NAG Library Routine Document

D02TYF

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

D02TYF interpolates on the solution of a general two-point boundary value problem computed by D02TLF.

2 Specification

```
SUBROUTINE D02TYF (X, Y, NEQ, MMAX, RCOMM, ICOMM, IFAIL)
INTEGER            NEQ, MMAX, ICOMM(*), IFAIL
REAL (KIND=nag_wp) X, Y(NEQ,MMAX), RCOMM(*)
```

3 Description

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

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

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 mth derivative of the ith solution component. Hence $y_i^{(0)}(x) = y_i(x)$. The left boundary conditions at a are defined as

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

and the right boundary conditions at b as

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

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

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

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 and other details of the solution procedure, and 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

Grossman C (1992) Enclosures of the solution of the Thomas–Fermi equation by monotone discretization *J. Comput. Phys.* **98** 26–32

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

5 Arguments

1: X – REAL (KIND=nag_wp) *Input*

On entry: x, the independent variable.

Constraint: $a \leq \mathrm{X} \leq b$, i.e., not outside the range of the original mesh specified in the initialization call to D02TVF.

2: Y(NEQ, MMAX) – REAL (KIND=nag_wp) array *Output*

On exit: $\mathrm{Y}(i,j)$ contains an approximation to $y_i^{(j)}(x)$, for $i = 1, 2, \ldots, \mathrm{NEQ}$ and $j = 0, 1, \ldots, m_i - 1$. The remaining elements of Y (where $m_i < \mathrm{MMAX}$) are initialized to 0.0.

3: NEQ – INTEGER *Input*

On entry: the number of differential equations.

Constraint: NEQ must be the same value as supplied to D02TVF.

4: MMAX – INTEGER *Input*

On entry: the maximal order of the differential equations, $\max(m_i)$, for $i = 1, 2, \ldots, \mathrm{NEQ}$.

Constraint: MMAX must contain the maximum value of the components of the argument M as supplied to D02TVF.

5: 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.

6: 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.

7: 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 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: 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 IFAIL $= 0$ or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Note: D02TYF 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, MMAX $= \langle value \rangle$ and $\max \mathrm{M}(i) = \langle value \rangle$.
Constraint: MMAX $= \max \mathrm{M}(i)$.

On entry, NEQ $= \langle value \rangle$ and NEQ $= \langle value \rangle$ in D02TVF.
Constraint: NEQ $=$ NEQ in D02TVF.

On entry, X $= \langle value \rangle$.
Constraint: X $\leq \langle value \rangle$.

On entry, X $= \langle value \rangle$.
Constraint: X $\geq \langle value \rangle$.

The solver routine did not produce any results suitable for interpolation.

The solver routine does not appear to have been called.

IFAIL $= 2$

The solver routine did not converge to a suitable solution.
A converged intermediate solution has been used.
Interpolated values should be treated with caution.

The solver routine did not satisfy the error requirements.
Interpolated values should be treated with caution.

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

If D02TYF returns the value IFAIL $= 0$, the computed values of the solution components y_i should be of similar accuracy to that specified by the argument TOLS of D02TVF. Note that during the solution process the error in the derivatives $y_i^{(j)}$, for $j = 1, 2, \ldots, m_i - 1$, has not been controlled and that the derivative values returned by D02TYF are computed via differentiation of the piecewise polynomial approximation to y_i. See also Section 9.

8 Parallelism and Performance

D02TYF makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

If D02TYF returns the value IFAIL $= 2$ in this routine and IFAIL $= 5$ in D02TLF, then the accuracy of the interpolated values may be proportional to the quantity ERMX as returned by D02TZF.

If D02TLF returned a value for IFAIL other than IFAIL $= 0$, then nothing can be said regarding either the quality or accuracy of the values computed by D02TYF.

10 Example

The following example is used to illustrate that a system with singular coefficients can be treated without modification of the system definition. See also D02TLF, D02TVF, D02TXF and D02TZF, for the illustration of other facilities.

Consider the Thomas–Fermi equation used in the investigation of potentials and charge densities of ionized atoms. See Grossman (1992), for example, and the references therein. The equation is

$$y'' = x^{-1/2} y^{3/2}$$

with boundary conditions

$$y(0) = 1, \quad y(a) = 0, \quad a > 0.$$

The coefficient $x^{-1/2}$ implies a singularity at the left-hand boundary $x = 0$.

We use the initial approximation $y(x) = 1 - x/a$, which satisfies the boundary conditions, on a uniform mesh of six points. For illustration we choose $a = 1$, as in Grossman (1992). Note that in FFUN and FJAC (see D02TLF) we have taken the precaution of setting the function value and Jacobian value to 0.0 in case a value of y becomes negative, although starting from our initial solution profile this proves unnecessary during the solution phase. Of course the true solution $y(x)$ is positive for all $x < a$.

10.1 Program Text

```
!   D02TYF Example Program Text
!   Mark 26 Release. NAG Copyright 2016.

    Module d02tyfe_mod

!     D02TYF 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, nmesh_out = 11, nout = 6,  &
                                          nrbc = 1
!     .. Local Scalars ..
      Real (Kind=nag_wp), Public, Save :: a
!     .. 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)
!       .. Intrinsic Procedures ..
        Intrinsic                      :: sqrt
!       .. Executable Statements ..
        If (y(1,0)<=0.0E0_nag_wp) Then
          f(1) = 0.0_nag_wp
        Else
          f(1) = (y(1,0))**1.5_nag_wp/sqrt(x)
        End If
        Return
      End Subroutine ffun
      Subroutine fjac(x,y,neq,m,dfdy,iuser,ruser)

!       .. 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)
!       .. Intrinsic Procedures ..
        Intrinsic                      :: sqrt
!       .. Executable Statements ..
        If (y(1,0)<=0.0E0_nag_wp) Then
          dfdy(1,1,0) = 0.0_nag_wp
        Else
          dfdy(1,1,0) = 1.5_nag_wp*sqrt(y(1,0))/sqrt(x)
        End If
        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) - 1.0_nag_wp
        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)
        Return
      End Subroutine gbfun
      Subroutine gajac(ya,neq,m,nlbc,dgady,iuser,ruser)

!       .. 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) = 1.0_nag_wp
        Return
      End Subroutine gajac
      Subroutine gbjac(yb,neq,m,nrbc,dgbdy,iuser,ruser)

!       .. 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) = 1.0_nag_wp
        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) = 1.0_nag_wp - x/a
        y(1,1) = -1.0_nag_wp/a
        dym(1) = 0.0_nag_wp
        Return
      End Subroutine guess
    End Module d02tyfe_mod
    Program d02tyfe

!     D02TYF Example Main Program

!     .. Use Statements ..
      Use nag_library, Only: d02tlf, d02tvf, d02tyf, d02tzf, nag_wp
      Use d02tyfe_mod, Only: a, ffun, fjac, gafun, gajac, gbfun, gbjac, guess, &
                             m, mmax, neq, nin, nlbc, nmesh_out, nout, nrbc
!     .. Implicit None Statement ..
      Implicit None
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: ainc, ermx, x
      Integer                          :: i, iermx, ifail, ijermx, 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)
!     .. Intrinsic Procedures ..
      Intrinsic                          :: real
!     .. Executable Statements ..
      Write (nout,*) 'D02TYF 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,*) a
      Read (nin,*) tol(1:neq)

      ainc = a/real(nmesh-1,kind=nag_wp)
      mesh(1) = 0.0E0_nag_wp
      Do i = 2, nmesh - 1
        mesh(i) = mesh(i-1) + ainc
      End Do
      mesh(nmesh) = a

      ipmesh(1) = 1
      ipmesh(2:nmesh-1) = 2
      ipmesh(nmesh) = 1

!     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)

      Write (nout,99999) tol(1), a

!     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)

      If (ifail/=1) Then
!       Print mesh statistics
        Write (nout,99998) nmesh, ermx, iermx, ijermx
        Write (nout,99997)(i,ipmesh(i),mesh(i),i=1,nmesh)
      End If
      If (.Not. failed) Then
!       Print solution on output mesh.
        Write (nout,99996)
        x = 0.0_nag_wp
        ainc = a/real(nmesh_out-1,kind=nag_wp)
        Do i = 1, nmesh_out
          ifail = 0
          Call d02tyf(x,y,neq,mmax,rcomm,icomm,ifail)
          Write (nout,99995) x, y(1,0:1)
          x = x + ainc
        End Do
      End If
```

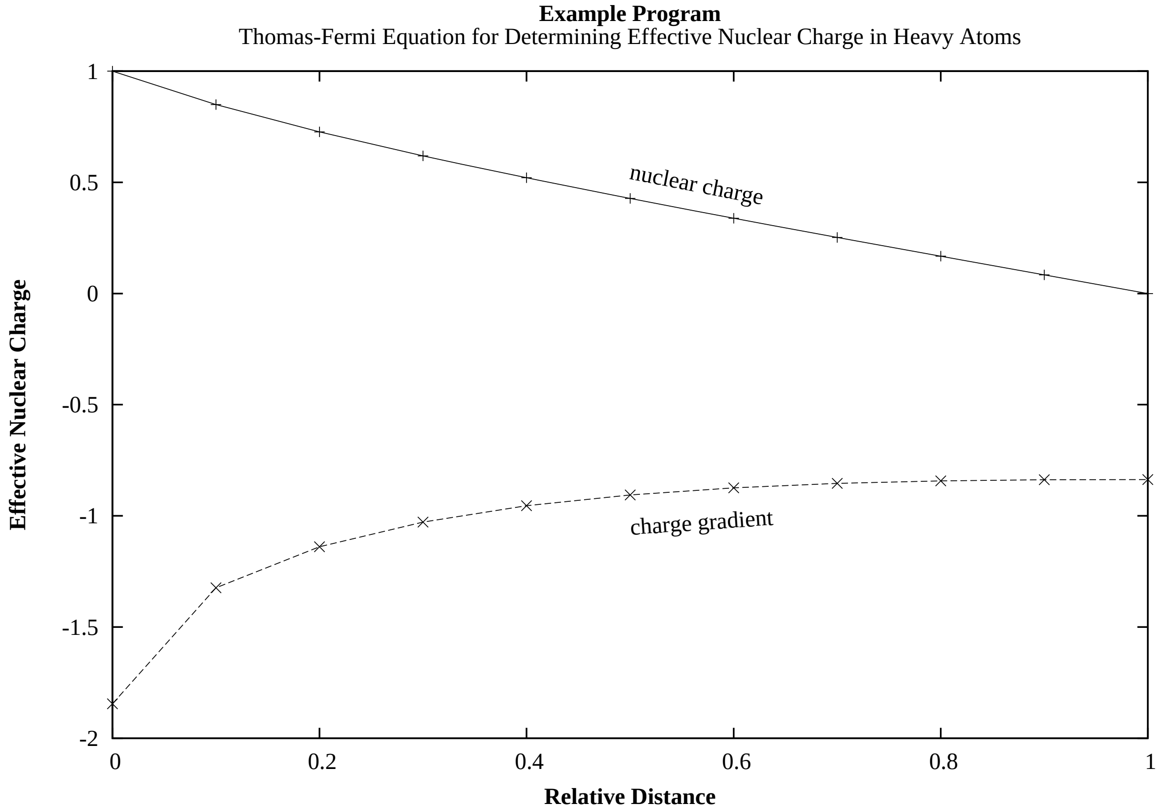
```
99999 Format (/,/,' Tolerance = ',E8.1,' A = ',F8.2)
99998 Format (/,' Used a mesh of ',I4,' points',/,' Maximum error = ',E10.2,   &
        '  in interval ',I4,' for component ',I4,/)
99997 Format (/,' Mesh points:',/,4(I4,'(',I1,')',E11.4))
99996 Format (/,' Computed solution',/,'       x     solution   derivative')
99995 Format (' ',F8.2,2F11.5)

    End Program d02tyfe
```

10.2 Program Data

```
D02TYF Example Program Data
   4  6  100                    : ncol, nmesh, mxmesh
   1.0                          : a
   1.0E-5                       : tol
```

10.3 Program Results

```
 D02TYF Example Program Results



 Tolerance =  0.1E-04 A =     1.00

 Used a mesh of   11 points
 Maximum error =   0.31E-05  in interval    1 for component    1


 Mesh points:
   1(1) 0.0000E+00   2(3) 0.1000E+00   3(2) 0.2000E+00   4(3) 0.3000E+00
   5(2) 0.4000E+00   6(3) 0.5000E+00   7(2) 0.6000E+00   8(3) 0.7000E+00
   9(2) 0.8000E+00  10(3) 0.9000E+00  11(1) 0.1000E+01

 Computed solution
       x     solution   derivative
     0.00    1.00000   -1.84496
     0.10    0.84944   -1.32330
     0.20    0.72721   -1.13911
     0.30    0.61927   -1.02776
     0.40    0.52040   -0.95468
     0.50    0.42754   -0.90583
     0.60    0.33867   -0.87372
     0.70    0.25239   -0.85369
     0.80    0.16764   -0.84248
     0.90    0.08368   -0.83756
     1.00    0.00000   -0.83655
```


Example Program
Thomas-Fermi Equation for Determining Effective Nuclear Charge in Heavy Atoms
Effective Nuclear Charge
Relative Distance
nuclear charge
charge gradient
1
0.5
0
-0.5
-1
-1.5
-2
0
0.2
0.4
0.6
0.8
1