

# NAG Library Routine Document

## D03PWF

**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

D03PWF calculates a numerical flux function using a modified HLL (Harten–Lax–van Leer) Approximate Riemann Solver for the Euler equations in conservative form. It is designed primarily for use with the upwind discretization schemes D03PFF, D03PLF or D03PSF, but may also be applicable to other conservative upwind schemes requiring numerical flux functions.

### 2 Specification

```
SUBROUTINE D03PWF (ULEFT, URIGHT, GAMMA, FLUX, IFAIL)
  INTEGER          IFAIL
  REAL (KIND=nag_wp) ULEFT(3), URIGHT(3), GAMMA, FLUX(3)
```

### 3 Description

D03PWF calculates a numerical flux function at a single spatial point using a modified HLL (Harten–Lax–van Leer) Approximate Riemann Solver (see Toro (1992), Toro (1996) and Toro *et al.* (1994)) for the Euler equations (for a perfect gas) in conservative form. You 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 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 you may call D03PWF.

The Euler equations for a perfect gas in conservative form are:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0, \quad (1)$$

with

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

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

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

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

The routine calculates an approximation to 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

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial y} = 0, \quad (4)$$

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.

## 4 References

Toro E F (1992) The weighted average flux method applied to the Euler equations *Phil. Trans. R. Soc. Lond.* **A341** 499–530

Toro E F (1996) *Riemann Solvers and Upwind Methods for Fluid Dynamics* Springer–Verlag

Toro E F, Spruce M and Spears W (1994) Restoration of the contact surface in the HLL Riemann solver *J. Shock Waves* **4** 25–34

## 5 Arguments

- 1: ULEFT(3) – REAL (KIND=nag\_wp) 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  $\rho$ , ULEFT(2) must contain the left value of  $m$  and ULEFT(3) must contain the left value of  $e$ .

*Constraints:*

$$\text{ULEFT}(1) \geq 0.0;$$

Left pressure,  $pl \geq 0.0$ , where  $pl$  is calculated using (3).

- 2: URIGHT(3) – REAL (KIND=nag\_wp) 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  $\rho$ , URIGHT(2) must contain the right value of  $m$  and URIGHT(3) must contain the right value of  $e$ .

*Constraints:*

$$\text{URIGHT}(1) \geq 0.0;$$

Right pressure,  $pr \geq 0.0$ , where  $pr$  is calculated using (3).

- 3: GAMMA – REAL (KIND=nag\_wp) *Input*

*On entry:* the ratio of specific heats,  $\gamma$ .

*Constraint:* GAMMA > 0.0.

- 4: FLUX(3) – REAL (KIND=nag\_wp) array *Output*

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

- 5: 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, if you are not familiar with this argument, the recommended value is 0. **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).

**Note:** if the left and/or right values of  $\rho$  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 NUMFLX 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 NUMFLX argument IRES (see D03PFF or D03PLF).

## 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,  $GAMMA \leq 0.0$ .

$IFAIL = 2$

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

$IFAIL = -99$

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

D03PWF performs an exact calculation of the HLL (Harten–Lax–van Leer) numerical flux function, and so the result will be accurate to *machine precision*.

## 8 Parallelism and Performance

D03PWF is not thread safe and should not be called from a multithreaded user program. Please see Section 3.12.1 in How to Use the NAG Library and its Documentation for more information on thread safety.

D03PWF is not threaded in any implementation.

## 9 Further Comments

D03PWF 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  $\rho, m$  and  $e$ , for  $i = 1, 2, 3$ , respectively. The time taken is independent of the input arguments.

## 10 Example

This example uses D03PLF and D03PWF to solve the Euler equations in the domain  $0 \leq x \leq 1$  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

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

This test problem is taken from Toro (1996) 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 Toro (1996)) but the calculation is lengthy and has therefore been omitted.

## 10.1 Program Text

```

!   D03PWF Example Program Text
!   Mark 26 Release. NAG Copyright 2016.

Module d03pwfe_mod

!       D03PWF 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                                :: bndary, numflx
!       .. Parameters ..
Real (Kind=nag_wp), Parameter, Public :: alpha_l = 460.894_nag_wp
Real (Kind=nag_wp), Parameter, Public :: alpha_r = 46.095_nag_wp
Real (Kind=nag_wp), Parameter, Public :: beta_l = 19.5975_nag_wp
Real (Kind=nag_wp), Parameter, Public :: beta_r = 6.19633_nag_wp
Real (Kind=nag_wp), Parameter, Public :: half = 0.5_nag_wp
Integer, Parameter, Public           :: itrace = 0, ncode = 0, nin = 5,      &
                                     nout = 6, npde = 3, nxi = 0
!       .. Local Scalars ..
Real (Kind=nag_wp), Public, Save :: el0, er0, gamma, rl0, rr0, ul0, ur0
Contains
Subroutine bndary(npde,npts,t,x,u,ncode,v,vdot,ibnd,g,ires)

!       .. Scalar Arguments ..
Real (Kind=nag_wp), Intent (In) :: t
Integer, Intent (In)           :: ibnd, ncode, npde, npts
Integer, Intent (Inout)        :: ires
!       .. Array Arguments ..
Real (Kind=nag_wp), Intent (Out) :: g(npde)
Real (Kind=nag_wp), Intent (In)  :: u(npde,npts), v(ncode),      &
                                     vdot(ncode), x(npts)
!       .. Executable Statements ..
If (ibnd==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 bndary
Subroutine numflx(npde,t,x,ncode,v,uleft,uright,flux,ires)

!       .. Use Statements ..
Use nag_library, Only: d03pwf
!       .. Scalar Arguments ..
Real (Kind=nag_wp), Intent (In) :: t, x
Integer, Intent (Inout)          :: ires
Integer, Intent (In)             :: ncode, npde
!       .. Array Arguments ..
Real (Kind=nag_wp), Intent (Out) :: flux(npde)
Real (Kind=nag_wp), Intent (In)  :: uleft(npde), uright(npde), v(ncode)
!       .. Local Scalars ..
Integer                          :: ifail
!       .. Executable Statements ..
ifail = 0
Call d03pwf(uleft,uright,gamma,flux,ifail)
Return
End Subroutine numflx
End Module d03pwfe_mod
Program d03pwfe

```

```

!      D03PWF Example Main Program

!      .. Use Statements ..
Use nag_library, Only: d03pek, d03plf, d03plp, nag_wp
Use d03pwfe_mod, Only: alpha_l, alpha_r, beta_l, beta_r, bndary, el0,      &
                      er0, gamma, half, itrace, ncode, nin, nout, npde, &
                      numflx, nxi, rl0, rr0, ul0, ur0

!      .. Implicit None Statement ..
Implicit None

!      .. Local Scalars ..
Real (Kind=nag_wp)                :: d, p, tout, ts, v
Integer                          :: i, ifail, ind, itask, itol, k,      &
                                lenode, mlu, neqn, niw, npts, nw,      &
                                nwkres
Character (1)                    :: laopt, norm

!      .. Local Arrays ..
Real (Kind=nag_wp)                :: algopt(30), atol(1), rtol(1),      &
                                ue(3,9), xi(1)
Real (Kind=nag_wp), Allocatable :: u(:, :), w(:, :), x(:)
Integer, Allocatable              :: iw(:)

!      .. Intrinsic Procedures ..
Intrinsic                        :: real

!      .. Executable Statements ..
Write (nout,*) 'D03PWF Example Program Results'
Skip heading in data file
Read (nin,*)
Read (nin,*) npts

nwkres = npde*(2*npts+3*npde+32) + 7*npts + 4
mlu = 3*npde - 1
neqn = npde*npts + ncode
niw = neqn + 24
lenode = 9*neqn + 50
nw = (3*mlu+1)*neqn + nwkres + lenode
Allocate (u(npde,npts),w(nw),x(npts),iw(niw))

Read (nin,*) gamma, rl0, rr0, ul0, ur0

el0 = alpha_l/(gamma-1.0_nag_wp) + half*rl0*beta_l**2
er0 = alpha_r/(gamma-1.0_nag_wp) + half*rr0*beta_r**2

!      Initialize mesh
Do i = 1, npts
    x(i) = real(i-1,kind=nag_wp)/real(npts-1,kind=nag_wp)
End Do
xi(1) = 0.0_nag_wp

!      Initial values
Do i = 1, npts
    If (x(i)<half) Then
        u(1,i) = rl0
        u(2,i) = ul0
        u(3,i) = el0
    Else If (x(i)==half) Then
        u(1,i) = half*(rl0+rr0)
        u(2,i) = half*(ul0+ur0)
        u(3,i) = half*(el0+er0)
    Else
        u(1,i) = rr0
        u(2,i) = ur0
        u(3,i) = er0
    End If
End Do

Read (nin,*) itol
Read (nin,*) norm
Read (nin,*) atol(1), rtol(1)
Read (nin,*) laopt
ind = 0
itask = 1

```

```

      algopt(1:30) = 0.0_nag_wp

!      Theta integration
      algopt(1) = 2.0_nag_wp
      algopt(6) = 2.0_nag_wp
      algopt(7) = 2.0_nag_wp

!      Max. time step
      algopt(13) = 0.5E-2_nag_wp

      ts = 0.0_nag_wp
      tout = 0.035_nag_wp

!      ifail: behaviour on error exit
!      =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
      ifail = 0
      Call d03plf(npde,ts,tout,d03plp,numflx,bndary,u,npts,x,ncode,d03pek,nxi, &
        xi,neqn,rtol,atol,itol,norm,laopt,algot,w,nw,iw,niw,itask,itrac,ind, &
        ifail)

      Write (nout,99998) ts
      Write (nout,99999)

!      Read exact data at output points

      Do i = 1, 9
        Read (nin,*) ue(1:3,i)
      End Do

!      Calculate density, velocity and pressure

      k = 0
      Do i = 15, npts - 14, 14
        d = u(1,i)
        v = u(2,i)/d
        p = d*(gamma-1.0_nag_wp)*(u(3,i)/d-half*v**2)
        k = k + 1
        Write (nout,99996) x(i), d, ue(1,k), v, ue(2,k), p, ue(3,k)
      End Do

      Write (nout,99997) iw(1), iw(2), iw(3), iw(5)

99999 Format (4X,'X',7X,'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,E9.2,6(E11.4))
      End Program d03pwfe

```

## 10.2 Program Data

D03PWF Example Program Data

141			: npts
1.4	5.99924	5.99242	
	1.175701059E2	-3.71310118186E1	: gamma, rl0, rr0, ul0, ur0
1			: itol
'2'			: norm
0.5E-2	0.5E-3		: atol(1), rtol(1)
'B'			: laopt
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	: ue

### 10.3 Program Results

D03PWF 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	0.1422E+02	0.1428E+02	0.8658E+01	0.8690E+01	0.1687E+04	0.1692E+04
0.70E+00	0.1426E+02	0.1428E+02	0.8670E+01	0.8690E+01	0.1688E+04	0.1692E+04
0.80E+00	0.1944E+02	0.1428E+02	0.8678E+01	0.8690E+01	0.1691E+04	0.1692E+04
0.90E+00	0.3100E+02	0.3104E+02	0.8676E+01	0.8690E+01	0.1687E+04	0.1692E+04

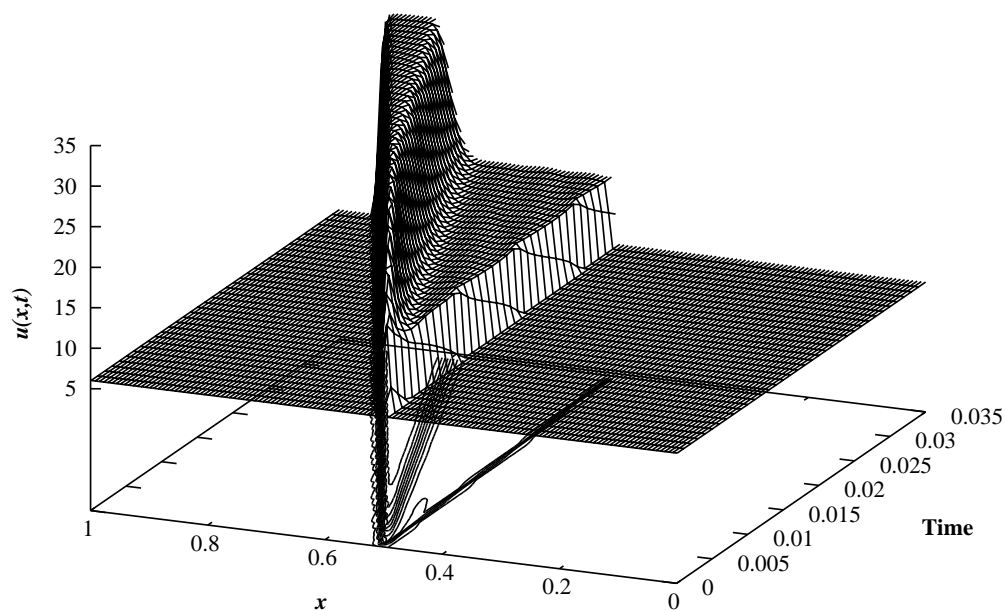
Number of integration steps in time = 699

Number of function evaluations = 1714

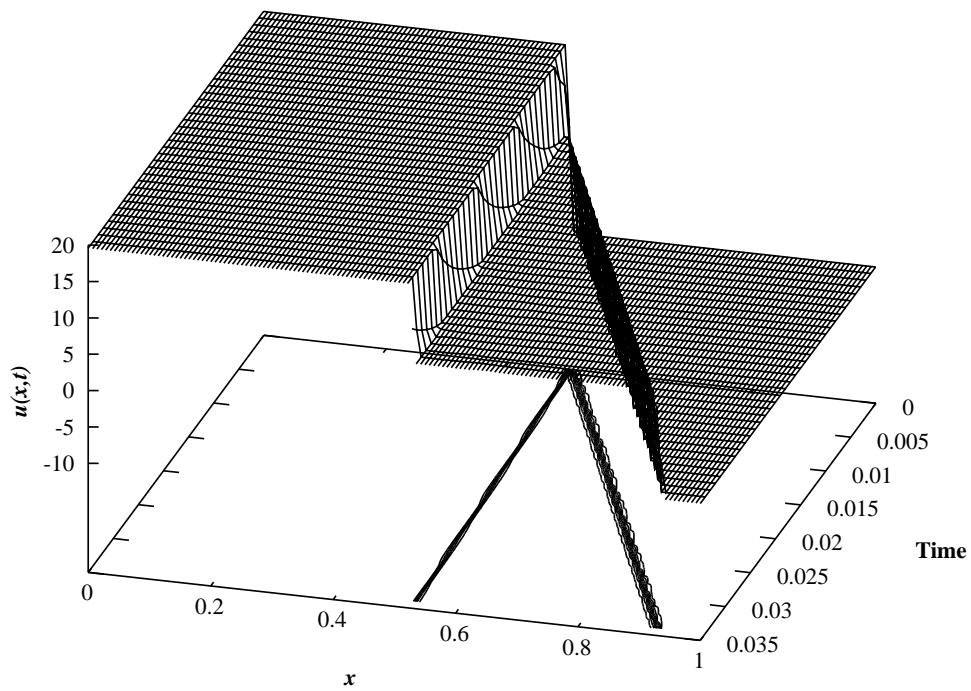
Number of Jacobian evaluations = 1

Number of iterations = 2

**Example Program**  
Euler Equation Solution Showing Collision of Two Strong Shocks  
DENSITY



Euler Equation Solution Showing Collision of Two Strong Shocks  
VELOCITY



Euler Equation Solution Showing Collision of Two Strong Shocks  
PRESSURE

