D03PXF – NAG Fortran Library Routine Document

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

D03PXF calculates a numerical flux function using an Exact Riemann Solver for the Euler equations in conservative form. The routine is designed primarily for use with the upwind discretisation routines D03PFF, D03PLF or D03PSF, but may also be applicable to other conservative upwind schemes requiring numerical flux functions.

2 Specification

```
SUBROUTINE D03PXF(ULEFT, URIGHT, GAMMA, TOL, NITER, FLUX, IFAIL)
INTEGER           NITER, IFAIL
real              ULEFT(3), URIGHT(3), GAMMA, TOL, FLUX(3)
```

3 Description

D03PXF calculates a numerical flux function at a single spatial point using an Exact Riemann Solver (see [1] and [2]) for the Euler equations (for a perfect gas) in conservative form. The user must supply the *left* and *right* solution values at the point where the numerical flux is required, i.e., the initial left and right states of the Riemann problem defined below. In the routines D03PFF, D03PLF and D03PSF, the left and right solution values are derived automatically from the solution values at adjacent spatial points and supplied to the subroutine argument NUMFLX from which the user may call D03PXF. The Euler equations for a perfect gas in conservative form are:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0, \tag{1}$$

with

$$U = \begin{bmatrix} \rho \\ m \\ e \end{bmatrix} \quad \text{and} \quad F = \begin{bmatrix} m \\ \frac{m^2}{\rho} + (\gamma - 1)\left(e - \frac{m^2}{2\rho}\right) \\ \frac{me}{\rho} + \frac{m}{\rho}(\gamma - 1)\left(e - \frac{m^2}{2\rho}\right) \end{bmatrix}, \tag{2}$$

where ρ is the density, m is the momentum, e is the specific total energy and γ is the (constant) ratio of specific heats. The pressure p is given by

$$p = (\gamma - 1)\left(e - \frac{\rho u^2}{2}\right), \tag{3}$$

where $u = m/\rho$ is the velocity.

The routine calculates the numerical flux function $F(U_L, U_R) = F(U^*(U_L, U_R))$, where $U = U_L$ and $U = U_R$ are the left and right solution values, and $U^*(U_L, U_R)$ is the intermediate state $\omega(0)$ arising from the similarity solution $U(y,t) = \omega(y/t)$ of the Riemann problem defined by

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial y} = 0, \tag{4}$$

with U and F as in (2), and initial piecewise constant values $U = U_L$ for $y < 0$ and $U = U_R$ for $y > 0$. The spatial domain is $-\infty < y < \infty$, where $y = 0$ is the point at which the numerical flux is required.

The algorithm is termed an Exact Riemann Solver although it does in fact calculate an approximate solution to a true Riemann problem, as opposed to an Approximate Riemann Solver which involves some form of alternative modelling of the Riemann problem. The approximation part of the Exact Riemann Solver is a Newton-Raphson iterative procedure to calculate the pressure, and the user must supply a tolerance TOL and a maximum number of iterations NITER. Default values for these parameters can be chosen.

A solution can not be found by this routine if there is a vacuum state in the Riemann problem (loosely characterised by zero density), or if such a state is generated by the interaction of two non-vacuum data states. In this case a Riemann solver which can handle vacuum states has to be used (see [1]).

4 References

[1] Toro E F (1996) *Riemann Solvers and Upwind Methods for Fluid Dynamics* Springer-Verlag

[2] Toro E F (1989) A weighted average flux method for hyperbolic conservation laws *Proc. Roy. Soc. Lond.* **A423** 401–418

5 Parameters

1: ULEFT(3) — ***real*** array *Input*

On entry: ULEFT(i) must contain the left value of the component U_i for $i = 1,2,3$. That is, ULEFT(1) must contain the left value of ρ, ULEFT(2) must contain the left value of m and ULEFT(3) must contain the left value of e.

2: URIGHT(3) — ***real*** array *Input*

On entry: URIGHT(i) must contain the right value of the component U_i for $i = 1,2,3$. That is, URIGHT(1) must contain the right value of ρ, URIGHT(2) must contain the right value of m and URIGHT(3) must contain the right value of e.

3: GAMMA — ***real*** *Input*

On entry: the ratio of specific heats γ.

Constraint: GAMMA > 0.0.

4: TOL — ***real*** *Input*

On entry: the tolerance to be used in the Newton-Raphson procedure to calculate the pressure. If TOL is set to zero then the default value of 1.0×10^{-6} is used.

Constraint: TOL ≥ 0.0.

5: NITER — INTEGER *Input*

On entry: the maximum number of Newton-Raphson iterations allowed. If NITER is set to zero then the default value of 20 is used.

Constraint: NITER ≥ 0.

6: FLUX(3) — ***real*** array *Output*

On exit: FLUX(i) contains the numerical flux component $\hat{F}_i$ for $i = 1,2,3$.

7: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

Note. If the left and/or right values of ρ or p (from (3)) are found to be negative, then the routine will terminate with an error exit (IFAIL $= 2$). If the routine is being called from the user-supplied subroutine NUMFLX in D03PFF etc., then a **soft fail** option (IFAIL $= 1$ or -1) is recommended so that a recalculation of the current time step can be forced using the IRES parameter.

On exit: IFAIL $= 0$ unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

On entry, GAMMA ≤ 0.0,
or TOL < 0.0,
or NITER < 0.

IFAIL = 2

On entry, the left and/or right density or derived pressure value is less than 0.0.

IFAIL = 3

A vacuum condition has been detected therefore a solution can not be found using this routine. You are advised to check your problem formulation.

IFAIL = 4

The internal Newton-Raphson iterative procedure used to solve for the pressure has failed to converge. The value of TOL or NITER may be too small, but if the problem persists try an Approximate Riemann Solver (D03PUF, D03PVF or D03PWF).

7 Accuracy

The algorithm is exact apart from the calculation of the pressure which uses a Newton-Raphson iterative procedure, the accuracy of which is controlled by the parameter TOL. In some cases the initial guess for the Newton-Raphson procedure is exact and no further iterations are required.

8 Further Comments

The routine must only be used to calculate the numerical flux for the Euler equations in exactly the form given by (2), with ULEFT(i) and URIGHT(i) containing the left and right values of ρ, m and e for $i = 1, 2, 3$ respectively.

For some problems the routine may fail or be highly inefficient in comparison with an Approximate Riemann Solver (e.g., D03PUF, D03PVF or D03PWF). Hence it is advisable to try more than one Riemann solver and to compare the performance and the results.

The time taken by the routine is independent of all input parameters other than TOL.

9 Example

This example uses D03PLF and D03PXF to solve the Euler equations in the domain $0 \leq \mathrm{x} \leq 1$ for $0 < t \leq 0.035$ with initial conditions for the primitive variables $\rho(x,t)$, $u(x,t)$ and $p(x,t)$ given by

$$\begin{array}{llll} \rho(x,0) = 5.99924, & u(x,0) = 19.5975, & p(x,0) = 460.894, & \text{for } x < 0.5, \\ \rho(x,0) = 5.99242, & u(x,0) = -6.19633, & p(x,0) = 46.095, & \text{for } x > 0.5. \end{array}$$

This test problem is taken from [1] and its solution represents the collision of two strong shocks travelling in opposite directions, consisting of a left facing shock (travelling slowly to the right), a right travelling contact discontinuity and a right travelling shock wave. There is an exact solution to this problem (see [1]) but the calculation is lengthy and has therefore been omitted.

9.1 Program Text

```
*     D03PXF Example Program Text
*     Mark 18 Release. NAG Copyright 1997.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NPDE, NPTS, NCODE, NXI, NEQN, NIW, NWKRES,
     +                 LENODE, MLU, NW
      PARAMETER        (NPDE=3,NPTS=141,NCODE=0,NXI=0,
     +                 NEQN=NPDE*NPTS+NCODE,NIW=NEQN+24,
     +                 NWKRES=NPDE*(2*NPTS+3*NPDE+32)+7*NPTS+4,
     +                 LENODE=9*NEQN+50,MLU=3*NPDE-1,NW=(3*MLU+1)
     +                 *NEQN+NWKRES+LENODE)
*     .. Scalars in Common ..
      real             EL0, ER0, GAMMA, RL0, RR0, UL0, UR0
*     .. Local Scalars ..
      real             D, P, TOUT, TS, V
      INTEGER          I, IFAIL, IND, ITASK, ITOL, ITRACE, K
      CHARACTER        LAOPT, NORM
*     .. Local Arrays ..
      real             ALGOPT(30), ATOL(1), RTOL(1), U(NPDE,NPTS),
     +                 UE(3,9), W(NW), X(NPTS), XI(1)
      INTEGER          IW(NIW)
*     .. External Subroutines ..
      EXTERNAL         BNDARY, D03PEK, D03PLF, D03PLP, NUMFLX
*     .. Common blocks ..
      COMMON           /INIT/EL0, ER0, RL0, RR0, UL0, UR0
      COMMON           /PARAMS/GAMMA
*     .. Executable Statements ..
      WRITE (NOUT,*) 'D03PXF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
*
*     Problem parameters
*
      GAMMA = 1.4e0
      RL0 = 5.99924e0
      RR0 = 5.99242e0
      UL0 = 5.99924e0*19.5975e0
      UR0 = -5.99242e0*6.19633e0
      EL0 = 460.894e0/(GAMMA-1.0e0) + 0.5e0*RL0*19.5975e0**2
      ER0 = 46.095e0/(GAMMA-1.0e0) + 0.5e0*RR0*6.19633e0**2
*
*     Initialise mesh
*
      DO 20 I = 1, NPTS
         X(I) = 1.0e0*(I-1.0e0)/(NPTS-1.0e0)
   20 CONTINUE
*
*     Initial values
*
      DO 40 I = 1, NPTS
         IF (X(I).LT.0.5e0) THEN
            U(1,I) = RL0
            U(2,I) = UL0
            U(3,I) = EL0
         ELSE IF (X(I).EQ.0.5e0) THEN
```

```
            U(1,I) = 0.5e0*(RL0+RR0)
            U(2,I) = 0.5e0*(UL0+UR0)
            U(3,I) = 0.5e0*(EL0+ER0)
         ELSE
            U(1,I) = RR0
            U(2,I) = UR0
            U(3,I) = ER0
         END IF
   40 CONTINUE
*
      ITRACE = 0
      ITOL = 1
      NORM = '2'
      ATOL(1) = 0.5e-2
      RTOL(1) = 0.5e-3
      XI(1) = 0.0e0
      LAOPT = 'B'
      IND = 0
      ITASK = 1
      DO 60 I = 1, 30
         ALGOPT(I) = 0.0e0
   60 CONTINUE
*
*     Theta integration
*
      ALGOPT(1) = 2.0e0
      ALGOPT(6) = 2.0e0
      ALGOPT(7) = 2.0e0
*
*     Max. time step
*
      ALGOPT(13) = 0.5e-2
*
      TS = 0.0e0
      TOUT = 0.035e0
      IFAIL = 0
*
      CALL D03PLF(NPDE,TS,TOUT,D03PLP,NUMFLX,BNDARY,U,NPTS,X,NCODE,
     +            D03PEK,NXI,XI,NEQN,RTOL,ATOL,ITOL,NORM,LAOPT,ALGOPT,W,
     +            NW,IW,NIW,ITASK,ITRACE,IND,IFAIL)
*
      WRITE (NOUT,99998) TS
      WRITE (NOUT,99999)
*
*     Read exact data at output points
*
      DO 80 I = 1, 9
         READ (NIN,*) UE(1,I), UE(2,I), UE(3,I)
   80 CONTINUE
*
*     Calculate density, velocity and pressure
*
      K = 0
      DO 100 I = 15, NPTS - 14, 14
         D = U(1,I)
         V = U(2,I)/D
         P = D*(GAMMA-1.0e0)*(U(3,I)/D-0.5e0*V**2)
         K = K + 1
```

```
            WRITE (NOUT,99996) X(I), D, UE(1,K), V, UE(2,K), P, UE(3,K)
  100    CONTINUE
*
         WRITE (NOUT,99997) IW(1), IW(2), IW(3), IW(5)
         STOP
*
99999 FORMAT (4X,'X',6X,'APPROX D',3X,'EXACT D',4X,'APPROX V',3X,'EXAC',
     +       'T V',4X,'APPROX P',3X,'EXACT P')
99998 FORMAT (/' T = ',F6.3,/)
99997 FORMAT (/' Number of integration steps in time = ',I6,/' Number ',
     +       'of function evaluations = ',I6,/' Number of Jacobian ',
     +       'evaluations =',I6,/' Number of iterations = ',I6,/)
99996 FORMAT (1X,e8.2,6(1X,e10.4))
      END
*
      SUBROUTINE BNDARY(NPDE,NPTS,T,X,U,NCODE,V,VDOT,IBND,G,IRES)
*     .. Scalar Arguments ..
      real              T
      INTEGER           IBND, IRES, NCODE, NPDE, NPTS
*     .. Array Arguments ..
      real              G(NPDE), U(NPDE,NPTS), V(*), VDOT(*), X(NPTS)
*     .. Scalars in Common ..
      real              EL0, ER0, RL0, RR0, UL0, UR0
*     .. Common blocks ..
      COMMON            /INIT/EL0, ER0, RL0, RR0, UL0, UR0
*     .. Executable Statements ..
      IF (IBND.EQ.0) THEN
         G(1) = U(1,1) - RL0
         G(2) = U(2,1) - UL0
         G(3) = U(3,1) - EL0
      ELSE
         G(1) = U(1,NPTS) - RR0
         G(2) = U(2,NPTS) - UR0
         G(3) = U(3,NPTS) - ER0
      END IF
      RETURN
      END
*
      SUBROUTINE NUMFLX(NPDE,T,X,NCODE,V,ULEFT,URIGHT,FLUX,IRES)
*     .. Scalar Arguments ..
      real              T, X
      INTEGER           IRES, NCODE, NPDE
*     .. Array Arguments ..
      real              FLUX(NPDE), ULEFT(NPDE), URIGHT(NPDE), V(*)
*     .. Scalars in Common ..
      real              GAMMA
*     .. Local Scalars ..
      real              TOL
      INTEGER           IFAIL, NITER
*     .. External Subroutines ..
      EXTERNAL          D03PXF
*     .. Common blocks ..
      COMMON            /PARAMS/GAMMA
*     .. Save statement ..
      SAVE              /PARAMS/
*     .. Executable Statements ..
*
      IFAIL = 0
```

```
      TOL = 0.0e0
      NITER = 0
      CALL D03PXF(ULEFT,URIGHT,GAMMA,TOL,NITER,FLUX,IFAIL)
      RETURN
      END
```

9.2 Program Data

```
D03PXF Example Program Data
 0.5999E+01   0.1960E+02   0.4609E+03
 0.5999E+01   0.1960E+02   0.4609E+03
 0.5999E+01   0.1960E+02   0.4609E+03
 0.5999E+01   0.1960E+02   0.4609E+03
 0.5999E+01   0.1960E+02   0.4609E+03
 0.1428E+02   0.8690E+01   0.1692E+04
 0.1428E+02   0.8690E+01   0.1692E+04
 0.1428E+02   0.8690E+01   0.1692E+04
 0.3104E+02   0.8690E+01   0.1692E+04
```

9.3 Program Results

```
 D03PXF Example Program Results

 T =  0.035

    X      APPROX D   EXACT D    APPROX V   EXACT V    APPROX P   EXACT P
 0.10E+00 0.5999E+01 0.5999E+01 0.1960E+02 0.1960E+02 0.4609E+03 0.4609E+03
 0.20E+00 0.5999E+01 0.5999E+01 0.1960E+02 0.1960E+02 0.4609E+03 0.4609E+03
 0.30E+00 0.5999E+01 0.5999E+01 0.1960E+02 0.1960E+02 0.4609E+03 0.4609E+03
 0.40E+00 0.5999E+01 0.5999E+01 0.1960E+02 0.1960E+02 0.4609E+03 0.4609E+03
 0.50E+00 0.5999E+01 0.5999E+01 0.1960E+02 0.1960E+02 0.4609E+03 0.4609E+03
 0.60E+00 0.1423E+02 0.1428E+02 0.8660E+01 0.8690E+01 0.1688E+04 0.1692E+04
 0.70E+00 0.1425E+02 0.1428E+02 0.8672E+01 0.8690E+01 0.1688E+04 0.1692E+04
 0.80E+00 0.1921E+02 0.1428E+02 0.8674E+01 0.8690E+01 0.1689E+04 0.1692E+04
 0.90E+00 0.3100E+02 0.3104E+02 0.8675E+01 0.8690E+01 0.1687E+04 0.1692E+04

 Number of integration steps in time =    697
 Number of function evaluations =   1708
 Number of Jacobian evaluations =     1
 Number of iterations =      2
```