NAG Fortran Library Routine Document

D03RBF

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

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 (see Blom and Verwer (1993) and Blom *et al.* (1996)).

2 Specification

```
SUBROUTINE DO3RBF (NPDE, TS, TOUT, DT, TOLS, TOLT, INIDOM, PDEDEF,
                    BNDARY, PDEIV, MONITR, OPTI, OPTR, RWK, LENRWK, IWK,
1
                    LENIWK, LWK, LENLWK, ITRACE, IND, IFAIL)
2
                    NPDE, OPTI(4), LENRWK, IWK(LENIWK), LENIWK, LENLWK,
 INTEGER
1
                    ITRACE, IND, IFAIL
double precision
                    TS, TOUT, DT(3), TOLS, TOLT, OPTR(3,NPDE),
                    RWK(LENRWK)
1
 LOGICAL
                    LWK(LENLWK)
 EXTERNAL
                    INIDOM, PDEDEF, BNDARY, PDEIV, MONITR
```

3 Description

D03RBF integrates the system of PDEs:

$$F_{j}(t, x, y, u, u_{t}, u_{x}, u_{y}, u_{xx}, u_{xy}, u_{yy}) = 0, \quad j = 1, 2, \dots, \text{NPDE}, \quad (x, y) \in \Omega, \quad t_{0} \le t \le t_{\text{out}}, \quad (1)$$

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

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

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

The functions F_j must be supplied by you in a (sub)program 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 (sub)program 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 you in a (sub)program BNDARY in the form

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

The domain is covered by a uniform coarse base grid specified by you, 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.

[NP3657/21]

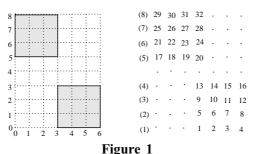
The system of PDEs and the boundary conditions are discretized in space on each grid using a standard second-order finite difference scheme (centred on the internal domain and one-sided at the boundaries), and the resulting system of ODEs is integrated in time using a second-order, two-step, implicit 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 $t = t_{out}$.

A modified Newton method is used to solve the nonlinear equations arising from the time integration. You 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 you in OPTI.

In order to define the base grid you 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 lefthand 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).



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 user-supplied (sub)program 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_v 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

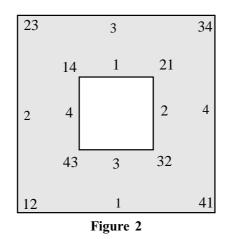
External corners (90°) :

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

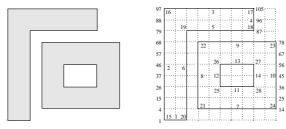
Internal corners (270°) :

- $21 {\rm lower-left \ corner}$
- 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).



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.





For this example we have

```
NROWS = 11
NPTS = 105
NBNDS = 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 the example in Section 9, and data statements are used to define the above arrays in that example program. For less complicated domains 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 you have specified in INIDOM.

Subgrids are stored internally using the same data structure, and solution information is communicated to you in the user-supplied (sub)programs 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_i 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 you extract the solution from these arrays, indeed the necessary information regarding these arrays is not provided. The user-supplied monitor (sub)program 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 parameter 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 Blom and Verwer (1993) and Blom *et al.* (1996) and the references therein.

4 **References**

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

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

Trompert R A (1993) Local uniform grid refinement and systems of coupled partial differential equations *Appl. Numer. Maths* **12** 331–355

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

5 **Parameters**

1:	NPDE –	INTEGER

On entry: the number of PDEs in the system.

Constraint: NPDE ≥ 1 .

2: TS – *double precision*

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 – *double precision*

On entry: the final value of t to which the integration is to be carried out.

4: DT(3) - double precision array

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 $DT(2) = 10.0 \times machine precision$ 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, DT(1) is unconstrained; $DT(1) \ge 0$ and $10.0 \times machine \ precision \times max(|TS|, |TOUT|) \le DT(1) \le TOUT - TS$ and $DT(2) \le DT(1) \le DT(3)$ otherwise.

Input/Output

Input

Input

Input/Output

Input

Input

External Procedure

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 $DT(i) \ge 0$, for i = 2, 3 and $DT(2) \le DT(3)$ for IND = 0 and IND = 1

5: TOLS – *double precision*

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 – *double precision*

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.

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 you have specified in INIDOM. D03RBF also checks the validity of the data, but you are 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, NROWS, NBNDS, NBPTS, LROW, IROW, ICOL, LLBND, 1 2 ILBND, LBND, IERR) INTEGER MAXPTS, NX, NY, NPTS, NROWS, NBNDS, NBPTS, LROW(*), IROW(*), ICOL(*), LLBND(*), ILBND(*), 1 2 LBND(*), IERR double precision XMIN, XMAX, YMIN, YMAX MAXPTS - INTEGER 1: Input On entry: the maximum number of base grid points allowed by the available workspace. Output 2: XMIN – *double precision* XMAX – double precision 3: Output On exit: the extents of the virtual grid in the x-direction, i.e., the x co-ordinates of the left and right boundaries respectively. YMIN – double precision Output 4: 5: YMAX – double precision Output On exit: the extents of the virtual grid in the y-direction, i.e., the y co-ordinates of the left and right boundaries respectively. NX - INTEGER Output 6: NY - INTEGER Output 7: On exit: the number of virtual grid points in the x- and y-direction respectively (including the boundary points).

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8:	NPTS – INTEGER Output
	On exit: 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.
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.
10:	NBNDS – INTEGER Output
	On exit: the total number of physical boundaries and corners in the base grid.
11:	NBPTS – INTEGER Output
	On exit: the total number of boundary points in the base grid.
12:	LROW(*) – INTEGER array Output
	Note: the dimension of the array LROW must be at least NROWS.
	On exit: LROW(i), for $i = 1, 2,$, NROWS, must contain the base grid index of the first grid point in base grid row <i>i</i> .
13:	IROW(*) – INTEGER array Output
	Note: the dimension of the array IROW must be at least NROWS.
	On exit: IROW(i), for $i = 1, 2,,$ NROWS, must contain the virtual row number v_y that corresponds to base grid row <i>i</i> .
14:	ICOL(*) – INTEGER array Output
	Note: the dimension of the array ICOL must be at least NPTS.
	On exit: ICOL(i), for $i = 1, 2,, NPTS$, must contain the virtual column number v_x that contains base grid point <i>i</i> .
15:	LLBND(*) – INTEGER array Output
	Note: the dimension of the array LLBND must be at least NBNDS.
	On exit: LLBND(i), for $i = 1, 2,,$ NBNDS, must contain the element of LBND corresponding to the start of the <i>i</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.
16:	ILBND(*) – INTEGER array Output
	Note: the dimension of the array ILBND must be at least NBNDS.
	On exit: ILBND(i), for $i = 1, 2,$, NBNDS, must contain the type of the <i>i</i> th boundary (or corner), as given in Section 3.
17:	LBND(*) – INTEGER array Output
	Note: the dimension of the array LBND must be at least NBPTS.
	On exit: LBND(i), for $i = 1, 2,, NBPTS$, must contain the grid index of the <i>i</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.

18: IERR – INTEGER

Input/Output

On entry: will be initialized by D03RBF to some value prior to internal calls to INIDOM.

On exit: 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 = 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 , for j = 1, 2, ..., 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 user-supplied (sub)program BNDARY. PDEDEF is called for each subgrid in turn.

Its specification is:

SUBROUTINE PDEDEF (NPTS, NPDE, T, X, Y, U, UT, UX, UY, UXX, UXY, 1 UYY, RES) NPTS, NPDE INTEGER double precision T, X(NPTS), Y(NPTS), U(NPTS, NPDE), UT(NPTS, NPDE), UX(NPTS,NPDE), UY(NPTS,NPDE), UXX(NPTS,NPDE), 1 UXY(NPTS,NPDE), UYY(NPTS,NPDE), RES(NPTS,NPDE) 2 NPTS - INTEGER 1: Input On entry: the number of grid points in the current grid. NPDE – INTEGER 2: Input On entry: the number of PDEs in the system. 3: T – double precision Input On entry: the current value of the independent variable t. 4: X(NPTS) - double precision array Input On entry: X(i) contains the x co-ordinate of the *i*th grid point, for i = 1, 2, ..., NPTS. Y(NPTS) – *double precision* array 5: Input On entry: Y(i) contains the y co-ordinate of the *i*th grid point, for i = 1, 2, ..., NPTS. U(NPTS,NPDE) – *double precision* array 6: Input On entry: U(i,j) contains the value of the *j*th PDE component at the *i*th grid point, for $i = 1, 2, \dots, \text{NPTS}; j = 1, 2, \dots, \text{NPDE}.$ UT(NPTS,NPDE) – *double precision* array 7: Input On entry: UT(*i*,*j*) contains the value of $\frac{\partial u}{\partial t}$ for the *j*th PDE component at the *i*th grid point, for i = 1, 2, ..., NPTS; j = 1, 2, ..., NPDE. 8: UX(NPTS,NPDE) – *double precision* array Input On entry: UX(i,j) contains the value of $\frac{\partial u}{\partial r}$ for the *j*th PDE component at the *i*th grid point, for i = 1, 2, ..., NPTS; j = 1, 2, ..., NPDE.

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9:	UY(NPTS,NPDE) – <i>double precision</i> array Inp	ut
	On entry: UY(<i>i</i> , <i>j</i>) contains the value of $\frac{\partial u}{\partial y}$ for the <i>j</i> th PDE component at the <i>i</i> th grid point, for $i = 1, 2,, NPTS$; $j = 1, 2,, NPDE$.	
10:	UXX(NPTS,NPDE) – <i>double precision</i> array Inp	ut
	On entry: UXX (i,j) contains the value of $\frac{\partial^2 u}{\partial x^2}$ for the <i>j</i> th PDE component at the <i>i</i> th graphing point, for $i = 1, 2,, NPTS$; $j = 1, 2,, NPDE$.	id
11:	UXY(NPTS,NPDE) – <i>double precision</i> array Inp	ut
	<i>On entry</i> : UXY (i,j) contains the value of $\frac{\partial^2 u}{\partial x \partial y}$ for the <i>j</i> th PDE component at the <i>i</i> th graphing point, for $i = 1, 2,, \text{NPTS}$; $j = 1, 2,, \text{NPDE}$.	id
12:	UYY(NPTS,NPDE) – <i>double precision</i> array Inp	ut
	On entry: UYY (i,j) contains the value of $\frac{\partial^2 u}{\partial y^2}$ for the <i>j</i> th PDE component at the <i>i</i> th graphing point, for $i = 1, 2,, \text{NPTS}$; $j = 1, 2,, \text{NPDE}$.	rid
13:	RES(NPTS,NPDE) – <i>double precision</i> array Outp	ut
	On exit: $\text{RES}(i,j)$ must contain the value of F_j for $j = 1, 2,, \text{NPDE}$, at the <i>i</i> th grid port for $i = 1, 2,, \text{NPTS}$, although the residuals at boundary points will be ignored (and overwritten later on) and so they need not be specified here.	nt

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 , for j = 1, 2, ..., 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 (sub)program.

Its specification is:

	SUBROUTINE BNDARY 1	(NPTS, NPDE, T, X, Y, U, UT, UX, UY, NBNDS, NB LLBND, ILBND, LBND, RES)	PTS,				
	INTEGER 1 <i>double precision</i> 1	NPTS, NPDE, NBNDS, NBPTS, LLBND(NBNDS), ILBND(NBNDS), LBND(NBPTS) T, X(NPTS), Y(NPTS), U(NPTS,NPDE), UT(NPTS,NP UX(NPTS,NPDE), UY(NPTS,NPDE), RES(NPTS,NPDE)	de),				
1:	NPTS – INTEGER		Input				
	On entry: the number	of grid points in the current grid.					
2:	NPDE – INTEGER		Input				
	On entry: the number of PDEs in the system.						
3:	T – double precision		Input				
	On entry: the current w	value of the independent variable t.					
4:	X(NPTS) – double pre	ecision array	Input				
	On entry: $X(i)$ contains the x co-ordinate of the <i>i</i> th grid point, for $i = 1, 2,, NPTS$.						

6: U(NPTS On entry i = 1, 2, 7: UT(NPT On entry point, fo 8: UX(NPT On entry point, fo 9: UY(NPT On entry point, fo 10: NBNDS On entry point, fo 10: NBNDS On entry 11: NBPTS On entry 11: NBPTS On entry 12: LLBND(On entry given in 14: LBND(N On entry solution 15: RES(NP	: $Y(i)$ contains the <i>y</i> co-ordinate of the <i>i</i> th grid point, for $i = 1, 2,,$ NPDE) – <i>double precision</i> array : $U(i,j)$ contains the value of the <i>j</i> th PDE component at the <i>i</i> th grid p	, NPTS.
On entry $i = 1, 2,$ 7:UT(NPT On entry point, fo8:UX(NPT On entry point, fo9:UY(NPT On entry point, fo9:UY(NPT On entry point, fo10:NBNDS On entry 11:11:NBPTS - On entry correspond13:ILBND(On entry given in14:LBND(N On entry solution15:RES(NP	: $U(i,j)$ contains the value of the <i>j</i> th PDE component at the <i>i</i> th grid p	
i = 1, 2,7:UT(NPT On entry point, fo8:UX(NPT On entry point, fo9:UY(NPT On entry point, fo9:UY(NPT On entry point, fo10:NBNDS On entry11:NBPTS On entry12:LLBND(On entry correspond13:ILBND(On entry given in14:LBND(N On entry point, where boundary solution15:RES(NP		Input
On entry point, fo8:UX(NPT On entry point, fo9:UY(NPT On entry point, fo9:UY(NPT On entry point, fo10:NBNDS On entry11:NBPTS On entry12:LLBND(On entry correspond13:ILBND(On entry given in14:LBND(N On entry solution15:RES(NP	, NPTS; $j = 1, 2,, NPDE$.	ooint, for
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 point, fo 10: NBNDS On entry 11: NBPTS On entry 12: LLBND(On entry correspond 13: ILBND(On entry given in 14: LBND(N On entry point, who boundary solution 15: RES(NP) 	S,NPDE) – <i>double precision</i> array	Input
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On entry given in 14: LBND(N On entry point, wi boundary solution 15: RES(NP	: LLBND(<i>i</i>), for $i = 1, 2,, NBNDS$, contains the element of LBND ding to the start of the <i>i</i> th boundary (or corner).	1
given in 14: LBND(N <i>On entry</i> point, wh boundary solution 15: RES(NP	NBNDS) – INTEGER array	Input
On entry point, wh boundary solution 15: RES(NP	: ILBND(<i>i</i>), for $i = 1, 2,$, NBNDS, contains the type of the <i>i</i> th bou Section 3.	indary, as
point, wh boundary solution 15: RES(NP	BPTS) – INTEGER array	Input
	LBND(i), for $i = 1, 2,, NBPTS$, contains the grid index of the <i>i</i> th there the order of the boundaries is as specified in LLBND. Hence the point has co-ordinates X(LBND(<i>i</i>)) and Y(LBND(<i>i</i>)), and the correspondence are U(LBND(<i>i</i>) <i>j</i>), for $j = 1, 2,, NPDE$.	e <i>i</i> th
On entry	TS,NPDE) – <i>double precision</i> array Inp	out/Output
On entry	contains function values returned by PDEDEF.	
		at the <i>i</i> th
Note: ele must not	RES(LBND(<i>i</i>) <i>j</i>) must contain the value of G_j , for $j = 1, 2,, NPDE$, point, for $i = 1, 2,, NBPTS$.	in LBND,

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)
	INTEGERNPTS, NPDEdouble precisionT, X(NPTS), Y(NPTS), U(NPTS,NPDE)
1:	NPTS – INTEGER Input
	On entry: the number of grid points in the base grid.
2:	NPDE – INTEGER Input
	On entry: the number of PDEs in the system.
3:	T – double precision Input
	On entry: the (initial) value of the independent variable t.
4:	X(NPTS) – <i>double precision</i> array Input
	On entry: $X(i)$ contains the x co-ordinate of the <i>i</i> th grid point, for $i = 1, 2,, NPTS$.
5:	Y(NPTS) – <i>double precision</i> array Input
	On entry: $Y(i)$ contains the y co-ordinate of the <i>i</i> th grid point, for $i = 1, 2,, NPTS$.
6:	U(NPTS,NPDE) – <i>double precision</i> array <i>Output</i>
	On exit: $U(i,j)$ must contain the value of the <i>j</i> th PDE component at the <i>i</i> th grid point, for $i = 1, 2,, NPTS$; $j = 1, 2,, NPDE$.

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, DXB,1DYB, LGRID, ISTRUC, LSOL, SOL, IERR)INTEGER
double precision
LOGICALNPDE, NLEV, LGRID(*), ISTRUC(*), LSOL(NLEV), IERR
T, DT, DTNEW, XMIN, YMIN, DXB, DYB, SOL(*)

1: NPDE – INTEGER

On entry: the number of PDEs in the system.

Input

2: T – double precision Input On entry: the current value of the independent variable t, i.e., the time at the end of the integration step just completed. 3: DT – double precision Input On entry: the current time step size Δt , i.e., the time step size used for the integration step just completed. DTNEW - double precision 4: Input On entry: the time step size that will be used for the next time step. 5: TLAST - LOGICAL Input On entry: indicates if intermediate or final time step. TLAST = .FALSE. for an intermediate step, TLAST = .TRUE. for the last call to MONITR before returning to your program. NLEV - INTEGER 6: Input On entry: the number of grid levels used at time T. 7: XMIN – double precision Input YMIN - double precision 8: Input On entry: the (x, y) co-ordinates of the lower-left corner of the virtual grid. DXB – double precision 9: Input DYB - double precision 10: Input On entry: the sizes of the base grid spacing in the x- and y-direction respectively. 11: LGRID(*) – INTEGER array Input Note: the dimension of the array LGRID must be at least NLEV + 1. On entry: 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 Input Note: the dimension of the array ISTRUC must be at least $3 \times NLEV$. On entry: contains the grid structures for each grid level and must be passed unchanged to D03RZF in order to extract the grid information. LSOL(NLEV) – INTEGER array 13: Input On entry: 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.) 14: SOL(*) – *double precision* array Input Note: the dimension of the array SOL must be at least NPDE \times $(n_1 + \ldots + n_{\text{NLEV}})$. On entry: contains the solution u at time T for each grid level l in turn, positioned according to LSOL. More precisely $U(i,j) = SOL(LSOL(l) + (j-1) \times n_l + i)$ 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

On entry: will be initialized by D03RBF to some value prior to internal calls to INIDOM.

On exit: should be set to 1 to force a termination of the integration and an immediate return to the calling program with IFAIL = 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.

OPTI(4) - INTEGER array 12:

On entry: may be set to control various options available in the integrator.

OPTI(1) = 0

All the default options are employed.

OPTI(1) > 0

The default value of OPTI(i), for i = 2, 3 or 4, can be obtained by setting OPTI(i) = 0.

Specifies the maximum number of grid levels allowed (including the base grid). $OPTI(1) \ge 0$. 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. $OPTI(4) \ge 0$. The default value is OPTI(4) = 100.

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

OPTR(3,NPDE) – *double precision* array 13:

On entry: 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_i^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. $OPTR(2, j) \ge 0.0$ 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 $(3, j) \ge 0.0$, for j = 1, 2, ..., NPDE.

Constraint: OPTR(1, j) > 0.0, for $j = 1, 2, \dots$, NPDE, and OPTR $(i, j) \ge 0.0$, for i = 2, 3 and $j = 1, 2, \dots, \text{NPDE}.$

14: RWK(LENRWK) – *double precision* array

LENRWK - INTEGER 15:

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

Input/Output

Input

Input

D03RBF.13

Input

Communication Array

OPTI(1)

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

$$LENRWK = maxpts \times NPDE \times (5 \times l + 18 \times NPDE + 9) + 2 \times maxpts,$$

where l = OPTI(1) if $OPTI(1) \neq 0$ 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 cannot 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

Communication Array

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. Here, m is the maximum number of grid levels allowed (m = OPTI(1) if OPTI(1) > 1 and m = 3 otherwise), and l is a grid level taking the values l = 1, 2, ..., nl, where nl is the number of levels used.

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*.

 $IWK(2 + 2 \times m + l)$

Contains the total number of Newton iterations performed at grid level *l*.

IWK $(2 + 3 \times m + l)$

Contains the total number of linear solver iterations performed at grid level *l*.

 $IWK(2 + 4 \times m + l)$

Contains the maximum number of Newton iterations performed at any one time step at grid level l.

 $IWK(2 + 5 \times m + l)$

Contains the maximum number of linear solver iterations performed at any one time step at grid level l.

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

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

The required value of LENIWK cannot 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

Input

Input/Output

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 cannot 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

LENLWK - INTEGER 19:

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

> The required value of LENLWK cannot 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 cannot be checked upon initial entry to D03RBF since the number of grid points on the base grid is not known.

20: ITRACE – INTEGER

On entry: the level of trace information required from D03RBF. ITRACE may take the value -1, 0, 1, 2, or 3.

ITRACE = -1

No output is generated.

ITRACE = 0

Only warning messages are printed.

ITRACE > 0

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.

If ITRACE < -1, then -1 is assumed and similarly if ITRACE > 3, then 3 is assumed.

The advisory messages are given in greater detail as ITRACE increases. Setting ITRACE = 1 allows you to monitor the progress of the integration without possibly excessive information.

IND – INTEGER 21.

On entry: 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 < IND < 1.

On exit: IND = 1.

IFAIL - INTEGER 22:

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Chapter P01 for details.

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

[NP3657/21]

Input/Output

Workspace Input

Input

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 parameter the recommended value is 0. When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.

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, NPDE < 1, 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 $0.0 < DT(1) < 10 \times machine precision \times max(|TS|, |TOUT|)$, 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 $(1, j) \le 0.0$, for some j = 1, 2, ..., NPDE, or OPTR(2, j) < 0.0, for some j = 1, 2, ..., NPDE, or OPTR(3, j) < 0.0, for some j = 1, 2, ..., NPDE, or IND \neq 0 or 1, or IND = 1 on initial entry to D03RBF. or

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 you are 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 because you set IERR to -1 in the user-supplied (sub)program 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 (sub)program MONITR, forcing control to be passed back to calling program. Integration was successful as far as T = 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-suppled (sub)program INIDOM was incorrectly specified, i.e.,

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

7 Accuracy

There are three sources of error in the algorithm: space and time discretization, and interpolation (linear) between grid levels. The space and time discretization errors are controlled separately using the parameters TOLS and TOLT described in the following section, and you 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 Trompert and Verwer (1993).

8 Further Comments

8.1 Algorithm Outline

The local uniform grid refinement method is summarized as follows.

- 1. Initialize 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) Go to 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 go to 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

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

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

$$\gamma_j = \frac{w_j^{\rm s}}{u_j^{\rm max}\,\sigma},\tag{4}$$

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 you. 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

$$\max\{\mu_i^s\} > 0.9 \quad \text{or} \quad 1.0,$$
 (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

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

where NGPTS(*l*) is the total number of points on grid level *l*; N = NGPTS(*l*) × 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

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

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

An integration step is rejected and retried at all levels if

$$\max_{l} \left\{ \mu_{l}^{i} \right\} > 1.0. \tag{8}$$

9 Example

This example is taken from Blom and Verwer (1993) and is the two dimensional Burgers' system

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

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

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

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 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.

```
DO3RBF Example Program Text
*
      Mark 19 Revised. NAG Copyright 1999.
*
       .. Parameters ..
*
       INTEGER
                           NOUT
                          (NOUT=6)
      PARAMETER
      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)
                          MXLEV, NPDE, NPTS
      +
                          LENRWK=NPTS*NPDE*(5*MXLEV+9+18*NPDE)+2*NPTS,
      +
                          LENLWK=2*NPTS)
       .. Scalars in Common .
*
      INTEGER
                          IOUT
       .. Arrays in Common ..
*
       DOUBLE PRECISION TWANT(2)
       .. Local Scalars ..
      DOUBLE PRECISION TOLS, TOLT, TOUT, TS
       INTEGER
                          I, IFAIL, IND, ITRACE, J, MAXLEV
      .. Local Arrays ..
DOUBLE PRECISION DT(3), OPTR(3,NPDE), RWK(LENRWK)
*
      INTEGER
                          IWK(LENIWK), OPTI(4)
      LOGICAL
                          LWK(LENLWK)
       .. External Subroutines ..
*
                          BNDRY, DO3RBF, INIDM, MONIT, PDEF, PDEIV
      EXTERNAL
       .. Common blocks .
       COMMON
                          /OTIME/TWANT, IOUT
       .. Executable Statements ..
*
       WRITE (NOUT, *) 'DO3RBF Example Program Results'
*
       IND = 0
       ITRACE = 0
       TS = 0.0D0
       TWANT(1) = 0.25D0
       TWANT(2) = 1.0D0
       DT(1) = 0.001D0
      DT(2) = 1.0D-7
       DT(3) = 0.0D0
      TOLS = 0.1D0
       TOLT = 0.05D0
```

```
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) = 1.0D0
   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, INIDM, PDEF, BNDRY, PDEIV,
     +
                      MONIT, 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,
           '(''
                             Total number of
     +
                                                             ( ( ) ( )
         WRITE (NOUT,
      '(''
                     Residual Jacobian
                                             Newton '' , '' Lin sys'')'
     +
     +
           )
         WRITE (NOUT,
                                                          , ''
      '(''
                                              iters ^{\prime\prime}
                                                                   iters'')'
     +
                         evals
                                    evals
     +
          )
         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,
           '(''
                             Maximum number '', '' of'')')
     +
         WRITE (NOUT,
           '(''
     +
                              Newton iters
                                               Lin sys iters '')')
         WRITE (NOUT, '('' At level '')')
         DO 100 J = 1, MAXLEV
            IF (IWK(J+2).NE.0) WRITE (NOUT, '(16,2114)') J,
                 IWK(J+2+4*MAXLEV), IWK(J+2+5*MAXLEV)
 100
         CONTINUE
         WRITE (NOUT, *)
*
 120 CONTINUE
*
      STOP
      END
*
      SUBROUTINE INIDM (MAXPTS, XMIN, XMAX, YMIN, YMAX, NX, NY, NPTS, NROWS,
     +
                        NBNDS, NBPTS, LROW, IROW, ICOL, LLBND, ILBND, LBND, IERR)
      .. Parameters ..
                        NOUT
      INTEGER
      PARAMETER
                        (NOUT=6)
      .. Scalar Arguments ..
*
      DOUBLE PRECISION XMAX, XMIN, YMAX, YMIN
      INTEGER
                        IERR, MAXPTS, NBNDS, NBPTS, NPTS, NROWS, NX, NY
      .. Array Arguments ..
      INTEGER
                        ICOL(*), ILBND(*), IROW(*), LBND(*), LLBND(*),
```

```
LROW(*)
        .. Local Scalars ..
       INTEGER
                              I, IFAIL, J, LENIWK
        .. Local Arrays ..
*
                               ICOLD(105), ILBNDD(28), IROWD(11), IWK(122),
       INTEGER
      +
                               LBNDD(72), LLBNDD(28), LROWD(11)
                            PGRID(11)
       CHARACTER*33
        .. External Subroutines ..
*
       EXTERNAL
                               D03RYF
        .. Data statements ..
                               ICOLD/0, 1, 2, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10,
       DATA
                               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/
ILBNDD/1, 2, 3, 4, 1, 4, 1, 2, 3, 4, 3, 4, 1, 2,
      +
       DATA
                               12, 23, 34, 41, 14, 41, 12, 23, 34, 41, 43, 14,
      +
      +
                               21, 32/
                               IROWD/0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10/
LBNDD/2, 4, 15, 26, 37, 46, 57, 68, 79, 88, 98,
       DATA
       DATA
                               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/
                               LLBNDD/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/
LROWD/1, 4, 15, 26, 37, 46, 57, 68, 79, 88, 97/
       DATA
      +
      +
       DATA
        .. 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 = 0.0D0
        YMIN = 0.0D0
       XMAX = 1.0D0
        YMAX = 1.0D0
*
       NROWS = 11
       NPTS = 105
       NBNDS = 28
       NBPTS = 72
        DO 20 I = 1, NROWS
            LROW(I) = LROWD(I)
            IROW(I) = IROWD(I)
   20 CONTINUE
*
        DO 40 I = 1, NBNDS
            LLBND(I) = LLBNDD(I)
            ILBND(I) = ILBNDD(I)
   40 CONTINUE
       DO 60 I = 1, NBPTS
           LBND(I) = LBNDD(I)
   60 CONTINUE
        DO 80 I = 1, NPTS
            ICOL(I) = ICOLD(I)
   80 CONTINUE
```

D03RBF

```
*
      WRITE (NOUT, *) 'Base grid:'
      WRITE (NOUT, *)
      LENIWK = 122
      IFAIL = -1
      CALL D03RYF(NX,NY,NPTS,NROWS,NBNDS,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 PDEIV(NPTS, NPDE, T, X, Y, U)
*
      .. Parameters ..
      DOUBLE PRECISION EPS
      PARAMETER
                       (EPS=1D-3)
      .. Scalar Arguments ..
      DOUBLE PRECISION T
      INTEGER
                       NPDE, NPTS
      .. Array Arguments ..
*
      DOUBLE PRECISION U(NPTS, NPDE), X(NPTS), Y(NPTS)
*
      .. Local Scalars ..
      DOUBLE PRECISION A
      INTEGER
                       Ι
      .. Intrinsic Functions ..
*
      INTRINSIC
                       EXP
      .. Executable Statements ..
      DO 20 I = 1, NPTS
         A = (-4.0D0 * X(I) + 4.0D0 * Y(I) - T) / (32.0D0 * EPS)
         IF (A.LE.O.ODO) THEN
            U(I,1) = 0.75D0 - 0.25D0/(1.0D0+EXP(A))
            U(1,2) = 0.75D0 + 0.25D0/(1.0D0+EXP(A))
         ELSE
            U(I,1) = 0.75D0 - 0.25D0 \times EXP(-A) / (EXP(-A) + 1.0D0)
            U(I,2) = 0.75D0 + 0.25D0 \times EXP(-A) / (EXP(-A) + 1.0D0)
         END TF
   20 CONTINUE
*
      RETURN
      END
*
      SUBROUTINE PDEF(NPTS,NPDE,T,X,Y,U,UT,UX,UY,UXX,UXY,UYY,RES)
*
      .. Parameters ..
      DOUBLE PRECISION EPS
      PARAMETER
                       (EPS=1D-3)
      .. Scalar Arguments ..
      DOUBLE PRECISION T
      INTEGER
                      NPDE, NPTS
      .. Array Arguments .
      DOUBLE PRECISION 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
                      Т
      .. 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)+UYY(I,1)))
     +
         RES(I,2) = UT(I,2) - (-U(I,1)*UX(I,2)-U(I,2)*UY(I,2))
     +
                    +EPS*(UXX(I,2)+UYY(I,2)))
   20 CONTINUE
```

```
RETURN
     END
     SUBROUTINE BNDRY (NPTS, NPDE, T, X, Y, U, UT, UX, UY, NBNDS, NBPTS, LLBND,
                       ILBND,LBND,RES)
     ^{+}
      .. Parameters ..
*
     DOUBLE PRECISION EPS
     PARAMETER
                        (EPS=1D-3)
      .. Scalar Arguments ..
      DOUBLE PRECISION T
     INTEGER
                       NBNDS, NBPTS, NPDE, NPTS
      .. Array Arguments ..
     DOUBLE PRECISION RES(NPTS,NPDE), U(NPTS,NPDE), UT(NPTS,NPDE),
     +
                       UX(NPTS,NPDE), UY(NPTS,NPDE), X(NPTS), Y(NPTS)
     INTEGER
                        ILBND(NBNDS), LBND(NBPTS), LLBND(NBNDS)
      .. Local Scalars ..
     DOUBLE PRECISION A
     INTEGER
                        I, K
      .. Intrinsic Functions ..
     INTRINSIC
                       EXF
      .. Executable Statements ..
*
     DO 20 K = LLBND(1), NBPTS
         I = LBND(K)
         A = (-4.0D0 * X(I) + 4.0D0 * Y(I) - T) / (32.0D0 * EPS)
         IF (A.LE.O.ODO) THEN
            RES(I,1) = U(I,1) - (0.75D0 - 0.25D0 / (1.0D0 + EXP(A)))
            RES(I,2) = U(I,2) - (0.75D0+0.25D0/(1.0D0+EXP(A)))
         ELSE
            RES(I,1) = U(I,1) - (0.75D0 - 0.25D0 * EXP(-A) / (EXP(-A) + 1.0D0))
            RES(I,2) = U(I,2) - (0.75D0+0.25D0*EXP(-A)/(EXP(-A)+1.0D0))
         END IF
  20 CONTINUE
*
      RETURN
     END
      SUBROUTINE MONIT(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 ..
      DOUBLE PRECISION DT, DTNEW, DXB, DYB, T, XMIN, YMIN
     INTEGER
                       IERR, NLEV, NPDE
      LOGICAL
                        TLAST
      .. Array Arguments ..
     DOUBLE PRECISION SOL(*)
                       ISTRUC(*), LGRID(*), LSOL(NLEV)
      INTEGER
      .. Scalars in Common ..
*
      INTEGER
                       IOUT
      .. Arrays in Common .
*
     DOUBLE PRECISION TWANT(2)
      .. Local Scalars ..
*
      INTEGER
                        IFAIL, IPSOL, IPT, LEVEL, NPTS
      .. Local Arrays ..
      DOUBLE PRECISION UEX(105,2), X(MAXPTS), Y(MAXPTS)
      .. External Subroutines ..
*
                       DO3RZF, PDEIV
     EXTERNAL
*
      .. Common blocks ..
      COMMON
                        /OTIME/TWANT, IOUT
      .. Executable Statements ..
*
      IFAIL = -1
      IF (TLAST) THEN
         DO 40 LEVEL = 1, NLEV
            IPSOL = LSOL(LEVEL)
            Get grid information
*
*
            CALL DO3RZF(LEVEL,NLEV,XMIN,YMIN,DXB,DYB,LGRID,ISTRUC,NPTS,
     +
                         X,Y,MAXPTS,IFAIL)
            IF (IFAIL.NE.O) THEN
               IERR = 1
```

```
RETURN
            END IF
*
            IF (IOUT.EQ.2 .AND. LEVEL.EQ.1) THEN
*
               Get exact solution
*
*
               CALL PDEIV(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,A,10X,A,8X,A,5X,A,4X,A,4X,A)') 'x', 'y',
                 'approx u', 'exact u', 'approx v', 'exact v'
     +
               WRITE (NOUT, *)
               IPSOL = LSOL(LEVEL)
               DO 20 IPT = 1, NPTS, 2
                  WRITE (NOUT, '(6(1X,E11.4))') 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
```

9.2 Program Data

None.

9.3 **Program Results**

DO3RBF Example Program Results 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	ХХ	
2	•••	4	23	3	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	1	41	
12	1	41	XX	XX							

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

	sidual Jacob evals ev	ian Newto als iter	-		
At level 1 2 3 4 5	196119611961	4 28 4 28 4 28 4 28 0 21	14 22 25 31 29		
At level	M a x i m u Newton iter				
1	2	1			
2 3	2 2	1 1			
4 5	2 3	2 2			
5	3	2			
Solution at	every 2nd gr	id point in	level 1 at t	ime 1.0000	:
Х	У	approx u	exact u	approx v	exact v
0.0000E+00 0.2000E+00		0.5000E+00 0.5000E+00	0.5000E+00 0.5000E+00	0.1000E+01 0.1000E+01	0.1000E+01 0.1000E+01
0.1000E+00		0.5002E+00	0.5000E+00	0.9998E+00	0.1000E+01 0.1000E+01
0.3000E+00		0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.5000E+00 0.7000E+00		0.5000E+00 0.5000E+00	0.5000E+00 0.5000E+00	0.1000E+01 0.1000E+01	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 0.5000E+00	0.5005E+00 0.5000E+00	0.9995E+00 0.1000E+01	0.9995E+00 0.1000E+01
0.4000E+00	0.2000E+00	0.5001E+00	0.5000E+00	0.9999E+00	0.1000E+01
0.6000E+00 0.8000E+00		0.4999E+00 0.5000E+00	0.5000E+00 0.5000E+00	0.1000E+01 0.1000E+01	0.1000E+01 0.1000E+01
0.1000E+01		0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.1000E+00 0.3000E+00		0.5000E+00 0.5000E+00	0.5005E+00 0.5000E+00	0.1000E+01 0.1000E+01	0.9995E+00 0.1000E+01
0.5000E+00		0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.7000E+00		0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.9000E+00 0.0000E+00		0.5000E+00 0.7500E+00	0.5000E+00 0.7500E+00	0.1000E+01 0.7500E+00	0.1000E+01 0.7500E+00
0.2000E+00		0.5005E+00	0.5005E+00	0.9995E+00	0.9995E+00
0.4000E+00 0.8000E+00	0.4000E+00 0.4000E+00	0.5002E+00 0.5000E+00	0.5000E+00 0.5000E+00	0.9998E+00 0.1000E+01	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 0.3000E+00	0.5000E+00 0.5000E+00	0.7500E+00 0.5005E+00	0.7500E+00 0.5005E+00	0.7500E+00 0.9995E+00	0.7500E+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 0.9000E+00	0.5000E+00 0.5000E+00	0.5000E+00 0.5001E+00	0.5000E+00 0.5000E+00	0.1000E+01 0.9999E+00	0.1000E+01 0.1000E+01
0.0000E+00	0.6000E+00	0.7500E+00	0.7500E+00	0.7500E+00	0.7500E+00
0.2000E+00 0.4000E+00	0.6000E+00 0.6000E+00	0.7500E+00 0.5000E+00	0.7500E+00 0.5005E+00	0.7500E+00 0.1000E+01	0.7500E+00 0.9995E+00
0.6000E+00	0.6000E+00	0.4999E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.8000E+00 0.1000E+01	0.6000E+00	0.4998E+00 0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.1000E+01 0.1000E+00	0.6000E+00 0.7000E+00	0.7500E+00	0.5000E+00 0.7500E+00	0.1000E+01 0.7500E+00	0.1000E+01 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	0.7000E+00 0.7000E+00	0.5005E+00 0.5000E+00	0.5005E+00 0.5000E+00	0.9995E+00 0.1000E+01	0.9995E+00 0.1000E+01
0.9000E+00	0.7000E+00	0.5000E+00	0.5000E+00	0.1000E+01	0.1000E+01
0.0000E+00 0.2000E+00	0.8000E+00 0.8000E+00	0.7500E+00 0.7500E+00	0.7500E+00 0.7500E+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	0.8000E+00 0.8000E+00	0.5005E+00 0.5000E+00	0.5005E+00 0.5000E+00	0.9995E+00 0.1000E+01	0.9995E+00 0.1000E+01
0.1000E+00	0.9000E+00	0.7500E+00	0.7500E+00	0.7500E+00	0.7500E+00
0.3000E+00 0.5000E+00	0.9000E+00 0.9000E+00	0.7500E+00 0.7500E+00	0.7500E+00 0.7500E+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+0 0.2000E+0 0.4000E+0 0.6000E+0 0.8000E+0	0 0.1000E+01 0 0.1000E+01 0 0.1000E+01	0.7500E+00 0.7500E+00 0.7500E+00	0.7500E+00	0.7500E+00 0.7500E+00 0.7500E+00 0.7500E+00 0.9995E+00	0.7500E+00 0.7500E+00 0.7500E+00 0.7500E+00 0.9995E+00
Statistics	:				
	.0000				
	er of accepte er of rejecte				
IOCAL HUMD	er or rejecte	a timesteps -	- 0		
		number			
R	esidual Jaco evals e	bian Newto vals iter	- 1		
At level	evais e	vais itei	is iters		
1	630	45 90	45		
2		45 90	78		
3		45 90	87		
4		45 90	124		
5	575	41 83	122		
	Maximu	mnumbe	er of		
	Newton ite	rs Lin sys	s iters		
At level					
1	2	1			
2	2	1			
3	2	1			
4	2	2			
5	3	2			