

D03RBF – 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.

Note. This routine was introduced into the NAG Fortran Library at Mark 19 and may therefore not be available to all users of the NAG Fortran SMP Library.

1 Purpose

D03RBF integrates a system of linear or nonlinear, time-dependent partial differential equations (PDEs) in two space dimensions on a rectilinear domain. The method of lines is employed to reduce the PDEs to a system of ordinary differential equations (ODEs) which are solved using a backward differentiation formula (BDF) method. The resulting system of nonlinear equations is solved using a modified Newton method and a Bi-CGSTAB iterative linear solver with ILU preconditioning. Local uniform grid refinement is used to improve the accuracy of the solution. D03RBF originates from the VLUGR2 package [1] [2].

2 Specification

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SUBROUTINE D03RBF(NPDE, TS, TOUT, DT, TOLS, TOLT, INIDOM, PDEDEF,
1      BNDARY, PDEIV, MONITR, OPTI, OPTR, RWK, LENRWK,
2      IWK, LENIWK, LWK, LENLWK, ITRACE, IND, IFAIL)
  INTEGER      NPDE, OPTI(4), LENRWK, IWK(LENIWK), LENIWK,
1      LENLWK, ITRACE, IND, IFAIL
  real        TS, TOUT, DT(3), TOLS, TOLT, OPTR(3,NPDE),
1      RWK(LENRWK)
  LOGICAL      LWK(LENLWK)
  EXTERNAL     INIDOM, PDEDEF, BNDARY, PDEIV, MONITR

```

3 Description

D03RBF integrates the system of PDEs:

$$F_j(t, x, y, u, u_t, u_x, u_y, u_{xx}, u_{xy}, u_{yy}) = 0, \quad j = 1, 2, \dots, \text{NPDE}, \quad (x, y) \in \Omega, \quad t_0 \leq t \leq t_{\text{out}}, \quad (1)$$

where Ω is an arbitrary rectilinear domain, i.e., a domain bounded by perpendicular straight lines. If the domain is rectangular then it is recommended that D03RAF is used.

The vector u is the set of solution values

$$u(x, y, t) = [u_1(x, y, t), \dots, u_{\text{NPDE}}(x, y, t)]^T,$$

and u_t denotes partial differentiation with respect to t , and similarly for u_x etc.

The functions F_j must be supplied by the user in a subroutine PDEDEF. Similarly the initial values of the functions $u(x, y, t)$ for $(x, y) \in \Omega$ must be specified at $t = t_0$ in a subroutine PDEIV.

Note that whilst complete generality is offered by the master equations (1), D03RBF is not appropriate for all PDEs. In particular, hyperbolic systems should not be solved using this routine. Also, at least one component of u_t must appear in the system of PDEs.

The boundary conditions must be supplied by the user in a subroutine BNDARY in the form

$$G_j(t, x, y, u, u_t, u_x, u_y) = 0 \quad j = 1, 2, \dots, \text{NPDE}, \quad (x, y) \in \partial\Omega, \quad t_0 \leq t \leq t_{\text{out}}. \quad (2)$$

The domain is covered by a uniform coarse base grid specified by the user, and nested finer uniform subgrids are subsequently created in regions with high spatial activity. The refinement is controlled using a space monitor which is computed from the current solution and a user-supplied space tolerance TOLS. A number of optional parameters, e.g., the maximum number of grid levels at any time, and some weighting factors, can be specified in the arrays OPTI and OPTR. Further details of the refinement strategy can be found in Section 8.

The system of PDEs and the boundary conditions are discretised in space on each grid using a standard second-order finite difference scheme (centred on the internal domain and one-sided at the boundaries), and the resulting system of ODEs is integrated in time using a second-order, two-step, implicit BDF method with variable step size. The time integration is controlled using a time monitor computed at each grid level from the current solution and a user-supplied time tolerance TOLT, and some further optional user-specified weighting factors held in OPTR (see Section 8 for details). The time monitor is used to compute a new step size, subject to restrictions on the size of the change between steps, and (optional) user-specified maximum and minimum step sizes held in DT. The step size is adjusted so that the remaining integration interval is an integer number times Δt . In this way a solution is obtained at $t = t_{\text{out}}$.

A modified Newton method is used to solve the nonlinear equations arising from the time integration. The user may specify (in OPTI) the maximum number of Newton iterations to be attempted. A Jacobian matrix is calculated at the beginning of each time step. If the Newton process diverges or the maximum number of iterations is exceeded, a new Jacobian is calculated using the most recent iterates and the Newton process is restarted. If convergence is not achieved after the (optional) user-specified maximum number of new Jacobian evaluations, the time step is retried with $\Delta t = \Delta t/4$. The linear systems arising from the Newton iteration are solved using a Bi-CGSTAB iterative method, in combination with ILU preconditioning. The maximum number of iterations can be specified by the user in OPTI.

In order to define the base grid the user must first specify a virtual uniform rectangular grid which contains the entire base grid. The position of the virtual grid in physical (x, y) space is given by the (x, y) co-ordinates of its boundaries. The number of points n_x and n_y in the x and y directions must also be given, corresponding to the number of columns and rows respectively. This is sufficient to determine precisely the (x, y) co-ordinates of all virtual grid points. Each virtual grid point is then referred to by integer co-ordinates (v_x, v_y) , where $(0, 0)$ corresponds to the lower-left corner and $(n_x - 1, n_y - 1)$ corresponds to the upper-right corner. v_x and v_y are also referred to as the virtual column and row indices respectively.

The base grid is then specified with respect to the virtual grid, with each base grid point coinciding with a virtual grid point. Each base grid point must be given an index, starting from 1, and incrementing row-wise from the leftmost point of the lowest row. Also, each base grid row must be numbered consecutively from the lowest row in the grid, so that row 1 contains grid point 1.

As an example, consider the domain consisting of the two separate squares shown in Figure 1. The left-hand diagram shows the virtual grid and its integer co-ordinates (i.e., its column and row indices), and the right-hand diagram shows the base grid point indices and the base row indices (in brackets).

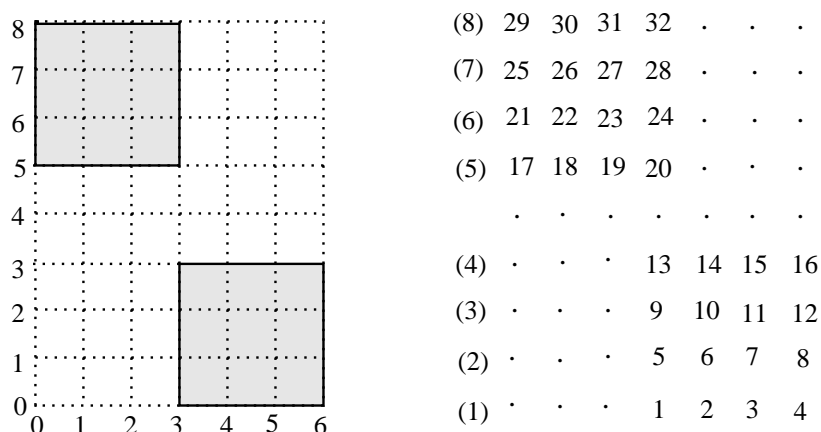


Figure 1

Hence the base grid point with index 6 say is in base row 2, virtual column 4, and virtual row 1, i.e., virtual grid integer co-ordinates $(4, 1)$; and the base grid point with index 19 say is in base row 5, virtual column 2, and virtual row 5, i.e., virtual grid integer co-ordinates $(2, 5)$.

The base grid must then be defined in the subroutine INIDOM by specifying the number of base grid rows, the number of base grid points, the number of boundaries, the number of boundary points, and the following integer arrays:

LROW contains the base grid indices of the starting points of the base grid rows.

IROW contains the virtual row numbers v_y of the base grid rows.

ICOL contains the virtual column numbers v_x of the base grid points.

LBND contains the grid indices of the boundary edges (without corners) and corner points.

LLBND contains the starting elements of the boundaries and corners in LBND.

Finally, ILBND contains the types of the boundaries and corners, as follows:

Boundaries:

- 1** – lower boundary
- 2** – left boundary
- 3** – upper boundary
- 4** – right boundary

External corners (90°):

- 12** – lower-left corner
- 23** – upper-left corner
- 34** – upper-right corner
- 41** – lower-right corner

Internal corners (270°):

- 21** – lower-left corner
- 32** – upper-left corner
- 43** – upper-right corner
- 14** – lower-right corner

Figure 2 shows the boundary types of a domain with a hole. Notice the logic behind the labelling of the corners: each one includes the types of the two adjacent boundary edges, in a clockwise fashion (outside the domain).

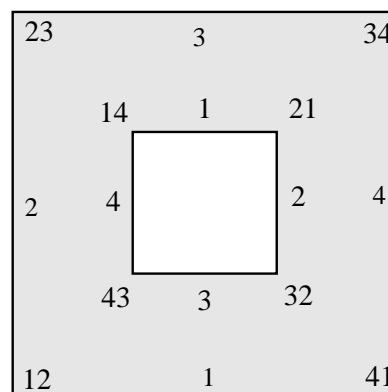


Figure 2

As an example, consider the domain shown in Figure 3. The left-hand diagram shows the physical domain and the right-hand diagram shows the base and virtual grids. The numbers outside the base grid are the indices of the left and rightmost base grid points, and the numbers inside the base grid are the boundary or corner numbers, indicating the order in which the boundaries are stored in LBND.

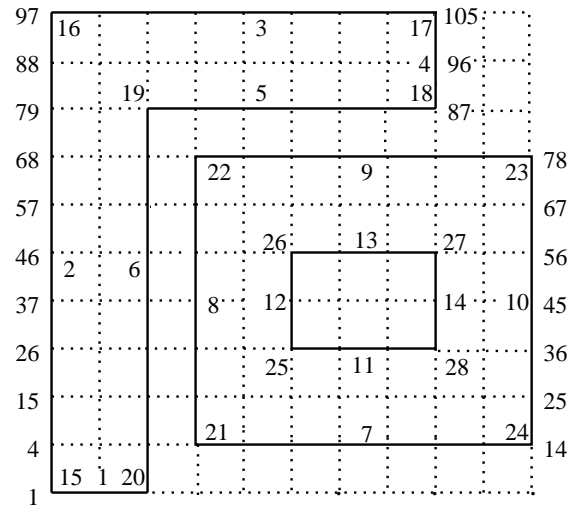
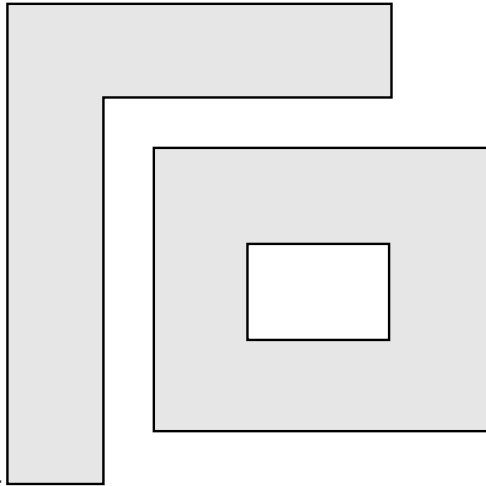


Figure 3

For this example we have

```
NROWS = 11
NPTS = 105
NBND = 28
NBPTS = 72
```

```
LROW = (1,4,15,26,37,46,57,68,79,88,97)
```

```
IROW = (0,1,2,3,4,5,6,7,8,9,10)
```

```
ICOL = (0,1,2,
         0,1,2,3,4,5,6,7,8,9,10,
         0,1,2,3,4,5,6,7,8,9,10,
         0,1,2,3,4,5,6,7,8,9,10,
         0,1,2,3,4,5,8,9,10,
         0,1,2,3,4,5,6,7,8,9,10,
         0,1,2,3,4,5,6,7,8,9,10,
         0,1,2,3,4,5,6,7,8,9,10,
         0,1,2,3,4,5,6,7,8,
         0,1,2,3,4,5,6,7,8,
         0,1,2,3,4,5,6,7,8)
```

```
LBND = (2,
        4,15,26,37,46,57,68,79,88,
        98,99,100,101,102,103,104,
        96,
        86,85,84,83,82,
        70,59,48,39,28,17,6,
        8,9,10,11,12,13,
        18,29,40,49,60,
        72,73,74,75,76,77,
        67,56,45,36,25,
        33,32,
        42,
        52,53,
        43,
        1,97,105,87,81,3,7,71,78,14,31,51,54,34)
```

LLBND = (1,2,11,18,19,24,31,37,42,48,53,55,56,58,59,60,
61,62,63,64,65,66,67,68,69,70,71,72)

ILBND = (1,2,3,4,1,4,1,2,3,4,3,4,1,2,12,23,34,41,14,41,12,23,34,41,43,14,21,32)

This particular domain is used in Example 1 in Section 9.1, and data statements are used to define the above arrays in that example program. In Example 2 a less complicated domain is used, and in that case it is simpler to assign the values of the arrays in do-loops. This also allows flexibility in the number of base grid points.

The routine D03RYF can be called from INIDOM to obtain a simple graphical representation of the base grid, and to verify the data that the user has specified in INIDOM.

Subgrids are stored internally using the same data structure, and solution information is communicated to the user in the subroutines PDEIV, PDEDEF and BNDARY in arrays according to the grid index on the particular level, e.g., $X(i)$ and $Y(i)$ contain the (x, y) co-ordinates of grid point i , and $U(i, j)$ contains the j th solution component u_j at grid point i .

The grid data and the solutions at all grid levels are stored in the workspace arrays, along with other information needed for a restart (i.e., a continuation call). It is not intended that the user extracts the solution from these arrays, indeed the necessary information regarding these arrays is not provided. The user-supplied monitor routine MONITR should be used to obtain the solution at particular levels and times. MONITR is called at the end of every time step, with the last step being identified via the input argument TLAST. The routine D03RZF should be called from MONITR to obtain grid information at a particular level.

Further details of the underlying algorithm can be found in Section 8 and in [1] and [2] and the references therein.

4 References

- [1] Blom J G and Verwer J G (1993) VLUGR2: A vectorized local uniform grid refinement code for PDEs in 2D *Report NM-R9306* CWI, Amsterdam
- [2] Blom J G, Trompert R A and Verwer J G (1996) Algorithm 758. VLUGR2: A vectorizable adaptive grid solver for PDEs in 2D *Trans. Math. Software* **22** 302–328
- [3] Trompert R A and Verwer J G (1993) Analysis of the implicit Euler local uniform grid refinement method *SIAM J. Sci. Comput.* **14** 259–278
- [4] Trompert R A (1993) Local uniform grid refinement and systems of coupled partial differential equations *Appl. Numer. Maths* **12** 331–355

5 Parameters

- 1: NPDE — INTEGER *Input*
On entry: the number of PDEs in the system.
Constraint: NPDE \geq 1.
- 2: TS — *real* *Input/Output*
On entry: the initial value of the independent variable t .
On exit: the value of t which has been reached. Normally TS = TOUT.
Constraint: TS < TOUT.
- 3: TOUT — *real* *Input*
On entry: the final value of t to which the integration is to be carried out.

4: DT(3) — *real* array *Input/Output*

On entry: the initial, minimum and maximum time step sizes respectively. DT(1) specifies the initial time step size to be used on the first entry, i.e., when IND = 0. If DT(1) = 0.0 then the default value $DT(1) = 0.01 \times (TOUT - TS)$ is used. On subsequent entries (IND = 1), the value of DT(1) is not referenced.

DT(2) specifies the minimum time step size to be attempted by the integrator. If DT(2) = 0.0 the default value $DT(2) = 10.0 \times \text{machine precision}$ is used.

DT(3) specifies the maximum time step size to be attempted by the integrator. If DT(3) = 0.0 the default value $DT(3) = TOUT - TS$ is used.

On exit: DT(1) contains the time step size for the next time step. DT(2) and DT(3) are unchanged or set to their default values if zero on entry.

Constraints: if IND = 1 then DT(1) is unconstrained. Otherwise $DT(1) \geq 0$ and if $DT(1) > 0.0$ then it must satisfy the constraints:

$$10.0 \times \text{machine precision} \times \max(|TS|, |TOUT|) \leq DT(1) \leq TOUT - TS$$

$$DT(2) \leq DT(1) \leq DT(3)$$

where the values of DT(2) and DT(3) will have been reset to their default values if zero on entry.

DT(2) and DT(3) must satisfy $DT(i) \geq 0$, $i = 2, 3$ and $DT(2) \leq DT(3)$ for IND = 0 and IND = 1.

5: TOLS — *real* *Input*

On entry: the space tolerance used in the grid refinement strategy (σ in equation (4)). See Section 8.2.

Constraint: TOLS > 0.0.

6: TOLT — *real* *Input*

On entry: the time tolerance used to determine the time step size (τ in equation (7)). See Section 8.3.

Constraint: TOLT > 0.0.

7: INIDOM — SUBROUTINE, supplied by the user. *External Procedure*

INIDOM must specify the base grid in terms of the data structure described in Section 3. INIDOM is not referenced if, on entry, IND = 1. D03RYF can be called from INIDOM to obtain a simple graphical representation of the base grid, and to verify the data that the user has specified in INIDOM. D03RBF also checks the validity of the data, but the user is strongly advised to call D03RYF to ensure that the base grid is exactly as required.

Note. The boundaries of the base grid should consist of as many points as are necessary to employ second-order space discretization, i.e., a boundary enclosing the internal part of the domain must include at least 3 grid points including the corners. If Neumann boundary conditions are to be applied the minimum is 4.

Its specification is:

```

SUBROUTINE INIDOM(MAXPTS, XMIN, XMAX, YMIN, YMAX, NX, NY, NPTS,
1      NROWS, NBND, NBPTS, LROW, IROW, ICOL, LLBND,
2      ILBND, LBND, IERR)
  INTEGER      MAXPTS, NX, NY, NPTS, NROWS, NBND, NBPTS,
1      LROW(*), IROW(*), ICOL(*), LLBND(*), ILBND(*),
2      LBND(*), IERR
  real         XMIN, XMAX, YMIN, YMAX
```

1:	MAXPTS — INTEGER	Input
	<i>On entry:</i> the maximum number of base grid points allowed by the available workspace.	
2:	XMIN — <i>real</i>	Output
3:	XMAX — <i>real</i>	Output
	<i>On exit:</i> the extents of the virtual grid in the x -direction, i.e., the x co-ordinates of the left and right boundaries respectively.	
	<i>Constraints:</i> XMIN < XMAX and XMAX must be sufficiently distinguishable from XMIN for the precision of the machine being used.	
4:	YMIN — <i>real</i>	Output
5:	YMAX — <i>real</i>	Output
	<i>On exit:</i> the extents of the virtual grid in the y -direction, i.e., the y co-ordinates of the left and right boundaries respectively.	
	<i>Constraints:</i> YMIN < YMAX and YMAX must be sufficiently distinguishable from YMIN for the precision of the machine being used.	
6:	NX — INTEGER	Output
7:	NY — INTEGER	Output
	<i>On exit:</i> the number of virtual grid points in the x - and y -direction respectively (including the boundary points).	
	<i>Constraints:</i> NX and NY ≥ 4 .	
8:	NPTS — INTEGER	Output
	<i>On exit:</i> the total number of points in the base grid. If the required number of points is greater than MAXPTS then INIDOM must be exited immediately with IERR set to -1 to avoid overwriting memory.	
	<i>Constraints:</i> NPTS $\leq NX \times NY$ and if IERR $\neq -1$ on exit, NPTS \leq MAXPTS.	
9:	NROWS — INTEGER	Output
	<i>On exit:</i> the total number of rows of the virtual grid that contain base grid points. This is the maximum base row index.	
	<i>Constraint:</i> $4 \leq NROWS \leq NY$.	
10:	NBND — INTEGER	Output
	<i>On exit:</i> the total number of physical boundaries and corners in the base grid.	
	<i>Constraint:</i> NBND ≥ 8 .	
11:	NBPTS — INTEGER	Output
	<i>On exit:</i> the total number of boundary points in the base grid.	
	<i>Constraint:</i> $12 \leq NBPTS < NPTS$.	
12:	LROW(*) — INTEGER array	Output
	<i>On exit:</i> LROW(i) for $i = 1, 2, \dots, NROWS$ must contain the base grid index of the first grid point in base grid row i .	
	<i>Constraints:</i> $1 \leq LROW(i) \leq NPTS$ for $i = 1, 2, \dots, NROWS$, LROW($i - 1$) < LROW(i) for $i = 2, 3, \dots, NROWS$.	
13:	IROW(*) — INTEGER array	Output
	<i>On exit:</i> IROW(i) for $i = 1, 2, \dots, NROWS$ must contain the virtual row number v_y that corresponds to base grid row i .	
	<i>Constraints:</i> $0 \leq IROW(i) \leq NY$ for $i = 1, 2, \dots, NROWS$, IROW($i - 1$) < IROW(i) for $i = 2, 3, \dots, NROWS$.	
14:	ICOL(*) — INTEGER array	Output
	<i>On exit:</i> ICOL(i) for $i = 1, 2, \dots, NPTS$ must contain the virtual column number v_x that contains base grid point i .	
	<i>Constraint:</i> $0 \leq ICOL(i) \leq NX$ for $i = 1, 2, \dots, NPTS$.	

15: LLBND(*) — INTEGER array	<i>Output</i>
<i>On exit:</i> LLBND(i) for $i = 1, 2, \dots, \text{NBND}$ must contain the element of LBND corresponding to the start of the i th boundary or corner.	
Note. The order of the boundaries and corners in LLBND must be first all the boundaries and then all the corners. The end points of a boundary (i.e., the adjacent corner points) must not be included in the list of points on that boundary. Also, if a corner is shared by two pairs of physical boundaries then it has two types and must therefore be treated as two corners.	
<i>Constraints:</i> $1 \leq \text{LLBND}(i) \leq \text{NBPTS}$ for $i = 1, 2, \dots, \text{NBND}$, $\text{LLBND}(i-1) < \text{LLBND}(i)$ for $i = 2, 3, \dots, \text{NBND}$.	
16: ILBND(*) — INTEGER array	<i>Output</i>
<i>On exit:</i> ILBND(i) for $i = 1, 2, \dots, \text{NBND}$ must contain the type of the i th boundary (or corner), as given in Section 3.	
<i>Constraint:</i> ILBND(i) must be equal to one of the following: 1, 2, 3, 4, 12, 23, 34, 41, 21, 32, 43 or 14, for $i = 1, 2, \dots, \text{NBND}$.	
17: LBND(*) — INTEGER array	<i>Output</i>
<i>On exit:</i> LBND(i) for $i = 1, 2, \dots, \text{NBPTS}$ must contain the grid index of the i th boundary point. The order of the boundaries is as specified in LLBND, but within this restriction the order of the points in LBND is arbitrary.	
<i>Constraint:</i> $1 \leq \text{LBND}(i) \leq \text{NPTS}$ for $i = 1, 2, \dots, \text{NBPTS}$.	
18: IERR — INTEGER	<i>Output</i>
<i>On exit:</i> if the required number of grid points is larger than MAXPTS, IERR must be set to -1 to force a termination of the integration and an immediate return to the calling program with IFAIL set to 3. Otherwise, IERR should remain unchanged.	

INIDOM must be declared as EXTERNAL in the (sub)program from which D03RBF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

8: PDEDEF — SUBROUTINE, supplied by the user. *External Procedure*

PDEDEF must evaluate the functions F_j , $j = 1, 2, \dots, \text{NPDE}$, in equation (1) which define the system of PDEs (i.e., the residuals of the resulting ODE system) at all interior points of the domain. Values at points on the boundaries of the domain are ignored and will be overwritten by the subroutine BNDARY. PDEDEF is called for each subgrid in turn.

Its specification is:

<pre> SUBROUTINE PDEDEF(NPTS, NPDE, T, X, Y, U, UT, UX, UY, UXX, UXY, 1 UYY, RES) INTEGER NPTS, NPDE <i>real</i> T, X(NPTS), Y(NPTS), U(NPTS,NPDE), 1 UT(NPTS,NPDE), UX(NPTS,NPDE), UY(NPTS,NPDE), 2 UXX(NPTS,NPDE), UXY(NPTS,NPDE), UYY(NPTS,NPDE), 3 RES(NPTS,NPDE) </pre>	
1: NPTS — INTEGER	<i>Input</i>
<i>On entry:</i> the number of grid points in the current grid.	
2: NPDE — INTEGER	<i>Input</i>
<i>On entry:</i> the number of PDEs in the system.	
3: T — <i>real</i>	<i>Input</i>
<i>On entry:</i> the current value of the independent variable t .	

4:	X(NPTS) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> X(<i>i</i>) contains the <i>x</i> co-ordinate of the <i>i</i> th grid point, for $i = 1, 2, \dots, \text{NPTS}$.	
5:	Y(NPTS) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> Y(<i>i</i>) contains the <i>y</i> co-ordinate of the <i>i</i> th grid point, for $i = 1, 2, \dots, \text{NPTS}$.	
6:	U(NPTS,NPDE) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> U(<i>i,j</i>) contains the value of the <i>j</i> th PDE component at the <i>i</i> th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$.	
7:	UT(NPTS,NPDE) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> UT(<i>i,j</i>) contains the value of $\partial u / \partial t$ for the <i>j</i> th PDE component at the <i>i</i> th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$.	
8:	UX(NPTS,NPDE) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> UX(<i>i,j</i>) contains the value of $\partial u / \partial x$ for the <i>j</i> th PDE component at the <i>i</i> th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$.	
9:	UY(NPTS,NPDE) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> UY(<i>i,j</i>) contains the value of $\partial u / \partial y$ for the <i>j</i> th PDE component at the <i>i</i> th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$.	
10:	UXX(NPTS,NPDE) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> UXX(<i>i,j</i>) contains the value of $\partial^2 u / \partial x^2$ for the <i>j</i> th PDE component at the <i>i</i> th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$.	
11:	UXY(NPTS,NPDE) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> UXY(<i>i,j</i>) contains the value of $\partial^2 u / \partial x \partial y$ for the <i>j</i> th PDE component at the <i>i</i> th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$.	
12:	UYU(NPTS,NPDE) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> UYU(<i>i,j</i>) contains the value of $\partial^2 u / \partial y^2$ for the <i>j</i> th PDE component at the <i>i</i> th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$.	
13:	RES(NPTS,NPDE) — <i>real</i> array	<i>Output</i>
	<i>On exit:</i> RES(<i>i,j</i>) must contain the value of F_j for $j = 1, 2, \dots, \text{NPDE}$, at the <i>i</i> th grid point for $i = 1, 2, \dots, \text{NPTS}$, although the residuals at boundary points will be ignored (and overwritten later on) and so they need not be specified here.	

PDEDEF must be declared as EXTERNAL in the (sub)program from which D03RBF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

- 9:** BNDARY — SUBROUTINE, supplied by the user. *External Procedure*
- BNDARY must evaluate the functions G_j , $j = 1, 2, \dots, \text{NPDE}$, in equation (2) which define the boundary conditions at all boundary points of the domain. Residuals at interior points must **not** be altered by this subroutine.

Its specification is:

	SUBROUTINE BNDARY(NPTS, NPDE, T, X, Y, U, UT, UX, UY, NBND,
1	NBPTS, LLBND, ILBND, LBND, RES)
INTEGER	NPTS, NPDE, NBND, NBPTS, LLBND(NBND),
1	ILBND(NBND), LBND(NBPTS)
<i>real</i>	T, X(NPTS), Y(NPTS), U(NPTS,NPDE),
1	UT(NPTS,NPDE), UX(NPTS,NPDE), UY(NPTS,NPDE),
2	RES(NPTS,NPDE)

- | | | |
|-----|---|---------------|
| 1: | NPTS — INTEGER | <i>Input</i> |
| | <i>On entry:</i> the number of grid points in the current grid. | |
| 2: | NPDE — INTEGER | <i>Input</i> |
| | <i>On entry:</i> the number of PDEs in the system. | |
| 3: | T — real | <i>Input</i> |
| | <i>On entry:</i> the current value of the independent variable t . | |
| 4: | X(NPTS) — real array | <i>Input</i> |
| | <i>On entry:</i> X(i) contains the x co-ordinate of the i th grid point, for $i = 1, 2, \dots, \text{NPTS}$. | |
| 5: | Y(NPTS) — real array | <i>Input</i> |
| | <i>On entry:</i> Y(i) contains the y co-ordinate of the i th grid point, for $i = 1, 2, \dots, \text{NPTS}$. | |
| 6: | U(NPTS, NPDE) — real array | <i>Input</i> |
| | <i>On entry:</i> U(i, j) contains the value of the j th PDE component at the i th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$. | |
| 7: | UT(NPTS, NPDE) — real array | <i>Input</i> |
| | <i>On entry:</i> UT(i, j) contains the value of $\partial u / \partial t$ for the j th PDE component at the i th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$. | |
| 8: | UX(NPTS, NPDE) — real array | <i>Input</i> |
| | <i>On entry:</i> UX(i, j) contains the value of $\partial u / \partial x$ for the j th PDE component at the i th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$. | |
| 9: | UY(NPTS, NPDE) — real array | <i>Input</i> |
| | <i>On entry:</i> UY(i, j) contains the value of $\partial u / \partial y$ for the j th PDE component at the i th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$. | |
| 10: | NBNDS — INTEGER | <i>Input</i> |
| | <i>On entry:</i> the total number of physical boundaries and corners in the grid. | |
| 11: | NBPTS — INTEGER | <i>Input</i> |
| | <i>On entry:</i> the total number of boundary points in the grid. | |
| 12: | LLBND(NBNDS) — INTEGER array | <i>Input</i> |
| | <i>On entry:</i> LLBND(i) for $i = 1, 2, \dots, \text{NBNDS}$ contains the element of LBND corresponding to the start of the i th boundary (or corner). | |
| 13: | ILBND(NBNDS) — INTEGER array | <i>Input</i> |
| | <i>On entry:</i> ILBND(i) for $i = 1, 2, \dots, \text{NBNDS}$ contains the type of the i th boundary, as given in Section 3. | |
| 14: | LBND(NBPTS) — INTEGER array | <i>Input</i> |
| | <i>On entry:</i> LBND(i) for $i = 1, 2, \dots, \text{NBPTS}$ contains the grid index of the i th boundary point, where the order of the boundaries is as specified in LLBND. Hence the i th boundary point has co-ordinates X(LBND(i)) and Y(LBND(i)), and the corresponding solution values are U(LBND(i), j), $j = 1, 2, \dots, \text{NPDE}$. | |
| 15: | RES(NPTS, NPDE) — real array | <i>Output</i> |
| | <i>On exit:</i> RES(LBND(i), j) must contain the value of G_j for $j = 1, 2, \dots, \text{NPDE}$, at the i th boundary point for $i = 1, 2, \dots, \text{NBPTS}$. | |
- Note.** Elements of RES corresponding to interior points, i.e., points not included in LBND, must **not** be altered.

BNDARY must be declared as EXTERNAL in the (sub)program from which D03RBF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

10: PDEIV — SUBROUTINE, supplied by the user. *External Procedure*

PDEIV must specify the initial values of the PDE components u at all points in the base grid. PDEIV is not referenced if, on entry, IND = 1.

Its specification is:

```
SUBROUTINE PDEIV(NPTS, NPDE, T, X, Y, U)
  INTEGER          NPTS, NPDE
  real            T, X(NPTS), Y(NPTS), U(NPTS, NPDE)
```

- | | | |
|----|---|---------------|
| 1: | NPTS — INTEGER
<i>On entry:</i> the number of grid points in the base grid. | <i>Input</i> |
| 2: | NPDE — INTEGER
<i>On entry:</i> the number of PDEs in the system. | <i>Input</i> |
| 3: | T — <i>real</i>
<i>On entry:</i> the (initial) value of the independent variable t . | <i>Input</i> |
| 4: | X(NPTS) — <i>real</i> array
<i>On entry:</i> X(i) contains the x co-ordinate of the i th grid point, for $i = 1, 2, \dots, \text{NPTS}$. | <i>Input</i> |
| 5: | Y(NPTS) — <i>real</i> array
<i>On entry:</i> Y(i) contains the y co-ordinate of the i th grid point, for $i = 1, 2, \dots, \text{NPTS}$. | <i>Input</i> |
| 6: | U(NPTS, NPDE) — <i>real</i> array
<i>On exit:</i> U(i, j) must contain the value of the j th PDE component at the i th grid point, for $i = 1, 2, \dots, \text{NPTS}$, $j = 1, 2, \dots, \text{NPDE}$. | <i>Output</i> |

PDEIV must be declared as EXTERNAL in the (sub)program from which D03RBF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

11: MONITR — SUBROUTINE, supplied by the user. *External Procedure*

MONITR is called by D03RBF at the end of every successful time step, and may be used to examine or print the solution or perform other tasks such as error calculations, particularly at the final time step, indicated by the parameter TLAST.

The input arguments contain information about the grid and solution at all grid levels used. D03RZF should be called from MONITR in order to extract the number of points and their (x, y) co-ordinates on a particular grid.

MONITR can also be used to force an immediate tidy termination of the solution process and return to the calling program.

Its specification is:

```
SUBROUTINE MONITR(NPDE, T, DT, DTNEW, TLAST, NLEV, XMIN, YMIN,
1  DXB, DYB, LGRID, ISTRUC, LSOL, SOL, IERR)
  INTEGER          NPDE, NLEV, LGRID(*), ISTRUC(*), LSOL(NLEV), IERR
  real            T, DT, DTNEW, XMIN, YMIN, DXB, DYB, SOL(*)
  LOGICAL          TLAST
```

- | | | |
|----|--|--------------|
| 1: | NPDE — INTEGER
<i>On entry:</i> the number of PDEs in the system. | <i>Input</i> |
|----|--|--------------|

2:	T — <i>real</i>	<i>Input</i>
	<i>On entry:</i> the current value of the independent variable t , i.e., the time at the end of the integration step just completed.	
3:	DT — <i>real</i>	<i>Input</i>
	<i>On entry:</i> the current time step size DT, i.e., the time step size used for the integration step just completed.	
4:	DTNEW — <i>real</i>	<i>Input</i>
	<i>On entry:</i> the time step size that will be used for the next time step.	
5:	TLAST — LOGICAL	<i>Input</i>
	<i>On entry:</i> indicates if intermediate or final time step. TLAST = .FALSE. for an intermediate step, TLAST = .TRUE. for the last call to MONITR before returning to the user's program.	
6:	NLEV — INTEGER	<i>Input</i>
	<i>On entry:</i> the number of grid levels used at time T.	
7:	XMIN — <i>real</i>	<i>Input</i>
8:	YMIN — <i>real</i>	<i>Input</i>
	<i>On entry:</i> the (x, y) co-ordinates of the lower-left corner of the virtual grid.	
9:	DXB — <i>real</i>	<i>Input</i>
10:	DYB — <i>real</i>	<i>Input</i>
	<i>On entry:</i> the sizes of the base grid spacing in the x - and y -direction respectively.	
11:	LGRID(*) — INTEGER array	<i>Input</i>
	<i>On entry:</i> LGRID contains pointers to the start of the grid structures in ISTRUC, and must be passed unchanged to D03RZF in order to extract the grid information.	
12:	ISTRUC(*) — INTEGER array	<i>Input</i>
	<i>On entry:</i> ISTRUC contains the grid structures for each grid level and must be passed unchanged to D03RZF in order to extract the grid information.	
13:	LSOL(NLEV) — INTEGER array	<i>Input</i>
	<i>On entry:</i> LSOL(l) contains the pointer to the solution in SOL at grid level l and time T. (LSOL(l) actually contains the array index immediately preceding the start of the solution in SOL. See below.)	
14:	SOL(*) — <i>real</i> array	<i>Input</i>
	<i>On entry:</i> SOL contains the solution u at time T for each grid level l in turn, positioned according to LSOL. More precisely	
	$U(i, j) = \text{SOL}(\text{LSOL}(l) + (j - 1) \times n_l + i)$	
	represents the j th component of the solution at the i th grid point in the l th level, for $i = 1, \dots, n_l$, $j = 1, \dots, \text{NPDE}$, $l = 1, \dots, \text{NLEV}$, where n_l is the number of grid points at level l (obtainable by a call to D03RZF).	
15:	IERR — INTEGER	<i>Output</i>
	<i>On exit:</i> IERR should be set to 1 to force a termination of the integration and an immediate return to the calling program with IFAIL set to 4. IERR should remain unchanged otherwise.	

MONITR must be declared as EXTERNAL in the (sub)program from which D03RBF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

12: OPTI(4) — INTEGER array*Input*

On entry: OPTI may be set to control various options available in the integrator. If OPTI(1) = 0 then **all** the default options are employed.

If OPTI(1) > 0 then the default value of OPTI(*i*) for *i* = 2, 3, 4, can be obtained by setting OPTI(*i*) = 0.

OPTI(1) specifies the maximum number of grid levels allowed (including the base grid). OPTI(1) ≥ 0. The default value is OPTI(1) = 3.

OPTI(2) specifies the maximum number of Jacobian evaluations allowed during each nonlinear equations solution. OPTI(2) ≥ 0. The default value is OPTI(2) = 2.

OPTI(3) specifies the maximum number of Newton iterations in each nonlinear equations solution. OPTI(3) ≥ 0. The default value is OPTI(3) = 10.

OPTI(4) specifies the maximum number of iterations in each linear equations solution. OPTI(4) ≥ 0. The default value is OPTI(4) = 100.

Constraint: OPTI(1) ≥ 0 and if OPTI(1) > 0 then OPTI(*i*) ≥ 0 for *i* = 2, 3, 4.

13: OPTR(3, NPDE) — *real* array*Input*

On entry: OPTR may be used to specify the optional vectors u^{max} , w^s and w^t in the space and time monitors (see Section 8).

If an optional vector is not required then all its components should be set to 1.0.

OPTR(1, *j*), for *j* = 1, 2, ..., NPDE, specifies u_j^{max} , the approximate maximum absolute value of the *j*th component of u , as used in (4) and (7). OPTR(1, *j*) > 0.0 for *j* = 1, 2, ..., NPDE.

OPTR(2, *j*), for *j* = 1, 2, ..., NPDE, specifies w_j^s , the weighting factors used in the space monitor (see (4)) to indicate the relative importance of the *j*th component of u on the space monitor. OPTR(2, *j*) ≥ 0.0 for *j* = 1, 2, ..., NPDE.

OPTR(3, *j*), for *j* = 1, 2, ..., NPDE, specifies w_j^t , the weighting factors used in the time monitor (see (6)) to indicate the relative importance of the *j*th component of u on the time monitor. OPTR(3, *j*) ≥ 0.0 for *j* = 1, 2, ..., NPDE.

Constraint: OPTR(1, *j*) > 0.0 for *j* = 1, 2, ..., NPDE and OPTR(*i*, *j*) ≥ 0.0 for *i* = 2, 3 and *j* = 1, 2, ..., NPDE.

14: RWK(LENRWK) — *real* array*Workspace***15: LENRWK — INTEGER***Input*

On entry: the dimension of the array RWK as declared in the (sub)program from which D03RBF is called.

The required value of LENRWK can not be determined exactly in advance, but a suggested value is

$$\text{LENRWK} = \text{MAXPTS} \times \text{NPDE} \times (5 \times l + 18 \times \text{NPDE} + 9) + 2 \times \text{MAXPTS},$$

where $l = \text{OPTI}(1)$ if $\text{OPTI}(1) \neq 0$ and $l = 3$ otherwise, and MAXPTS is the expected maximum number of grid points at any one level. If during the execution the supplied value is found to be too small then the routine returns with IFAIL = 3 and an estimated required size is printed on the current error message unit (see X04AAF).

Note. The size of LENRWK can not be checked upon initial entry to D03RBF since the number of grid points on the base grid is not known.

16: IWK(LENIWK) — INTEGER array*Input/Output*

On entry: if $IND = 0$, IWK need not be set. Otherwise IWK must remain unchanged from a previous call to D03RBF.

On exit: the following components of the array IWK concern the efficiency of the integration.

IWK(1) contains the number of steps taken in time;

IWK(2) contains the number of rejected time steps;

IWK(2+l) contains the total number of residual evaluations performed (i.e., the number of times PDEDEF was called) at grid level l ;

IWK(2+m+l) contains the total number of Jacobian evaluations performed at grid level l ;

IWK(2+2×m+l) contains the total number of Newton iterations performed at grid level l ;

IWK(2+3×m+l) contains the total number of linear solver iterations performed at grid level l ;

IWK(2+4×m+l) contains the maximum number of Newton iterations performed at any one time step at grid level l ;

IWK(2+5×m+l) contains the maximum number of linear solver iterations performed at any one time step at grid level l ;

for $l = 1, 2, \dots, nl$, where nl is the number of levels used and $m = OPTI(1)$ if $OPTI(1) > 0$ and $m = 3$ otherwise.

Note. The total and maximum numbers are cumulative over all calls to D03RBF. If the specified maximum number of Newton or linear solver iterations is exceeded at any stage, then the maximums above are set to the specified maximum plus one.

17: LENIWK — INTEGER*Input*

On entry: the dimension of the array IWK as declared in the (sub)program from which D03RBF is called.

The required value of LENIWK can not be determined exactly in advance, but a suggested value is

$$LENIWK = MAXPTS \times (14 + 5 \times m) + 7 \times m + 2,$$

where MAXPTS is the expected maximum number of grid points at any one level and $m = OPTI(1)$ if $OPTI(1) > 0$ and $m = 3$ otherwise. If during the execution the supplied value is found to be too small then the routine returns with $IFAIL = 3$ and an estimated required size is printed on the current error message unit (see X04AAF).

Note. The size of LENIWK can not be checked upon initial entry to D03RBF since the number of grid points on the base grid is not known.

18: LWK(LENLWK) — LOGICAL array*Workspace***19: LENLWK — INTEGER***Input*

On entry: the dimension of the array LWK as declared in the (sub)program from which D03RBF is called.

The required value of LENLWK can not be determined exactly in advance, but a suggested value is

$$LENLWK = MAXPTS + 1,$$

where MAXPTS is the expected maximum number of grid points at any one level. If during the execution the supplied value is found to be too small then the routine returns with $IFAIL = 3$ and an estimated required size is printed on the current error message unit (see X04AAF).

Note. The size of LENLWK can not be checked upon initial entry to D03RBF since the number of grid points on the base grid is not known.

20: ITRACE — INTEGER*Input*

On entry: the level of trace information required from D03RBF. ITRACE may take the value -1 , 0 , 1 , 2 , or 3 . If $ITRACE < -1$, then -1 is assumed and similarly if $ITRACE > 3$, then 3 is assumed. If $ITRACE = -1$, no output is generated. If $ITRACE = 0$, only warning messages are printed, and if $ITRACE > 0$, then output from the underlying solver is printed on the current advisory message unit (see X04ABF). This output contains details of the time integration, the nonlinear iteration and the linear solver. The advisory messages are given in greater detail as ITRACE increases. Setting $ITRACE = 1$ allows the user to monitor the progress of the integration without possibly excessive information.

21: IND — INTEGER*Input/Output*

On entry: IND must be set to 0 or 1 .

IND = 0

starts the integration in time.

IND = 1

continues the integration after an earlier exit from the routine. In this case, only the following parameters may be reset between calls to D03RBF: TOUT, DT(2), DT(3), TOLS, TOLT, OPTI, OPTR, ITRACE and IFAIL.

Constraint: $0 \leq \text{IND} \leq 1$.

On exit: IND = 1 .

22: 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 .

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, NPDE < 1 ,
 or TOUT \leq TS,
 or TOUT is too close to TS,
 or IND = 0 and DT(1) < 0.0 ,
 or DT(i) < 0.0 for $i = 2$ or 3 ,
 or DT(2) $>$ DT(3),
 or IND = 0 and
 $0.0 < \text{DT}(1) < 10 \times \text{machine precision} \times \max(|\text{TS}|, |\text{TOUT}|)$,
 or IND = 0 and DT(1) $>$ TOUT – TS,
 or IND = 0 and DT(1) $<$ DT(2) or DT(1) $>$ DT(3),
 or TOLS or TOLT ≤ 0.0 ,
 or OPTI(1) < 0 ,
 or OPTI(1) > 0 and OPTI(j) < 0 for $j = 2, 3$ or 4 ,
 or OPTR(1, j) ≤ 0.0 for some $j = 1, 2, \dots, \text{NPDE}$,
 or OPTR(2, j) < 0.0 for some $j = 1, 2, \dots, \text{NPDE}$,
 or OPTR(3, j) < 0.0 for some $j = 1, 2, \dots, \text{NPDE}$,
 or IND $\neq 0$ or 1 ,

or $\text{IND} = 1$ on initial entry to D03RBF.

IFAIL = 2

The time step size to be attempted is less than the specified minimum size. This may occur following time step failures and subsequent step size reductions caused by one or more of the following:

- the requested accuracy could not be achieved, i.e., TOLT is too small,
- the maximum number of linear solver iterations, Newton iterations or Jacobian evaluations is too small,
- ILU decomposition of the Jacobian matrix could not be performed, possibly due to singularity of the Jacobian.

Setting ITRACE to a higher value may provide further information.

In the latter two cases the user is advised to check their problem formulation in PDEDEF and/or BNDARY, and the initial values in PDEIV if appropriate.

IFAIL = 3

One or more of the workspace arrays is too small for the required number of grid points. At the initial time step this error may result from either the user setting IERR to -1 in INIDOM, or the internal check on the number of grid points following the call to INIDOM. An estimate of the required sizes for the current stage is output, but more space may be required at a later stage.

IFAIL = 4

IERR was set to 1 in the user-supplied subroutine MONITR, forcing control to be passed back to calling program. Integration was successful as far as $T = \text{TS}$.

IFAIL = 5

The integration has been completed but the maximum number of levels specified in OPTI(1) was insufficient at one or more time steps, meaning that the requested space accuracy could not be achieved. To avoid this warning either increase the value of OPTI(1) or decrease the value of TOLS.

IFAIL = 6

One or more of the output arguments of the user-supplied subroutine INIDOM was incorrectly specified, i.e.,

- $\text{XMIN} \geq \text{XMAX}$,
- or XMAX too close to XMIN ,
- or $\text{YMIN} \geq \text{YMAX}$,
- or YMAX too close to YMIN ,
- or NX or $\text{NY} < 4$,
- or $\text{NROWS} < 4$,
- or $\text{NROWS} > \text{NY}$,
- or $\text{NPTS} > \text{NX} \times \text{NY}$,
- or $\text{NBND} < 8$,
- or $\text{NBPTS} < 12$,
- or $\text{NBPTS} \geq \text{NPTS}$,
- or $\text{LROW}(i) < 1$ or $\text{LROW}(i) > \text{NPTS}$ for some $i = 1, 2, \dots, \text{NROWS}$,
- or $\text{LROW}(i) \leq \text{LROW}(i - 1)$ for some $i = 2, 3, \dots, \text{NROWS}$,
- or $\text{IROW}(i) < 0$ or $\text{IROW}(i) > \text{NY}$ for some $i = 1, 2, \dots, \text{NROWS}$,
- or $\text{IROW}(i) \leq \text{IROW}(i - 1)$ for some $i = 2, 3, \dots, \text{NROWS}$,
- or $\text{ICOL}(i) < 0$ or $\text{ICOL}(i) > \text{NX}$ for some $i = 1, 2, \dots, \text{NPTS}$,
- or $\text{LLBND}(i) < 1$ or $\text{LLBND}(i) > \text{NBPTS}$ for some $i = 1, 2, \dots, \text{NBND}$,
- or $\text{LLBND}(i) \leq \text{LLBND}(i - 1)$ for some $i = 2, 3, \dots, \text{NBND}$,
- or $\text{ILBND}(i) \neq 1, 2, 3, 4, 12, 23, 34, 41, 21, 32, 43$ or 14 , for some $i = 1, 2, \dots, \text{NBND}$,
- or $\text{LBND}(i) < 1$ or $\text{LBND}(i) > \text{NPTS}$ for some $i = 1, 2, \dots, \text{NBPTS}$.

7 Accuracy

There are three sources of error in the algorithm: space and time discretisation, and interpolation (linear) between grid levels. The space and time discretisation errors are controlled separately using the parameters TOLS and TOLT described in the following section, and the user should test the effects of varying these parameters. Interpolation errors are generally implicitly controlled by the refinement criterion since in areas where interpolation errors are potentially large, the space monitor will also be large. It can be shown that the global spatial accuracy is comparable to that which would be obtained on a uniform grid of the finest grid size. A full error analysis can be found in [3].

8 Further Comments

8.1 Algorithm Outline

The local uniform grid refinement method is summarised as follows

- (1) Initialise the course base grid, an initial solution and an initial time step,
- (2) Solve the system of PDEs on the current grid with the current time step,
- (3) If the required accuracy in space and the maximum number of grid levels have not yet been reached:
 - (a) Determine new finer grid at forward time level,
 - (b) Get solution values at previous time level(s) on new grid,
 - (c) Interpolate internal boundary values from old grid at forward time,
 - (d) Get initial values for the Newton process at forward time,
 - (e) Goto 2,
- (4) Update the coarser grid solution using the finer grid values,
- (5) Estimate error in time integration. If time error is acceptable advance time level,
- (6) Determine new step size then goto 2 with coarse base as current grid.

8.2 Refinement Strategy

For each grid point i a space monitor μ_i^s is determined by

$$\mu_i^s = \max_{j=1, \text{NPDE}} \{ \gamma_j (| \Delta x^2 \frac{\partial^2}{\partial x^2} u_j(x_i, y_i, t) | + | \Delta y^2 \frac{\partial^2}{\partial y^2} u_j(x_i, y_i, t) |) \}, \quad (3)$$

where Δx and Δy are the grid widths in the x and y directions; and x_i, y_i are the (x, y) co-ordinates at grid point i . The parameter γ_j is obtained from

$$\gamma_j = \frac{w_j^s}{u_j^{max} \sigma}, \quad (4)$$

where σ is the user-supplied space tolerance; w_j^s is a weighting factor for the relative importance of the j th PDE component on the space monitor; and u_j^{max} is the approximate maximum absolute value of the j th component. A value for σ must be supplied by the user. Values for w_j^s and u_j^{max} must also be supplied but may be set to the values 1.0 if little information about the solution is known.

A new level of refinement is created if

$$\max_i \{ \mu_i^s \} > 0.9 \text{ or } 1.0, \quad (5)$$

depending on the grid level at the previous step in order to avoid fluctuations in the number of grid levels between time steps. If (5) is satisfied then all grid points for which $\mu_i^s > 0.25$ are flagged and surrounding cells are quartered in size.

No derefinement takes place as such, since at each time step the solution on the base grid is computed first and new finer grids are then created based on the new solution. Hence derefinement occurs implicitly. See Section 8.1.

8.3 Time Integration

The time integration is controlled using a time monitor calculated at each level l up to the maximum level used, given by

$$\mu_l^t = \sqrt{\frac{1}{N} \sum_{j=1}^{\text{NPDE}} w_j^t \sum_{i=1}^{\text{NGPTS}(l)} \left(\frac{\Delta t}{\alpha_{ij}} u_t(x_i, y_i, t) \right)^2} \quad (6)$$

where $\text{NGPTS}(l)$ is the total number of points on grid level l ; $N = \text{NGPTS}(l) \times \text{NPDE}$; Δt is the current time step; u_t is the time derivative of u which is approximated by first-order finite differences; w_j^t is the time equivalent of the space weighting factor w_j^s ; and α_{ij} is given by

$$\alpha_{ij} = \tau \left(\frac{u_j^{\max}}{100} + |u(x_i, y_i, t)| \right) \quad (7)$$

where u_j^{\max} is as before, and τ is the user-specified time tolerance.

An integration step is rejected and retried at all levels if

$$\max_l \{\mu_l^t\} > 1.0. \quad (8)$$

9 Example

For this routine two examples are presented, in Section 9.1 and Section 9.2. In the example programs distributed to sites, there is a single example program for D03RBF, with a main program:

```
*      D03RBF Example Program Text
*      Mark 18 Release. NAG Copyright 1997.
*      .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*      .. External Subroutines ..
      EXTERNAL         EX1, EX2
*      .. Executable Statements ..
      WRITE (NOUT,*) 'D03RBF Example Program Results'
      CALL EX1
      CALL EX2
      STOP
      END
```

The code to solve the two example problems is given in the subroutines EX1 and EX2, in Section 9.1.1 and Section 9.2.1 respectively.

9.1 Example 1

This example is taken from [1] and is the two dimensional Burgers' system

$$\begin{aligned} \frac{\partial u}{\partial t} &= -u \frac{\partial u}{\partial x} - v \frac{\partial u}{\partial y} + \epsilon \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \\ \frac{\partial v}{\partial t} &= -u \frac{\partial v}{\partial x} - v \frac{\partial v}{\partial y} + \epsilon \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right), \end{aligned}$$

with $\epsilon = 10^{-3}$ on the domain given in Figure 3. Dirichlet boundary conditions are used on all boundaries using the exact solution

$$\begin{aligned} u &= \frac{3}{4} - \frac{1}{4(1 + \exp((-4x + 4y - t)/(32\epsilon)))}, \\ v &= \frac{3}{4} + \frac{1}{4(1 + \exp((-4x + 4y - t)/(32\epsilon)))}. \end{aligned}$$

The solution contains a wave front at $y = x + 0.25t$ which propagates in a direction perpendicular to the front with speed $\sqrt{2}/8$.

9.1.1 Program Text

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.

```

*
  SUBROUTINE EX1
*
  .. Parameters ..
  INTEGER          NOUT
  PARAMETER        (NOUT=6)
  INTEGER          MXLEV, NPDE, NPTS
  PARAMETER        (MXLEV=5, NPDE=2, NPTS=3000)
  INTEGER          LENIWK, LENRWK, LENLWK
  PARAMETER        (LENIWK=NPTS*(5*MXLEV+14)+2+7*MXLEV,
+                  LENRWK=NPTS*NPDE*(5*MXLEV+9+18*NPDE)+2*NPTS,
+                  LENLWK=2*NPTS)
*
  .. Scalars in Common ..
  INTEGER          IOUT
*
  .. Arrays in Common ..
  real            TWANT(2)
*
  .. Local Scalars ..
  real            TOLS, TOLT, TOUT, TS
  INTEGER          I, IFAIL, IND, ITRACE, J, MAXLEV
*
  .. Local Arrays ..
  real            DT(3), OPTR(3, NPDE), RWK(LENRWK)
  INTEGER          IWK(LENIWK), OPTI(4)
  LOGICAL          LWK(LENLWK)
*
  .. External Subroutines ..
  EXTERNAL          BNDRY1, D03RBF, INIDM1, MONIT1, PDEF1, PDEIV1
*
  .. Common blocks ..
  COMMON            /OTIME1/TWANT, IOUT
*
  .. Save statement ..
  SAVE              /OTIME1/
*
  .. Executable Statements ..
  WRITE (NOUT,*)
  WRITE (NOUT,*)
  WRITE (NOUT,*) 'Example 1'
  WRITE (NOUT,*)

*
  IND = 0
  ITRACE = 0
  TS = 0.0e0
  TWANT(1) = 0.25e0
  TWANT(2) = 1.0e0
  DT(1) = 0.001e0
  DT(2) = 1.0e-7
  DT(3) = 0.0e0
  TOLS = 0.1e0
  TOLT = 0.05e0
  OPTI(1) = 5
  MAXLEV = OPTI(1)
  DO 20 I = 2, 4
    OPTI(I) = 0
20 CONTINUE
  DO 60 J = 1, NPDE
    DO 40 I = 1, 3
      OPTR(I, J) = 1.0e0
40 CONTINUE
60 CONTINUE

```

```

*
*   Call main routine
*
DO 120 IOUT = 1, 2
    IFAIL = -1
    TOUT = TWANT(IOUT)
    CALL D03RBF(NPDE,TS,TOUT,DT,TOLS,TOLT,INIDM1,PDEF1,BNDY1,
+             PDEIV1,MONIT1,OPTI,OPTR,RWK,LENRWK,IWK,LENIWK,LWK,
+             LENLWK,ITRACE,IND,IFAIL)
*
*   Print statistics
*
    WRITE (NOUT,(''Statistics:'''))
    WRITE (NOUT,('' Time = '',F8.4)') TS
    WRITE (NOUT,('' Total number of accepted timesteps = '', I5)')
+     IWK(1)
    WRITE (NOUT,('' Total number of rejected timesteps = '', I5)')
+     IWK(2)
    WRITE (NOUT,*)
    WRITE (NOUT,
+     '(''          T o t a l   n u m b e r   o f          '')')
    WRITE (NOUT,
+     '(''          Residual   Jacobian   Newton   '' , ''   Lin sys'')')
+     )
    WRITE (NOUT,
+     '(''          evals      evals      iters   '' , ''      iters'')')
+     )
    WRITE (NOUT,('' At level '''))
    MAXLEV = OPTI(1)
    DO 80 J = 1, MAXLEV
        IF (IWK(J+2).NE.0) WRITE (NOUT,('I6,4I10')) J, IWK(J+2),
+        IWK(J+2+MAXLEV), IWK(J+2+2*MAXLEV), IWK(J+2+3*MAXLEV)
*
80    CONTINUE
    WRITE (NOUT,*)
    WRITE (NOUT,
+     '(''          M a x i m u m   n u m b e r   '' , ''   o f'')')
    WRITE (NOUT,
+     '(''          Newton iters   Lin sys iters   '''))
    WRITE (NOUT,('' At level '''))
    DO 100 J = 1, MAXLEV
        IF (IWK(J+2).NE.0) WRITE (NOUT,('I6,2I14')) J,
+        IWK(J+2+4*MAXLEV), IWK(J+2+5*MAXLEV)
100    CONTINUE
    WRITE (NOUT,*)
*
120 CONTINUE
*
    RETURN
    END
*
    SUBROUTINE INIDM1(MAXPTS,XMIN,XMAX,YMIN,YMAX,NX,NY,NPTS,NROWS,
+                 NBND,NBPTS,LROW,IROW,ICOL,LLBND,ILBND,LBND,
+                 IERR)
*
    .. Parameters ..
    INTEGER          NOUT
    PARAMETER          (NOUT=6)

```

```

*    .. Scalar Arguments ..
    real                XMAX, XMIN, YMAX, YMIN
    INTEGER              IERR, MAXPTS, NBND, NBPTS, NPTS, NROWS, NX, NY
*    .. Array Arguments ..
    INTEGER              ICOL(*), ILBND(*), IROW(*), LBND(*), LLBND(*),
+                       LROW(*)
*    .. Local Scalars ..
    INTEGER              I, IFAIL, J, LENIWK
*    .. Local Arrays ..
    INTEGER              ICOLD(105), ILBND(28), IROW(11), IWK(122),
+                       LBND(72), LLBND(28), LROW(11)
    CHARACTER*33         PGRID(11)
*    .. External Subroutines ..
    EXTERNAL              D03RYF
*    .. Data statements ..
    DATA                ICOLD/0, 1, 2, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10,
+                       0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 0, 1, 2, 3, 4,
+                       5, 6, 7, 8, 9, 10, 0, 1, 2, 3, 4, 5, 8, 9, 10,
+                       0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 0, 1, 2, 3, 4,
+                       5, 6, 7, 8, 9, 10, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9,
+                       10, 0, 1, 2, 3, 4, 5, 6, 7, 8, 0, 1, 2, 3, 4, 5,
+                       6, 7, 8, 0, 1, 2, 3, 4, 5, 6, 7, 8/
    DATA                ILBND/1, 2, 3, 4, 1, 4, 1, 2, 3, 4, 3, 4, 1, 2,
+                       12, 23, 34, 41, 14, 41, 12, 23, 34, 41, 43, 14,
+                       21, 32/
    DATA                IROW/0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10/
    DATA                LBND/2, 4, 15, 26, 37, 46, 57, 68, 79, 88, 98,
+                       99, 100, 101, 102, 103, 104, 96, 86, 85, 84, 83,
+                       82, 70, 59, 48, 39, 28, 17, 6, 8, 9, 10, 11, 12,
+                       13, 18, 29, 40, 49, 60, 72, 73, 74, 75, 76, 77,
+                       67, 56, 45, 36, 25, 33, 32, 42, 52, 53, 43, 1,
+                       97, 105, 87, 81, 3, 7, 71, 78, 14, 31, 51, 54,
+                       34/
    DATA                LLBND/1, 2, 11, 18, 19, 24, 31, 37, 42, 48, 53,
+                       55, 56, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67,
+                       68, 69, 70, 71, 72/
    DATA                LROW/1, 4, 15, 26, 37, 46, 57, 68, 79, 88, 97/
*    .. Executable Statements ..
    NX = 11
    NY = 11

*
*    Check MAXPTS against rough estimate of NPTS
*
    NPTS = NX*NY
    IF (MAXPTS.LT.NPTS) THEN
        IERR = -1
        RETURN
    END IF

*
    XMIN = 0.0e0
    YMIN = 0.0e0
    XMAX = 1.0e0
    YMAX = 1.0e0

*
    NROWS = 11
    NPTS = 105
    NBND = 28
    NBPTS = 72

```

```

*
DO 20 I = 1, NROWS
  LROW(I) = LROWD(I)
  IROW(I) = IROWD(I)
20 CONTINUE
*
DO 40 I = 1, NBND
  LLBND(I) = LLBND(I)
  ILBND(I) = ILBND(I)
40 CONTINUE
*
DO 60 I = 1, NBPTS
  LBND(I) = LBND(I)
60 CONTINUE
*
DO 80 I = 1, NPTS
  ICOL(I) = ICOLD(I)
80 CONTINUE
*
WRITE (NOUT,*) 'Base grid:'
WRITE (NOUT,*)
LENIWK = 122
IFAIL = -1
*
CALL D03RYF(NX,NY,NPTS,NROWS,NBND,NBPTS,LROW,IROW,ICOL,LLBND,
+          ILBND,LBND,IWK,LENIWK,PGRID,IFAIL)
*
IF (IFAIL.EQ.0) THEN
  WRITE (NOUT,*) ' '
  DO 100 J = 1, NY
    WRITE (NOUT,*) PGRID(J)
    WRITE (NOUT,*) ' '
100  CONTINUE
  WRITE (NOUT,*) ' '
END IF
*
RETURN
END
*
SUBROUTINE PDEIV1(NPTS,NPDE,T,X,Y,U)
*
  .. Parameters ..
  real                EPS
  PARAMETER           (EPS=1e-3)
*
  .. Scalar Arguments ..
  real                T
  INTEGER              NPDE, NPTS
*
  .. Array Arguments ..
  real                U(NPTS,NPDE), X(NPTS), Y(NPTS)
*
  .. Local Scalars ..
  real                A
  INTEGER              I
*
  .. Intrinsic Functions ..
  INTRINSIC           EXP
*
  .. Executable Statements ..
  DO 20 I = 1, NPTS
    A = (-4.0e0*X(I)+4.0e0*Y(I)-T)/(32.0e0*EPS)
    IF (A.LE.0.0e0) THEN
      U(I,1) = 0.75e0 - 0.25e0/(1.0e0+EXP(A))

```

```

        U(I,2) = 0.75e0 + 0.25e0/(1.0e0+EXP(A))
    ELSE
        U(I,1) = 0.75e0 - 0.25e0*EXP(-A)/(EXP(-A)+1.0e0)
        U(I,2) = 0.75e0 + 0.25e0*EXP(-A)/(EXP(-A)+1.0e0)
    END IF
20 CONTINUE
*
    RETURN
    END
*
SUBROUTINE PDEF1(NPTS,NPDE,T,X,Y,U,UT,UX,UY,UXX,UXY,UY,Y,RES)
*
.. Parameters ..
real                EPS
PARAMETER            (EPS=1e-3)
*
.. Scalar Arguments ..
real                T
INTEGER              NPDE, NPTS
*
.. Array Arguments ..
real                RES(NPTS,NPDE), U(NPTS,NPDE), UT(NPTS,NPDE),
+                    UX(NPTS,NPDE), UXX(NPTS,NPDE), UXY(NPTS,NPDE),
+                    UY(NPTS,NPDE), UYY(NPTS,NPDE), X(NPTS), Y(NPTS)
*
.. Local Scalars ..
INTEGER              I
*
.. Executable Statements ..
DO 20 I = 1, NPTS
    RES(I,1) = UT(I,1) - (-U(I,1)*UX(I,1)-U(I,2)*UY(I,1)
+                    +EPS*(UXX(I,1)+UY(I,1)))
    RES(I,2) = UT(I,2) - (-U(I,1)*UX(I,2)-U(I,2)*UY(I,2)
+                    +EPS*(UXX(I,2)+UY(I,2)))
20 CONTINUE

    RETURN
    END
SUBROUTINE BNDY1(NPTS,NPDE,T,X,Y,U,UT,UX,UY,NBND,NBPTS,LLBND,
+                ILBND,LBND,RES)
*
.. Parameters ..
real                EPS
PARAMETER            (EPS=1e-3)
*
.. Scalar Arguments ..
real                T
INTEGER              NBND, NBPTS, NPDE, NPTS
*
.. Array Arguments ..
real                RES(NPTS,NPDE), U(NPTS,NPDE), UT(NPTS,NPDE),
+                    UX(NPTS,NPDE), UY(NPTS,NPDE), X(NPTS), Y(NPTS)
INTEGER              ILBND(NBND), LBND(NBPTS), LLBND(NBND)
*
.. Local Scalars ..
real                A
INTEGER              I, K
*
.. Intrinsic Functions ..
INTRINSIC            EXP
*
.. Executable Statements ..
DO 20 K = LLBND(1), NBPTS
    I = LBND(K)
    A = (-4.0e0*X(I)+4.0e0*Y(I)-T)/(32.0e0*EPS)
    IF (A.LE.0.0e0) THEN
        RES(I,1) = U(I,1) - (0.75e0-0.25e0/(1.0e0+EXP(A)))
        RES(I,2) = U(I,2) - (0.75e0+0.25e0/(1.0e0+EXP(A)))
    ELSE

```

```

      RES(I,1) = U(I,1) - (0.75e0-0.25e0*EXP(-A)/(EXP(-A)+1.0e0))
      RES(I,2) = U(I,2) - (0.75e0+0.25e0*EXP(-A)/(EXP(-A)+1.0e0))
    END IF
20 CONTINUE
*
    RETURN
    END
*
    SUBROUTINE MONIT1(NPDE,T,DT,DTNEW,TLAST,NLEV,XMIN,YMIN,DXB,DYB,
+      LGRID,ISTRUC,LSOL,SOL,IERR)
*
    .. Parameters ..
    INTEGER          MAXPTS, NOUT
    PARAMETER        (MAXPTS=2500,NOUT=6)
*
    .. Scalar Arguments ..
    real             DT, DTNEW, DXB, DYB, T, XMIN, YMIN
    INTEGER           IERR, NLEV, NPDE
    LOGICAL           TLAST
*
    .. Array Arguments ..
    real             SOL(*)
    INTEGER           ISTRUC(*), LGRID(*), LSOL(NLEV)
*
    .. Scalars in Common ..
    INTEGER           IOUT
*
    .. Arrays in Common ..
    real             TWANT(2)
*
    .. Local Scalars ..
    INTEGER           IFAIL, IPSOL, IPT, LEVEL, NPTS
*
    .. Local Arrays ..
    real             UEX(105,2), X(MAXPTS), Y(MAXPTS)
*
    .. External Subroutines ..
    EXTERNAL          D03RZF, PDEIV1
*
    .. Common blocks ..
    COMMON            /OTIME1/TWANT, IOUT
*
    .. Save statement ..
    SAVE              /OTIME1/
*
    .. Executable Statements ..
*
    IFAIL = -1
    IF (TLAST) THEN
      DO 40 LEVEL = 1, NLEV
        IPSOL = LSOL(LEVEL)
*
*       Get grid information
*
        CALL D03RZF(LEVEL,NLEV,XMIN,YMIN,DXB,DYB,LGRID,ISTRUC,NPTS,
+          X,Y,MAXPTS,IFAIL)
        IF (IFAIL.NE.0) THEN
          IERR = 1
          RETURN
        END IF
*
        IF (IOUT.EQ.2 .AND. LEVEL.EQ.1) THEN
*
*       Get exact solution
*
          CALL PDEIV1(NPTS,NPDE,T,X,Y,UEX)
          WRITE (NOUT,*)
          WRITE (NOUT,
+('' Solution at every 2nd grid point '', ''in level 1 at time '',

```



```

+ F8.4,':')) T
      WRITE (NOUT,*)
      WRITE (NOUT,
+ '(7X,':x',10X,':y',8X,':approx u',5X,':exact u',4X,
+ ':approx v',4X,':exact v'))
      WRITE (NOUT,*)
      IPSOL = LSOL(LEVEL)
      DO 20 IPT = 1, NPTS, 2
        WRITE (NOUT,'(6(1X,D11.4))') X(IPT), Y(IPT),
+      SOL(IPSOL+IPT), UEX(IPT,1), SOL(IPSOL+NPTS+IPT),
+      UEX(IPT,2)
20      CONTINUE
      WRITE (NOUT,*)
      END IF
*
40      CONTINUE
      END IF
*
      RETURN
      END

```

9.1.2 Program Data

None.

9.1.3 Program Results

D03RBF Example Program Results

Example 1

Base grid:

```

23  3  3  3  3  3  3  3 34 XX XX
2  .. .. .. .. .. 4 XX XX
2  .. 14  1  1  1  1  1 41 XX XX
2  ..  4 23  3  3  3  3  3 34
2  ..  4  2 .. .. .. .. 4
2  ..  4  2 .. 14  1  1 21 .. 4
2  ..  4  2 ..  4 XX XX  2 .. 4
2  ..  4  2 .. 43  3  3 32 .. 4
2  ..  4  2 .. .. .. .. 4
2  ..  4 12  1  1  1  1  1 41
12  1 41 XX XX XX XX XX XX XX

```

Statistics:

Time = 0.2500
 Total number of accepted timesteps = 14
 Total number of rejected timesteps = 0

	T o t a l n u m b e r o f			
	Residual	Jacobian	Newton	Lin sys
	evals	evals	iters	iters
At level				
1	196	14	28	14
2	196	14	28	22
3	196	14	28	25
4	196	14	28	31
5	141	10	21	29

	M a x i m u m n u m b e r o f	
	Newton iters	Lin sys iters
At level		
1	2	1
2	2	1
3	2	1
4	2	2
5	3	2

Solution at every 2nd grid point in level 1 at time 1.0000:

x	y	approx u	exact u	approx v	exact v
0.0000E+00	0.0000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.2000E+00	0.0000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.1000E+00	0.1000E+00	0.5002E+00	0.5000E+00	0.9998E+00	0.1000E+01
0.3000E+00	0.1000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.5000E+00	0.1000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.7000E+00	0.1000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.9000E+00	0.1000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.0000E+00	0.2000E+00	0.5005E+00	0.5005E+00	0.9995E+00	0.9995E+00
0.2000E+00	0.2000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.4000E+00	0.2000E+00	0.5001E+00	0.5000E+00	0.9999E+00	0.1000E+01
0.6000E+00	0.2000E+00	0.4999E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.8000E+00	0.2000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.1000E+01	0.2000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.1000E+00	0.3000E+00	0.5000E+00	0.5005E+00	0.1000E+01	0.9995E+00
0.3000E+00	0.3000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.5000E+00	0.3000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.7000E+00	0.3000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.9000E+00	0.3000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.0000E+00	0.4000E+00	0.7500E+00	0.7500E+00	0.7500E+00	0.7500E+00
0.2000E+00	0.4000E+00	0.5005E+00	0.5005E+00	0.9995E+00	0.9995E+00
0.4000E+00	0.4000E+00	0.5002E+00	0.5000E+00	0.9998E+00	0.1000E+01
0.8000E+00	0.4000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.1000E+01	0.4000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.1000E+00	0.5000E+00	0.7500E+00	0.7500E+00	0.7500E+00	0.7500E+00
0.3000E+00	0.5000E+00	0.5005E+00	0.5005E+00	0.9995E+00	0.9995E+00
0.5000E+00	0.5000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.7000E+00	0.5000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.9000E+00	0.5000E+00	0.5001E+00	0.5000E+00	0.9999E+00	0.1000E+01
0.0000E+00	0.6000E+00	0.7500E+00	0.7500E+00	0.7500E+00	0.7500E+00

```

0.2000E+00  0.6000E+00  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.4000E+00  0.6000E+00  0.5000E+00  0.5005E+00  0.1000E+01  0.9995E+00
0.6000E+00  0.6000E+00  0.4999E+00  0.5000E+00  0.1000E+01  0.1000E+01
0.8000E+00  0.6000E+00  0.4998E+00  0.5000E+00  0.1000E+01  0.1000E+01
0.1000E+01  0.6000E+00  0.5000E+00  0.5000E+00  0.1000E+01  0.1000E+01
0.1000E+00  0.7000E+00  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.3000E+00  0.7000E+00  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.5000E+00  0.7000E+00  0.5005E+00  0.5005E+00  0.9995E+00  0.9995E+00
0.7000E+00  0.7000E+00  0.5000E+00  0.5000E+00  0.1000E+01  0.1000E+01
0.9000E+00  0.7000E+00  0.5000E+00  0.5000E+00  0.1000E+01  0.1000E+01
0.0000E+00  0.8000E+00  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.2000E+00  0.8000E+00  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.4000E+00  0.8000E+00  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.6000E+00  0.8000E+00  0.5005E+00  0.5005E+00  0.9995E+00  0.9995E+00
0.8000E+00  0.8000E+00  0.5000E+00  0.5000E+00  0.1000E+01  0.1000E+01
0.1000E+00  0.9000E+00  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.3000E+00  0.9000E+00  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.5000E+00  0.9000E+00  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.7000E+00  0.9000E+00  0.4999E+00  0.5005E+00  0.1000E+01  0.9995E+00
0.0000E+00  0.1000E+01  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.2000E+00  0.1000E+01  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.4000E+00  0.1000E+01  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.6000E+00  0.1000E+01  0.7500E+00  0.7500E+00  0.7500E+00  0.7500E+00
0.8000E+00  0.1000E+01  0.5005E+00  0.5005E+00  0.9995E+00  0.9995E+00

```

Statistics:

Time = 1.0000

Total number of accepted timesteps = 45

Total number of rejected timesteps = 0

At level	T o t a l n u m b e r o f			
	Residual evals	Jacobian evals	Newton iters	Lin sys iters
1	630	45	90	45
2	630	45	90	78
3	630	45	90	87
4	630	45	90	124
5	575	41	83	122

At level	M a x i m u m n u m b e r o f	
	Newton iters	Lin sys iters
1	2	1
2	2	1
3	2	1
4	2	2
5	3	2

9.2 Example 2

This example comes from [1] and concerns brine transport in porous media. It involves an isothermal groundwater flow model consisting of an equation for the continuity for the fluid and a salt transport equation:

$$n\rho\gamma\frac{\partial w}{\partial t} + \nabla \cdot (\rho \underline{q}) = 0,$$

$$n\rho\frac{\partial w}{\partial t} + \rho \underline{q} \cdot \nabla w + \nabla \cdot (\rho \underline{J}^w) = 0,$$

where w is the salt mass fraction; n is the porosity parameter; γ is a salt coefficient; ρ is the density satisfying $\rho = \rho_0 \exp(\gamma w)$ where ρ_0 is the reference viscosity of fresh water; and \underline{q} is the fluid velocity given by

$$\underline{q} = -\frac{k}{\mu}(\nabla p - \rho \underline{g}),$$

where k is the permeability coefficient of the porous medium; p is the pressure; $\underline{g} = (0, -g)$ is the acceleration due to gravity; and μ is the viscosity given by

$$\mu = \mu_0 m(w), \quad m(w) = 1 + 1.85w - 4w^2,$$

where μ_0 is a reference viscosity. \underline{J}^w is the salt-dispersion flux vector given by

$$\underline{J}^w = -nD\nabla w,$$

where D is the dispersion tensor for the solute defined as

$$nD = (nD_{\text{mol}} + \alpha_T |\underline{q}|)I + \frac{(\alpha_L - \alpha_T)}{|\underline{q}|} \underline{q} \underline{q}^T, \quad |\underline{q}| = \sqrt{\underline{q}^T \underline{q}}.$$

The coefficients D_{mol} , α_T , α_L are the molecular diffusion and the transversal and longitudinal dispersion respectively.

The dependent variables are p and w , and the values for the constants are

$$\begin{array}{llll} n = 0.2, & D_{\text{mol}} = 0.0, & \rho_0 = 1000, & \mu_0 = 10^{-3}, \\ k = 10^{-10}, & \alpha_T = 0.002, & p_0 = 10^5, & w_0 = 0.25, \\ g = 9.81, & \alpha_L = 0.01, & \gamma = \ln(1.2), & q_c = 10^{-4}. \end{array}$$

This particular example is a simulation of a laboratory experiment looking at the displacement of fresh water by brine in a vertical column filled with porous media. The problem can be considered two-dimensional since the column is thin in one of its dimensions. High concentration brine is injected through a gate at the bottom of the column giving rise to a fresh-salt water front moving in all directions. There is a region of total impermeability in part of the column, and so the solution domain is non-rectangular, as shown in Figure 4. The inlet gate is situated between $(0.025, 0)$ and $(0.05, 0)$.

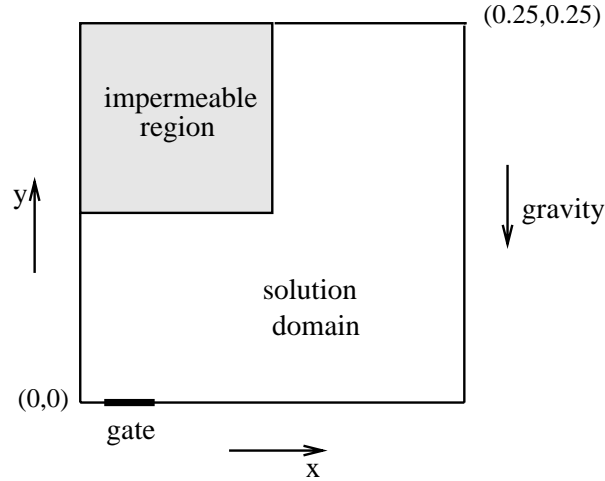


Figure 4

The initial values are

$$p(x, y, 0) = p_0 + (0.25 - y)\rho_0 g, \quad w(x, y, 0) = 0,$$

and the boundary conditions are

$$x = 0, 0 \leq y \leq 0.125 : p_x = 0, w_x = 0,$$

$$x = 0.25, 0 \leq y \leq 0.25 : p_x = 0, w_x = 0,$$

$$x = 0.125, 0.125 \leq y \leq 0.25 : p_x = 0, w_x = 0.$$

$$y = 0, 0 < x < 0.025 \text{ and } 0.05 < x < 0.25 : -\frac{k}{\mu}(p_y + \rho g) = 0, w_y = 0,$$

$$y = 0, 0.025 \leq x \leq 0.05 : -\frac{k}{\mu}(p_y + \rho g) = q_c, w = w_0,$$

$$y = 0.125, 0 < x < 0.125 : -\frac{k}{\mu}(p_y + \rho g) = 0, w_y = 0,$$

$$y = 0.25, 0.125 < x < 0.25 : p = p_0, w_y = 0,$$

Note that eventually the solution will reach steady state, with the whole of the domain being filled with brine to a constant concentration, but in the example program shown the solution process is terminated at an earlier stage.

9.2.1 Program Text

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.

```

*
SUBROUTINE EX2
*
  .. Parameters ..
  INTEGER          NOUT
  PARAMETER        (NOUT=6)
  INTEGER          MXLEV, NPDE, NPTS
  PARAMETER        (MXLEV=4, NPDE=2, NPTS=2000)
  INTEGER          LENIWK, LENRWK, LENLWK
  PARAMETER        (LENIWK=NPTS*(5*MXLEV+14)+2+7*MXLEV,
+                  LENRWK=NPTS*NPDE*(5*MXLEV+9+18*NPDE)+2*NPTS,
+                  LENLWK=2*NPTS)
*
  .. Scalars in Common ..
  INTEGER          IOUT
*
  .. Arrays in Common ..
  real             TWANT(2)

```

```

*      .. Local Scalars ..
      real          TOLS, TOLT, TOUT, TS
      INTEGER       I, IFAIL, IND, ITRACE, J, MAXLEV
*      .. Local Arrays ..
      real          DT(3), OPTR(3, NPDE), RWK(LENRWK)
      INTEGER       IWK(LENIWK), OPTI(4)
      LOGICAL       LWK(LENLWK)
*      .. External Subroutines ..
      EXTERNAL      BNDRY2, D03RBF, INIDM2, MONIT2, PDEF2, PDEIV2
*      .. Common blocks ..
      COMMON        /OTIME2/TWANT, IOUT
*      .. Save statement ..
      SAVE          /OTIME2/
*      .. Executable Statements ..
      WRITE (NOUT,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Example 2'
      WRITE (NOUT,*)

*
      IND = 0
      ITRACE = -1
      TS = 0.0e0
      TWANT(1) = 150.0e0
      TWANT(2) = 750.0e0
      DT(1) = 0.01e0
      DT(2) = 1.0e-3
      DT(3) = 5.0e4
      TOLS = 0.1e0
      TOLT = 0.1e0
      OPTI(1) = 4
      MAXLEV = OPTI(1)
      DO 20 I = 2, 4
         OPTI(I) = 0
20  CONTINUE
      OPTR(1,1) = 1.1e5
      OPTR(1,2) = 0.25e0
      DO 60 J = 1, NPDE
         DO 40 I = 2, 3
            OPTR(I,J) = 1.0e0
40  CONTINUE
60  CONTINUE

*
      DO 120 IOUT = 1, 2
         IFAIL = -1
         TOUT = TWANT(IOUT)
         CALL D03RBF(NPDE, TS, TOUT, DT, TOLS, TOLT, INIDM2, PDEF2, BNDRY2,
+              PDEIV2, MONIT2, OPTI, OPTR, RWK, LENRWK, IWK, LENIWK, LWK,
+              LENLWK, ITRACE, IND, IFAIL)

*
*      Print statistics
*
      MAXLEV = OPTI(1)
      WRITE (NOUT, '(Statistics:'))
      WRITE (NOUT, '(Time = ', F8.4)') TS
      WRITE (NOUT, '(Total number of accepted timesteps = ', I5)')
+      IWK(1)
      WRITE (NOUT, '(Total number of rejected timesteps = ', I5)')
+      IWK(2)

```

```

        WRITE (NOUT,*)
        WRITE (NOUT,
+          '( ' ' '          T o t a l   n u m b e r   o f   ' ' ' '))
        WRITE (NOUT,
+          '( ' ' '          R e s i d u a l   J a c o b i a n   N e w t o n   ' '   ,   ' '   L i n   s y s ' ' ' '))
+          )
        WRITE (NOUT,
+          '( ' ' '          e v a l s          e v a l s          i t e r s   ' '   ,   ' '   i t e r s ' ' ' '))
+          )
        WRITE (NOUT,'( ' ' ' At level ' ' ' '))
        MAXLEV = OPTI(1)
        DO 80 J = 1, MAXLEV
            IF (IWK(J+2).NE.0) WRITE (NOUT,'(I6,4I10)') J, IWK(J+2),
+              IWK(J+2+MAXLEV), IWK(J+2+2*MAXLEV), IWK(J+2+3*MAXLEV)
*
80      CONTINUE
        WRITE (NOUT,*)
        WRITE (NOUT,
+          '( ' ' '          M a x i m u m   n u m b e r   ' ' ,   ' '   o f ' ' ' '))
        WRITE (NOUT,
+          '( ' ' '          N e w t o n   i t e r s          L i n   s y s   i t e r s   ' ' ' '))
        WRITE (NOUT,'( ' ' ' At level ' ' ' '))
        DO 100 J = 1, MAXLEV
            IF (IWK(J+2).NE.0) WRITE (NOUT,'(I6,2I14)') J,
+              IWK(J+2+4*MAXLEV), IWK(J+2+5*MAXLEV)
100     CONTINUE
        WRITE (NOUT,*)
*
120 CONTINUE
*
        RETURN
        END
*
        SUBROUTINE INIDM2(MAXPTS,XMIN,XMAX,YMIN,YMAX,NX,NY,NPTS,NROWS,
+          NBND,NBPTS,LROW,IROW,ICOL,LLBND,ILBND,LBND,
+          IERR)
*
        .. Parameters ..
        INTEGER          NOUT
        PARAMETER        (NOUT=6)
*
        .. Scalar Arguments ..
        real            XMAX, XMIN, YMAX, YMIN
        INTEGER          IERR, MAXPTS, NBND, NBPTS, NPTS, NROWS, NX, NY
*
        .. Array Arguments ..
        INTEGER          ICOL(*), ILBND(*), IROW(*), LBND(*), LLBND(*),
+          LROW(*)
*
        .. Local Scalars ..
        INTEGER          I, IFAIL, IPT, J, LENIWK, NX1, NY1
*
        .. Local Arrays ..
        INTEGER          IWK(122)
        CHARACTER*33      PGRID(11)
*
        .. External Subroutines ..
        EXTERNAL          D03RYF
*
        .. Executable Statements ..
*
        NX = 11
        NY = 11
*
        Check MAXPTS against rough estimate of NPTS

```

```

*
  NPTS = NX*NY
  IF (MAXPTS.LT.NPTS) THEN
    IERR = -1
    RETURN
  END IF
  NROWS = NY
*
  XMIN = 0.0e0
  YMIN = 0.0e0
  XMAX = 0.25e0
  YMAX = 0.25e0
*
  NX1 = (NX-1)/2
  NY1 = (NY-1)/2
*
  * Make grid structure for general NX, NY
  *
  IPT = 1
  DO 40 J = 1, NY1 + 1
    LROW(J) = IPT
    IROW(J) = J - 1
    DO 20 I = 1, NX
      ICOL(IPT) = I - 1
      IPT = IPT + 1
    20 CONTINUE
  40 CONTINUE
  DO 80 J = NY1 + 2, NY
    LROW(J) = IPT
    IROW(J) = J - 1
    DO 60 I = NX1 + 1, NX
      ICOL(IPT) = I - 1
      IPT = IPT + 1
    60 CONTINUE
  80 CONTINUE
*
  NPTS = IPT - 1
*
  * Boundaries
  *
  NBND = 12
*
  ILBND(1) = 1
  ILBND(2) = 2
  ILBND(3) = 3
  ILBND(4) = 2
  ILBND(5) = 3
  ILBND(6) = 4
  ILBND(7) = 12
  ILBND(8) = 23
  ILBND(9) = 32
  ILBND(10) = 23
  ILBND(11) = 34
  ILBND(12) = 41
*
  LLBND(1) = 1
  LLBND(2) = LLBND(1) + NX - 2
  LLBND(3) = LLBND(2) + NY1 - 1

```



```

      LLBND(4) = LLBND(3) + NX1 - 1
      LLBND(5) = LLBND(4) + NY1 - 1
      LLBND(6) = LLBND(5) + NX1 - 1
      LLBND(7) = LLBND(6) + NY - 2
      LLBND(8) = LLBND(7) + 1
      LLBND(9) = LLBND(8) + 1
      LLBND(10) = LLBND(9) + 1
      LLBND(11) = LLBND(10) + 1
      LLBND(12) = LLBND(11) + 1
*
      NBPTS = LLBND(12)
*
*      Lower boundary
*
      DO 100 I = 1, NX - 2
        LBND(LLBND(1)+I-1) = I + 1
100 CONTINUE
*
*      Upper boundaries
*
      DO 120 I = 1, NX1 - 1
        LBND(LLBND(3)+I-1) = NY1*NX + 1 + I
120 CONTINUE
      DO 140 I = 1, NX1 - 1
        LBND(LLBND(5)+I-1) = NPTS - I
140 CONTINUE
*
*      Left boundaries
*
      DO 160 J = 1, NY1 - 1
        LBND(LLBND(2)+J-1) = J*NX + 1
160 CONTINUE
      DO 180 J = 1, NY1 - 1
        LBND(LLBND(4)+J-1) = (NY1+1)*NX + (J-1)*(NX1+1) + 1
180 CONTINUE
*
*      Right boundary
*
      DO 200 J = 1, NY1
        LBND(LLBND(6)+J-1) = (J+1)*NX
200 CONTINUE
      I = LLBND(6) + NY1 - 1
      DO 220 J = 1, NY1 - 1
        LBND(I+J) = LBND(I) + J*(NX1+1)
220 CONTINUE
*
*      Corners
*
      LBND(LLBND(7)) = 1
      LBND(LLBND(8)) = NY1*NX + 1
      LBND(LLBND(9)) = LBND(LLBND(8)) + NX1
      LBND(LLBND(10)) = LBND(LLBND(5)) - NX1 + 1
      LBND(LLBND(11)) = LBND(LLBND(5)) + 1
      LBND(LLBND(12)) = NX
*
      WRITE (NOUT,*) 'Base grid:'
      WRITE (NOUT,*)
      LENIWK = 122

```

```

      IFAIL = -1
*
      CALL D03RYF(NX,NY,NPTS,NROWS,NBND,NBPTS,LROW,IROW,ICOL,LLBND,
+               ILBND,LBND,IWK,LENIWK,PGRID,IFAIL)
*
      IF (IFAIL.EQ.0) THEN
        WRITE (NOUT,*) ' '
        DO 240 J = 1, NY
          WRITE (NOUT,*) PGRID(J)
          WRITE (NOUT,*) ' '
240      CONTINUE
        WRITE (NOUT,*) ' '
      END IF
*
      RETURN
      END
*
      SUBROUTINE PDEIV2(NPTS,NPDE,T,X,Y,U)
*
      .. Scalar Arguments ..
      real          T
      INTEGER       NPDE, NPTS
*
      .. Array Arguments ..
      real          U(NPTS,NPDE), X(NPTS), Y(NPTS)
*
      .. Scalars in Common ..
      real          AL, AT, DM, G, GAMMA, KAPPA, MUO, N, PO, QC,
+               RHOO, WO
*
      .. Local Scalars ..
      INTEGER       I
*
      .. Intrinsic Functions ..
      INTRINSIC     LOG
*
      .. Common blocks ..
      COMMON        /PARAMS/N, KAPPA, GAMMA, MUO, RHOO, PO, WO, G,
+               DM, AL, AT, QC
*
      .. Save statement ..
      SAVE          /PARAMS/
*
      .. Executable Statements ..
      N = 0.2e0
      KAPPA = 1.0e-10
      G = 9.81e0
      DM = 0.0e0
      AT = 0.002e0
      AL = 0.01e0
      RHOO = 1.0e+3
      PO = 1.0e+5
      GAMMA = LOG(1.2e0)
      MUO = 1.0e-3
      WO = 0.25e0
      QC = 1.0e-4
*
      DO 20 I = 1, NPTS
        U(I,1) = PO + (0.25e0-Y(I))*RHOO*G
        U(I,2) = 0.0e0
20    CONTINUE
*
      RETURN
      END
*
      SUBROUTINE PDEF2(NPTS,NPDE,T,X,Y,U,UT,UX,UY,UXX,UXY,UY,Y,RES)

```

```

*    .. Scalar Arguments ..
      real                T
      INTEGER             NPDE, NPTS
*    .. Array Arguments ..
      real                RES(NPTS,NPDE), U(NPTS,NPDE), UT(NPTS,NPDE),
+                        UX(NPTS,NPDE), UXX(NPTS,NPDE), UXY(NPTS,NPDE),
+                        UY(NPTS,NPDE), UYY(NPTS,NPDE), X(NPTS), Y(NPTS)
*    .. Scalars in Common ..
      real                AL, AT, DM, G, GAMMA, KAPPA, MU0, N, PO, QC,
+                        RH00, WO
*    .. Local Scalars ..
      real                JW1, JW1X, JW2, JW2Y, KAPMU, KAPMU2, KAPMUX,
+                        KAPMUY, MU, MUX, MUY, ND11, ND11Q1, ND11Q2,
+                        ND11X, ND12, ND12Q1, ND12Q2, ND12X, ND12Y, ND22,
+                        ND22Q1, ND22Q2, ND22Y, PX, PXX, PXY, PY, PYY, Q1,
+                        Q1L, Q1X, Q1Y, Q2, Q2L, Q2X, Q2Y, QL, RHO, RHOX,
+                        RHOY, W, WT, WX, WXX, WXY, WY, WYY
      INTEGER             I
*    .. Intrinsic Functions ..
      INTRINSIC           EXP, SQRT
*    .. Common blocks ..
      COMMON              /PARAMS/N, KAPPA, GAMMA, MU0, RH00, PO, WO, G,
+                        DM, AL, AT, QC
*    .. Save statement ..
      SAVE                /PARAMS/
*    .. Executable Statements ..
      DO 20 I = 1, NPTS
        PX = UX(I,1)
        PY = UY(I,1)
        W = U(I,2)
        WT = UT(I,2)
        WX = UX(I,2)
        WY = UY(I,2)
        RHO = RH00*EXP(GAMMA*W)
        RHOX = RHO*(GAMMA*WX)
        RHOY = RHO*(GAMMA*WY)
        MU = MU0*(1+1.85e0*W-4.0e0*W*W)
        MUX = MU0*(1.85e0*WX-8.0e0*W*WX)
        MUY = MU0*(1.85e0*WY-8.0e0*W*WY)
        KAPMU = KAPPA/MU
        KAPMU2 = -KAPMU/MU
        KAPMUX = KAPMU2*MUX
        KAPMUY = KAPMU2*MUY
        Q1 = -KAPMU*PX
        Q2 = -KAPMU*(PY+RHO*G)
        QL = SQRT(Q1*Q1+Q2*Q2)
        IF (QL.EQ.0.0e0) THEN
          Q1L = 0.0e0
          Q2L = 0.0e0
        ELSE
          Q1L = Q1/QL
          Q2L = Q2/QL
        END IF
        ND11 = N*DM + AT*QL + (AL-AT)*Q1*Q1L
        ND12 = (AL-AT)*Q1*Q2L
        ND22 = N*DM + AT*QL + (AL-AT)*Q2*Q2L
        PXX = UXX(I,1)
        PXY = UXY(I,1)

```

```

      PYY = UYY(I,1)
      WXX = UXX(I,2)
      WXY = UXY(I,2)
      WYY = UYY(I,2)
      ND11Q1 = (AT+(AL-AT)*(2-Q1L**2))*Q1L
      ND11Q2 = (AT-(AL-AT)*(Q1L**2))*Q2L
      ND12Q1 = (AL-AT)*Q2L**3
      ND12Q2 = (AL-AT)*Q1L**3
      ND22Q1 = (AT-(AL-AT)*(Q2L**2))*Q1L
      ND22Q2 = (AT+(AL-AT)*(2-Q2L**2))*Q2L
      Q1X = -(KAPMUX*PX+KAPMU*PXX)
      Q1Y = -(KAPMUY*PX+KAPMU*PXY)
      Q2X = -(KAPMUX*(PY+RHO*G)+KAPMU*(PXY+RHOX*G))
      Q2Y = -(KAPMUY*(PY+RHO*G)+KAPMU*(PYY+RHOY*G))
      ND11X = ND11Q1*Q1X + ND11Q2*Q2X
      ND12X = ND12Q1*Q1X + ND12Q2*Q2X
      ND12Y = ND12Q1*Q1Y + ND12Q2*Q2Y
      ND22Y = ND22Q1*Q1Y + ND22Q2*Q2Y
      JW1 = -(ND11*WX+ND12*WY)
      JW2 = -(ND12*WX+ND22*WY)
      JW1X = -(ND11X*WX+ND11*WXX+ND12X*WY+ND12*WXY)
      JW2Y = -(ND12Y*WX+ND12*WXY+ND22Y*WY+ND22*WYY)
*
      RES(I,1) = N*RHO*GAMMA*WT + RHOX*Q1 + RHO*Q1X + RHOY*Q2 +
+      RHO*Q2Y
      RES(I,2) = N*RHO*WT + RHO*Q1*WX + RHO*Q2*WY + RHOX*JW1 +
+      RHO*JW1X + RHOY*JW2 + RHO*JW2Y
20 CONTINUE
*
      RETURN
      END
*
      SUBROUTINE BNDRY2(NPTS,NPDE,T,X,Y,U,UT,UX,UY,NBND,NBPTS,LLBND,
+      ILBND,LBND,RES)
*      .. Scalar Arguments ..
      real          T
      INTEGER       NBND, NBPTS, NPDE, NPTS
*      .. Array Arguments ..
      real          RES(NPTS,NPDE), U(NPTS,NPDE), UT(NPTS,NPDE),
+      UX(NPTS,NPDE), UY(NPTS,NPDE), X(NPTS), Y(NPTS)
      INTEGER       ILBND(NBND), LBND(NBPTS), LLBND(NBND)
*      .. Scalars in Common ..
      real          AL, AT, DM, G, GAMMA, KAPPA, MUO, N, PO, QC,
+      RHOO, WO
*      .. Local Scalars ..
      real          KAPMU, MU, PY, Q2, RHO, W
      INTEGER       I, J, K
*      .. Intrinsic Functions ..
      INTRINSIC     EXP
*      .. Common blocks ..
      COMMON        /PARAMS/N, KAPPA, GAMMA, MUO, RHOO, PO, WO, G,
+      DM, AL, AT, QC
*      .. Save statement ..
      SAVE          /PARAMS/
*      .. Executable Statements ..
      J = 1
*
*      y = 0.0 boundary

```

```

*
DO 20 K = LLBND(J), LLBND(J+1) - 1
  I = LBND(K)
  IF ((0.LT.X(I) .AND. X(I).LT.0.025e0) .OR. (0.075e0.LT.X(I)
+    .AND. X(I).LT.0.25e0)) THEN
    PY = UY(I,1)
    W = U(I,2)
    RHO = RH00*EXP(GAMMA*W)
    MU = MU0*(1+1.85e0*W-4.0e0*W*W)
    KAPMU = KAPPA/MU
    Q2 = -KAPMU*(PY+RHO*G)
    RES(I,1) = Q2
    RES(I,2) = UY(I,2)
  ELSE
    PY = UY(I,1)
    W = U(I,2)
    RHO = RH00*EXP(GAMMA*W)
    MU = MU0*(1+1.85e0*W-4.0e0*W*W)
    KAPMU = KAPPA/MU
    Q2 = -KAPMU*(PY+RHO*G)
*
    RES(I,1) = Q2 - QC
    RES(I,2) = W - W0
  END IF
20 CONTINUE
*
J = 5
*
* y = 0.25 boundary
*
DO 40 K = LLBND(J), LLBND(J+1) - 1
  I = LBND(K)
  RES(I,1) = U(I,1) - P0
  RES(I,2) = UY(I,2)
40 CONTINUE
*
DO 80 J = 2, 6, 2
*
* x = 0.0, 0.125, 0.25 boundaries
*
DO 60 K = LLBND(J), LLBND(J+1) - 1
  I = LBND(K)
  RES(I,1) = UX(I,1)
  RES(I,2) = UX(I,2)
60 CONTINUE
80 CONTINUE
*
J = 3
*
* y = 0.125 boundary
*
DO 100 K = LLBND(J), LLBND(J+1) - 1
  I = LBND(K)
  PY = UY(I,1)
  W = U(I,2)
  RHO = RH00*EXP(GAMMA*W)
  RES(I,1) = UY(I,1) + RHO*G
  RES(I,2) = UY(I,2)

```

```

100 CONTINUE
*
      DO 140 J = 7, 11
*
*         Corners: dp/dx = dw/dx = 0
*
          DO 120 K = LLBND(J), LLBND(J+1) - 1
            I = LBND(K)
            RES(I,1) = UX(I,1)
            RES(I,2) = UX(I,2)
120      CONTINUE
140 CONTINUE
*
      DO 160 K = LLBND(12), NBPTS
        I = LBND(K)
        RES(I,1) = UX(I,1)
        RES(I,2) = UX(I,2)
160 CONTINUE
*
      RETURN
      END
*
      SUBROUTINE MONIT2(NPDE,T,DT,DTNEW,TLAST,NLEV,XMIN,YMIN,DXB,DYB,
+      LGRID,ISTRUC,LSOL,SOL,IERR)
*
      .. Parameters ..
      INTEGER          MAXPTS, NOUT
      PARAMETER        (MAXPTS=2000,NOUT=6)
*
      .. Scalar Arguments ..
      real            DT, DTNEW, DXB, DYB, T, XMIN, YMIN
      INTEGER          IERR, NLEV, NPDE
      LOGICAL          TLAST
*
      .. Array Arguments ..
      real            SOL(*)
      INTEGER          ISTRUC(*), LGRID(*), LSOL(NLEV)
*
      .. Scalars in Common ..
      INTEGER          IOUT
*
      .. Arrays in Common ..
      real            TWANT(2)
*
      .. Local Scalars ..
      INTEGER          IFAIL, IPSOL, IPT, LEVEL, NPTS
*
      .. Local Arrays ..
      real            X(MAXPTS), Y(MAXPTS)
*
      .. External Subroutines ..
      EXTERNAL          D03RZF
*
      .. Common blocks ..
      COMMON            /OTIME2/TWANT, IOUT
*
      .. Save statement ..
      SAVE              /OTIME2/
*
      .. Executable Statements ..
*
      IFAIL = -1
      IF (TLAST) THEN
        DO 40 LEVEL = 1, NLEV
          IPSOL = LSOL(LEVEL)
*
*         Get grid information
*
          CALL D03RZF(LEVEL,NLEV,XMIN,YMIN,DXB,DYB,LGRID,ISTRUC,NPTS,

```

```

+           X,Y,MAXPTS,IFAIL)
      IF (IFAIL.NE.0) THEN
        IERR = 1
        RETURN
      END IF
*
      IF (IOUT.EQ.2 .AND. LEVEL.EQ.1) THEN
        WRITE (NOUT,*)
        WRITE (NOUT,
+('' Solution at every 2nd grid point '', ''in level 1 at time '',
+ F8.4,'':'')) T
        WRITE (NOUT,*)
        WRITE (NOUT,'(7X,''x'',10X,''y'',8X,''approx w'')')
        WRITE (NOUT,*)
        IPSOL = LSOL(LEVEL)
        DO 20 IPT = 1, NPTS, 2
          WRITE (NOUT,'(3(1X,D11.4))') X(IPT), Y(IPT),
+           SOL(IPSOL+NPTS+IPT)
20      CONTINUE
        WRITE (NOUT,*)
      END IF
40    CONTINUE
      END IF
*
      RETURN
      END

```

9.2.2 Program Data

None.

9.2.3 Program Results

D03RBF Example Program Results

Example 2

Base grid:

```

XX XX XX XX XX 23  3  3  3  3 34
XX XX XX XX XX  2 .. .. .. .. 4
XX XX XX XX XX  2 .. .. .. .. 4
XX XX XX XX XX  2 .. .. .. .. 4
XX XX XX XX XX  2 .. .. .. .. 4
23  3  3  3  3 32 .. .. .. .. 4
 2 .. .. .. .. .. .. .. .. 4
 2 .. .. .. .. .. .. .. .. 4

```

```

2 .. .. . 4
2 .. .. . 4
12 1 1 1 1 1 1 1 1 1 41

```

Statistics:

```

Time = 150.0000
Total number of accepted timesteps = 111
Total number of rejected timesteps = 0

```

	T o t a l n u m b e r o f			
	Residual	Jacobian	Newton	Lin sys
	evals	evals	iters	iters
At level				
1	1554	111	222	492
2	1554	111	222	412
3	1555	111	223	484
4	1555	111	223	625

	M a x i m u m n u m b e r o f	
	Newton iters	Lin sys iters
At level		
1	2	7
2	2	7
3	3	6
4	3	9

Solution at every 2nd grid point in level 1 at time 750.0000:

x	y	approx w
0.0000E+00	0.0000E+00	0.2496E+00
0.5000E-01	0.0000E+00	0.2500E+00
0.1000E+00	0.0000E+00	0.2496E+00
0.1500E+00	0.0000E+00	0.2370E+00
0.2000E+00	0.0000E+00	0.1615E+00
0.2500E+00	0.0000E+00	0.1068E-01
0.2500E-01	0.2500E-01	0.2492E+00
0.7500E-01	0.2500E-01	0.2496E+00
0.1250E+00	0.2500E-01	0.2436E+00
0.1750E+00	0.2500E-01	0.1977E+00
0.2250E+00	0.2500E-01	0.6179E-01
0.0000E+00	0.5000E-01	0.2377E+00
0.5000E-01	0.5000E-01	0.2452E+00
0.1000E+00	0.5000E-01	0.2408E+00
0.1500E+00	0.5000E-01	0.2073E+00
0.2000E+00	0.5000E-01	0.1038E+00
0.2500E+00	0.5000E-01	0.2914E-02
0.2500E-01	0.7500E-01	0.2087E+00
0.7500E-01	0.7500E-01	0.2155E+00
0.1250E+00	0.7500E-01	0.1942E+00
0.1750E+00	0.7500E-01	0.1251E+00
0.2250E+00	0.7500E-01	0.1905E-01
0.0000E+00	0.1000E+00	0.1125E+00
0.5000E-01	0.1000E+00	0.1207E+00


```

0.1000E+00  0.1000E+00  0.1185E+00
0.1500E+00  0.1000E+00  0.1198E+00
0.2000E+00  0.1000E+00  0.4098E-01
0.2500E+00  0.1000E+00  0.5599E-03
0.2500E-01  0.1250E+00  0.1888E-01
0.7500E-01  0.1250E+00  0.2361E-01
0.1250E+00  0.1250E+00  0.5862E-01
0.1750E+00  0.1250E+00  0.5284E-01
0.2250E+00  0.1250E+00  0.3616E-02
0.1250E+00  0.1500E+00  0.4117E-01
0.1750E+00  0.1500E+00  0.2753E-01
0.2250E+00  0.1500E+00  0.1248E-02
0.1250E+00  0.1750E+00  0.2045E-01
0.1750E+00  0.1750E+00  0.1121E-01
0.2250E+00  0.1750E+00  0.3885E-03
0.1250E+00  0.2000E+00  0.8343E-02
0.1750E+00  0.2000E+00  0.3956E-02
0.2250E+00  0.2000E+00  0.1171E-03
0.1250E+00  0.2250E+00  0.3053E-02
0.1750E+00  0.2250E+00  0.1306E-02
0.2250E+00  0.2250E+00  0.4249E-04
0.1250E+00  0.2500E+00  0.1489E-02
0.1750E+00  0.2500E+00  0.6204E-03
0.2250E+00  0.2500E+00  0.1627E-04

```

Statistics:

Time = 750.0000

Total number of accepted timesteps = 164

Total number of rejected timesteps = 0

	T o t a l n u m b e r o f			
	Residual	Jacobian	Newton	Lin sys
	evals	evals	iters	iters
At level				
1	2296	164	328	854
2	2296	164	328	881
3	2297	164	329	970
4	1695	121	243	705

	M a x i m u m n u m b e r o f	
	Newton iters	Lin sys iters
At level		
1	2	7
2	2	11
3	3	9
4	3	9
