) nmesh, ermx, iermx, ijermx

    If (failed) Then
        Exit contn
    End If

! Print solution at every second point on final mesh.
    Write (nout,99999)
    Do i = 1, nmesh, 2
        ifail = -1
        Call d02tyf(mesh(i),y,neq,mmax,rcomm,icomm,ifail)
        Write (nout,99998) mesh(i), y(1,0), y(1,1)
    End Do

    If (j==1) Then
! Halve final mesh for new initial mesh and set up for continuation.
        nmesh = (nmesh+1)/2
        ifail = 0
        Call d02txf(mxmesh,nmesh,mesh,ipmesh,rcomm,icomm,ifail)

```





0.5000	-0.00000	0.00000
0.5500	0.00000	0.00000
0.6000	0.00000	0.00000
0.6500	0.00001	0.00354
0.7000	0.03333	1.00745
0.7375	0.07083	1.00202
0.7750	0.10833	1.00098
0.8125	0.14583	1.00059
0.8500	0.18333	1.00040
0.8875	0.22083	1.00029
0.9250	0.25833	1.00022
0.9625	0.29583	1.00018
1.0000	0.33333	1.00014



