D03RAF - 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

D03RAF integrates a system of linear or nonlinear, time-dependent partial differential equations (PDEs) in two space dimensions on a rectangular 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. D03RAF originates from the VLUGR2 package [1] [2].

2 Specification

```
SUBROUTINE DO3RAF(NPDE, TS, TOUT, DT, XMIN, XMAX, YMIN, YMAX, NX,
1
                   NY, TOLS, TOLT, PDEDEF, BNDARY, PDEIV, MONITR,
2
                   OPTI, OPTR, RWK, LENRWK, IWK, LENIWK, LWK, LENLWK,
                   ITRACE, IND, IFAIL)
3
 INTEGER
                   NPDE, NX, NY, OPTI(4), LENRWK, IWK(LENIWK),
                   LENIWK, LENLWK, ITRACE, IND, IFAIL
real
                   TS, TOUT, DT(3), XMIN, XMAX, YMIN, YMAX, TOLS,
                   TOLT, OPTR(3, NPDE), RWK(LENRWK)
1
 LOGICAL
                   LWK (LENLWK)
 EXTERNAL
                   PDEDEF, BNDARY, PDEIV, MONITR
```

3 Description

D03RAF integrates the system of PDEs:

$$F_{j}(t,x,y,u,u_{t},u_{x},u_{y},u_{xx},u_{xy},u_{yy})=0,\ \ j=1,2,\ldots, \text{NPDE}, \eqno(1)$$

for x and y in the rectangular domain $x_{\min} \le x \le x_{\max}$, $y_{\min} \le y \le y_{\max}$, and time interval $t_0 \le t \le t_{\text{out}}$, where 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) must be specified at $t = t_0$ in a subroutine PDEIV.

Note that whilst complete generality is offered by the master equations (1), D03RAF 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

$$G_j(t, x, y, u, u_t, u_x, u_y) = 0$$
 at $x = x_{\min}, x_{\max}, y = y_{\min}, y_{\max}$, for $j = 1, 2, ..., \text{NPDE}$. (2)

The domain is covered by a uniform coarse base grid of size $n_x \times n_y$ 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 $t = t_{\rm out}$.

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.

The solution at all grid levels is 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 included. 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.

Within the user-specified subroutines PDEIV, PDEDEF, BNDARY and MONITR the data structure is as follows. Each point on a particular grid is given an index (ranging from 1 to the total number of points on the grid) and all coordinate or solution information is stored in arrays according to this index, e.g., X(i) and Y(i) contain the x- and y-coordinate of point i, and U(i,j) contains the jth solution component u_j at point i.

Further details of the underlying algorithm can be found in Section 8 and in [1] [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] Adjerid S and Flaherty J E (1988) A local refinement finite element method for two dimensional parabolic systems SIAM J. Sci. Statist. Comput. 9 792–811
- [6] Brown P N, Hindmarsh A C and Petzold L R (1994) Using Krylov methods in the solution of large scale differential-algebraic systems SIAM J. Sci. Statist. Comput. 15 1467–1488

5 Parameters

1: NPDE — INTEGER Input

On entry: the number of PDEs in the system.

Constraint: NPDE > 1.

D03RAF.2 [NP3086/18/pdf]

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.

 $3: \quad TOUT - real$ 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 $DT(2) = 10.0 \times machine precision$ 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:

$$10.0 \times machine\ precision \times max(|TS|,|TOUT|) \le DT(1) \le TOUT - TS$$

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

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) ≥ 0 , i = 2,3 and DT(2) \leq DT(3) for IND = 0 and IND = 1.

5: XMIN - real

6: XMAX - real Input

On entry: the extents of the rectangular domain in the x-direction, i.e., the x-coordinates of the left and right boundaries respectively.

Constraint: XMIN < XMAX and XMAX must be sufficiently distinguishable from XMIN for the precision of the machine being used.

7: YMIN - real Input

8: YMAX - real Input

On entry: the extents of the rectangular domain in the y-direction, i.e., the y-coordinates of the lower and upper boundaries respectively.

Constraint: YMIN < YMAX and YMAX must be sufficiently distinguishable from YMIN for the precision of the machine being used.

9: NX — INTEGER Input

On entry: the number of grid points in the x-direction (including the boundary points).

Constraint: $NX \ge 4$.

10: NY — INTEGER

On entry: the number of grid points in the y-direction (including the boundary points).

Constraint: NY > 4.

11: 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.

12: TOLT-real

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

Constraint: TOLT > 0.0.

13: PDEDEF - SUBROUTINE, supplied by the user.

External Procedure

Input

PDEDEF must evaluate the functions F_j , 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 subroutine 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)

INTEGER NPTS, NPDE

real 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)

1: NPTS — INTEGER

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-real

On entry: the current value of the independent variable t.

4: X(NPTS) — real array Input

On entry: X(i) contains the x-coordinate of the ith grid point, for i = 1, 2, ..., NPTS.

5: Y(NPTS) - real array Input On entry: Y(i) contains the y-coordinate of the ith grid point, for i = 1, 2, ..., NPTS.

6: U(NPTS,NPDE) - real array

On entry: U(i,j) contains the value of the jth PDE component at the ith grid point, for

 $i=1,2,\ldots, \text{NPTS}, \ j=1,2,\ldots, \text{NPDE}.$ 7: UT(NPTS,NPDE) — \pmb{real} array Input

On entry: UT(i,j) contains the value of $\partial u/\partial t$ for the jth PDE component at the ith grid point, for $i=1,2,\ldots, \text{NPTS},\ j=1,2,\ldots, \text{NPDE}.$

8: UX(NPTS,NPDE) - real array Input On entry: UX(i,j) contains the value of $\partial u/\partial x$ for the jth PDE component at the ith grid point, for $i=1,2,\ldots,NPTS$, $j=1,2,\ldots,NPDE$.

9: UY(NPTS,NPDE) — real array Input On entry: UY(i,j) contains the value of $\partial u/\partial y$ for the jth PDE component at the ith grid point, for $i=1,2,\ldots,$ NPTS, $j=1,2,\ldots,$ NPDE.

10: UXX(NPTS,NPDE) — real array Input On entry: UXX(i,j) contains the value of $\partial^2 u/\partial x^2$ for the jth PDE component at the ith grid point, for $i=1,2,\ldots,$ NPTS, $j=1,2,\ldots,$ NPDE.

D03RAF.4 [NP3086/18/pdf]

11: UXY(NPTS,NPDE) — real array

Input

On entry: UXY(i,j) contains the value of $\partial^2 u/\partial x \partial y$ for the jth PDE component at the ith grid point, for i = 1, 2, ..., NPTS, j = 1, 2, ..., NPDE.

12: UYY(NPTS,NPDE) — real array

Input

On entry: UYY(i,j) contains the value of $\partial^2 u/\partial y^2$ for the jth PDE component at the ith grid point, for $i=1,2,\ldots,\text{NPTS},\ j=1,2,\ldots,\text{NPDE}$.

13: RES(NPTS,NPDE) — real array

Output

On exit: RES(i,j) must contain the value of F_j for $j=1,2,\ldots,NPDE$, at the *i*th grid point for $i=1,2,\ldots,NPTS$, 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 D03RAF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

14: BNDARY — SUBROUTINE, supplied by the user.

External Procedure

BNDARY must evaluate the functions G_j , 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 subroutine.

Its specification is:

SUBROUTINE BNDARY(NPTS, NPDE, T, X, Y, U, UT, UX, UY, NBPTS, LBND,

1 RES)

INTEGER NPTS, NPDE, NBPTS, LBND(NBPTS)
real 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

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-real

Input

On entry: the current value of the independent variable t.

4: X(NPTS) - real array

Input

On entry: X(i) contains the x-coordinate of the ith grid point, for i = 1, 2, ..., NPTS.

5: Y(NPTS) - real array

Input

On entry: Y(i) contains the y-coordinate of the ith grid point, for i = 1, 2, ..., NPTS.

6: U(NPTS,NPDE) — *real* array

Input

On entry: U(i,j) contains the value of the jth PDE component at the ith grid point, for $i=1,2,\ldots, \text{NPTS}, j=1,2,\ldots, \text{NPDE}.$

7: UT(NPTS,NPDE) — real array

Input

On entry: UT(i,j) contains the value of $\partial u/\partial t$ for the jth PDE component at the ith grid point, for $i=1,2,\ldots,\text{NPTS},\ j=1,2,\ldots,\text{NPDE}.$

8: UX(NPTS,NPDE) — real array

Input

On entry: UX(i,j) contains the value of $\partial u/\partial x$ for the jth PDE component at the ith grid point, for $i=1,2,\ldots,NPTS,\ j=1,2,\ldots,NPDE$.

9: UY(NPTS,NPDE) — *real* array

Input

On entry: UY(i,j) contains the value of $\partial u/\partial y$ for the jth PDE component at the ith grid point, for $i=1,2,\ldots,\text{NPTS},\ j=1,2,\ldots,\text{NPDE}$.

10: NBPTS — INTEGER

Input

On entry: the number of boundary points in the grid.

11: LBND(NBPTS) — INTEGER array

Input

On entry: LBND(i) contains the grid index for the ith boundary point for i = 1, 2, ..., NBPTS. Hence the ith boundary point has coordinates X(LBND(i)) and Y(LBND(i)), and the corresponding solution values are U(LBND(i), NPDE), etc.

12: RES(NPTS,NPDE) — real array

Output

On exit: RES(LBND(i),j) must contain the value of G_j for $j=1,2,\ldots,NPDE$, at the ith boundary point for $i=1,2,\ldots,NBPTS$.

Note. Elements of RES corresponding to interior points must **not** be altered.

BNDARY must be declared as EXTERNAL in the (sub)program from which D03RAF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

15: PDEIV — SUBROUTINE, supplied by the user.

External Procedure

PDEIV must specify the initial values of the PDE components u at all points in the 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

Input

On entry: the number of grid points in the grid.

2: NPDE — INTEGER

Input

On entry: the number of PDEs in the system.

3: T-real

Input

On entry: the (initial) value of the independent variable t.

4: X(NPTS) — real array

Input

On entry: X(i) contains the x-coordinate of the ith grid point, for i = 1, 2, ..., NPTS.

5: Y(NPTS) - real array

Input

On entry: Y(i) contains the y-coordinate of the ith grid point, for i = 1, 2, ..., NPTS.

6: U(NPTS,NPDE) — real array

Output

On exit: U(i,j) must contain the value of the jth PDE component at the ith grid point, for $i=1,2,\ldots, NPTS, j=1,2,\ldots, NPDE$.

PDEIV must be declared as EXTERNAL in the (sub)program from which D03RAF is called. Parameters denoted as Input must **not** be changed by this procedure.

16: MONITR — SUBROUTINE, supplied by the user.

External Procedure

MONITR is called by D03RAF 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

D03RAF.6 [NP3086/18/pdf]

step, indicated by the parameter TLAST. The input arguments contain information about the grid and solution at all grid levels used.

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, NGPTS, XPTS,

1 YPTS, LSOL, SOL, IERR)

LOGICAL TLAST

1: NPDE — INTEGER

Input

On entry: the number of PDEs in the system.

2: T-real

On entry: the current value of the independent variable t, i.e., the time at the end of the integration step just completed.

 $3: \quad DT-real$ Input

On entry: the current time step size DT, i.e., the time step size used for the integration step just completed.

4: DTNEW — real

On entry: the 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 the user's program.

6: NLEV — INTEGER Input

On entry: the number of grid levels used at time T.

7: NGPTS(NLEV) — INTEGER array Input On entry: NGPTS(l) contains the number of grid points at level l, for l = 1, 2, ..., NLEV.

8: XPTS(*) - real array Input

On entry: contains the x-coordinates of the grid points in each level in turn, i.e., X(i), for i = 1, 2, ..., NGPTS(1), l = 1, 2, ..., NLEV.

So for level l, X(i) = XPTS(k+i), where $k = NGPTS(1) + NGPTS(2) + \cdots + NGPTS(l-1)$, for $i = 1, 2, \dots, NGPTS(l)$, $l = 1, 2, \dots, NLEV$.

9: YPTS(*) - real array

Input

On entry: contains the y-coordinates of the grid points in each level in turn, i.e., Y(i), for i = 1, 2, ..., NGPTS(l), l = 1, 2, ..., NLEV.

So for level l, Y(i) = YPTS(k+i), where $k = NGPTS(1) + NGPTS(2) + \cdots + NGPTS(l-1)$, for $i = 1, 2, \dots, NGPTS(l)$, $l = 1, 2, \dots, NLEV$.

10: LSOL(NLEV) — INTEGER array

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. See below.)

11: $SOL(*) - real \operatorname{array}$

Inpu

On entry: SOL contains the solution U(NGPTS(l),NPDE) at time T for each grid level l in turn, positioned according to LSOL i.e., for level l,

$$U(i,j) = SOL(LSOL(l) + (j-1) \times NGPTS(l) + i),$$

for $i = 1, \dots, \text{NGPTS}(l), j = 1, \dots, \text{NPDE}, l = 1, \dots, \text{NLEV}.$

12: IERR — INTEGER

Output

On exit: IERR should be set to 1 to force a tidy termination 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 D03RAF is called. Parameters denoted as *Input* must **not** be changed by this procedure.

17: 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 $\mathrm{OPTI}(1) > 0$ then the default value of $\mathrm{OPTI}(i)$ for i = 2, 3, 4, can be obtained by setting $\mathrm{OPTI}(i) = 0$

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. $OPTI(2) \ge 0$. 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) \geq 0. The default value is OPTI(4) = 100.

Constraints: if $OPTI(1) \ge 0$ and OPTI(1) > 0 then $OPTI(i) \ge 0$, i = 2, 3, 4.

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

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

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

Constraints:

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\begin{aligned} & \text{OPTR}(1,j) > 0.0 \text{ for } j=1,2,\ldots, \text{NPDE and} \\ & \text{OPTR}(i,j) \geq 0.0 \text{ for } i=2,3 \text{ and } j=1,2,\ldots, \text{NPDE}. \end{aligned}
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D03RAF.8 [NP3086/18/pdf]

19: RWK(LENRWK) — real array

Work space

20: LENRWK — INTEGER

Input

On entry: the dimension of the array RWK as declared in the (sub)program from which D03RAF is called.

The required value of LENRWK can not 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 $\text{OPTI}(1) \neq 0$ 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).

Constraint: LENRWK \geq NX \times NY \times NPDE \times (14+18 \times NPDE) + 2 \times NX \times NY (the required size for the initial grid).

21: IWK(LENIWK) — INTEGER array

Output

On entry: if IND = 0, IWK need not be set. Otherwise IWK must remain unchanged from a previous call to D03RAF.

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;

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

 $\text{IWK}(2+3\times m+l)$ contains the total number of linear solver iterations performed at grid level l;

 $\text{IWK}(2+4\times m+l)$ contains the maximum number of Newton iterations performed at any one time step at grid level l;

 $\text{IWK}(2+5\times m+l)$ contains the maximum number of linear solver iterations performed at any one time step at grid level l;

for l = 1, 2, ..., 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 D03RAF. 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.

22: LENIWK — INTEGER

Input

On entry: the dimension of the array IWK as declared in the (sub)program from which D03RAF is called.

The required value of LENIWK can not be determined exactly in advance, but a suggested value is LENIWK = MAXPTS \times (14+5×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).

Constraint: LENIWK $\geq 19 \times NX \times NY + 9$ (the required size for the initial grid).

23: LWK(LENLWK) — LOGICAL array

Workspace

24: LENLWK — INTEGER

Input

On entry: the dimension of the array LWK as declared in the (sub)program from which D03RAF is called.

The required value of LENLWK can not be determined exactly in advanced, 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).

Constraint: LENLWK \geq NX \times NY + 1 (the required size for the initial grid).

25: ITRACE — INTEGER

Input

On entry: the level of trace information required from D03RAF. 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.

26: IND — INTEGER

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 D03RAF: TOUT, DT(2), DT(3), TOLS, TOLT, OPTI, OPTR, ITRACE and IFAIL.

Constraint: $0 \le IND \le 1$.

On exit: IND = 1.

27: IFAIL — INTEGER

Input/Output

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 = 0.0 and 0.0 < DT(1) < 10 × machine precision × max(|TS|,|TOUT|),
```

D03RAF.10 [NP3086/18/pdf]

```
or IND = 0.0 and DT(1) > TOUT - TS,
   IND = 0.0 \text{ and } DT(1) < DT(2) \text{ or } DT(1) > DT(3),
   XMIN \geq XMAX,
   XMAX too close to XMIN.
   YMIN \geq YMAX,
   YMAX too close to YMIN,
  NX \text{ or } NY < 4.
   TOLS or TOLT \leq 0.0,
   OPTI(1) < 0,
   OPTI(1) > 0 and OPTI(j) < 0 for j = 2, 3 or 4,
   OPTR(1,j) \leq 0.0 for some j = 1, 2, ..., NPDE,
   OPTR(2,j) < 0.0 for some j = 1, 2, ..., NPDE,
   OPTR(3,j) < 0.0 for some j = 1, 2, ..., NPDE,
  LENRWK, LENIWK or LENLWK too small for initial grid level,
   IND \neq 0 or 1,
or IND = 1 on initial entry to D03RAF,
```

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. 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 = 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.

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

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

where $\triangle x$ and $\triangle y$ are the grid widths in the x and y directions; and x_i , y_i are the x and y co-ordinates at grid point i. The parameter γ_j is obtained from

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

where σ is the user-supplied space tolerance; w_j^s is a weighting factor for the relative importance of the jth PDE component on the space monitor; and u_j^{max} is the approximate maximum absolute value of the jth 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 value 1.0 if little information about the solution is known.

A new level of refinement is created if

$$\max_{i} \{\mu_{i}^{s}\} > 0.9 \text{ or } 1.0, \tag{5}$$

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

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

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

$$\max_{l} \{\mu_l^t\} > 1.0. \tag{8}$$

D03RAF.12 [NP3086/18/pdf]

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 D03RAF, with a main program:

```
DO3RAF Example Program Text
Mark 18 Release. NAG Copyright 1997.
.. Parameters ..
INTEGER
                 NOUT
PARAMETER
                  (NOUT=6)
.. External Subroutines ..
                 EX1, EX2
EXTERNAL.
.. Executable Statements ..
WRITE (NOUT,*) 'DO3RAF 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 stems from combustion theory and is a model for a single, one-step reaction of a mixture of two chemicals [5]. The PDE for the temperature of the mixture u is

$$\frac{\partial u}{\partial t} = d\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + D(1 + \alpha - u) \exp\left(-\frac{\delta}{u}\right)$$

for $0 \le x, y \le 1$ and $t \ge 0$, with initial conditions u(x, y, 0) = 1 for $0 \le x, y \le 1$, and boundary conditions

$$u_x(0, y, t) = 0, u(1, y, t) = 1$$
 for $0 \le y \le 1$,

$$u_y(x, 0, t) = 0, u(x, 1, t) = 1 \text{ for } 0 \le x \le 1.$$

The heat release parameter $\alpha=1$, the Damkohler number $D=R\exp(\delta)/(\alpha\delta)$, the activation energy $\delta=20$, the reaction rate R=5, and the diffusion parameter d=0.1.

For small times the temperature gradually increases in a circular region about the origin, and at about t = 0.24 'ignition' occurs causing the temperature to suddenly jump from near unity to $1 + \alpha$, and a reaction front forms and propagates outwards, becoming steeper. Thus during the solution, just one grid level is used up to the ignition point, then two levels, and then three as the reaction front steepens.

9.1.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
SUBROUTINE EX1
.. Parameters ..
INTEGER
                 NOUT
PARAMETER
                  (NOUT=6)
INTEGER
                 MXLEV, NPDE, NPTS
PARAMETER
                 (MXLEV=3, NPDE=1, NPTS=2000)
INTEGER
                 LENIWK, LENRWK, LENLWK
PARAMETER
                 (LENIWK=NPTS*(5*MXLEV+14)+2+7*MXLEV,
                 LENRWK=NPTS*NPDE*(5*MXLEV+9+18*NPDE)+NPTS*2,
                 LENLWK=NPTS+1)
```

```
.. Scalars in Common ..
                  ALPHA, D, DELTA, DIFF, REAC
  INTEGER
   .. Arrays in Common ..
  real
                  TWANT(2)
  .. Local Scalars ..
  real
                  TOLS, TOLT, TOUT, TS, XMAX, XMIN, YMAX, YMIN
  INTEGER
                  I, IFAIL, IND, ITRACE, J, MAXLEV, NX, NY
  .. Local Arrays ..
  real DT(3), OPTR(3,NPDE), RWK(LENRWK)
  INTEGER
                 IWK(LENIWK), OPTI(4)
            LWK(LENLWK)
  LOGICAL
  .. External Subroutines ..
  EXTERNAL BNDRY1, DO3RAF, MONIT1, PDEF1, PDEIV1
  .. Intrinsic Functions ..
  INTRINSIC
  .. Common blocks ..
  COMMON
                  /OTIME1/TWANT, IOUT
  COMMON
                  /PARAM1/ALPHA, DELTA, REAC, DIFF, D
   .. Save statement ..
                 /OTIME1/, /PARAM1/
  SAVE
  .. Executable Statements ..
  WRITE (NOUT,*)
  WRITE (NOUT,*)
  WRITE (NOUT,*) 'Example 1'
  WRITE (NOUT,*)
  Problem Parameters
  ALPHA = 1.0e0
  DELTA = 20.0e0
  REAC = 5.0e0
  DIFF = 0.1e0
  D = REAC*EXP(DELTA)/(ALPHA*DELTA)
  IND = 0
  ITRACE = 0
  TS = 0.0e0
  DT(1) = 0.1e-2
  DT(2) = 0.0e0
  DT(3) = 0.0e0
  TOUT = 0.24e0
  TWANT(1) = 0.24e0
  TWANT(2) = 0.25e0
  XMIN = 0.0e0
  XMAX = 1.0e0
  YMIN = 0.0e0
  YMAX = 1.0e0
  NX = 21
  NY = 21
  TOLS = 0.5e0
  TOLT = 0.01e0
  DO 20 I = 1, 4
     OPTI(I) = 0
20 CONTINUE
  DO 60 J = 1, NPDE
     DO 40 I = 1, 3
        OPTR(I,J) = 1.0e0
```

D03RAF.14 [NP3086/18/pdf]

```
40
      CONTINUE
 60 CONTINUE
   DO 120 IOUT = 1, 2
      IFAIL = -1
      TOUT = TWANT(IOUT)
       CALL DO3RAF(NPDE,TS,TOUT,DT,XMIN,XMAX,YMIN,YMAX,NX,NY,TOLS,
                   TOLT, PDEF1, BNDRY1, 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)')
      WRITE (NOUT,*)
      WRITE (NOUT,
         ,(,,
                          Total number of '')')
      WRITE (NOUT,
   + '(''
                 Residual Jacobian
                                         Newton ''
                                                   , '' Lin sys'')'
        )
      WRITE (NOUT,
                                                     , ,,
                                          iters ''
                      evals
                                evals
                                                             iters'')'
        )
      WRITE (NOUT,'('' At level '')')
      MAXLEV = 3
      DO 80 J = 1, MAXLEV
          IF (IWK(J+2).NE.0) WRITE (NOUT, '(18,4110)') 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,
        ,(,,
                                          Lin sys iters '')')
                          Newton iters
      WRITE (NOUT,'('' At level '')')
      DO 100 J = 1, MAXLEV
          IF (IWK(J+2).NE.0) WRITE (NOUT, '(18,2114)') J,
              IWK(J+2+4*MAXLEV), IWK(J+2+5*MAXLEV)
100
       CONTINUE
      WRITE (NOUT,*)
120 CONTINUE
   RETURN
   END
   SUBROUTINE PDEIV1(NPTS, NPDE, T, X, Y, U)
    .. Scalar Arguments ..
   real
   INTEGER
                      NPDE, NPTS
    .. Array Arguments ..
   real
                      U(NPTS, NPDE), X(NPTS), Y(NPTS)
    .. Local Scalars ..
```

```
INTEGER
   .. Executable Statements ..
  DO 20 I = 1, NPTS
      U(I,1) = 1.0e0
20 CONTINUE
  RETURN
  END
  SUBROUTINE PDEF1(NPTS, NPDE, T, X, Y, U, UT, UX, UY, UXX, UXY, UYY, RES)
   .. Scalar Arguments ..
  real
  INTEGER
                    NPDE, NPTS
   .. Array Arguments ..
                    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 ..
                   ALPHA, D, DELTA, DIFF, REAC
  real
   .. Local Scalars ..
  INTEGER
   .. Intrinsic Functions ..
  INTRINSIC
                  EXP
   .. Common blocks ..
  COMMON
           /PARAM1/ALPHA, DELTA, REAC, DIFF, D
   .. Save statement ..
  SAVE
                   /PARAM1/
   .. Executable Statements ..
  DO 20 I = 1, NPTS
      RES(I,1) = UT(I,1) - DIFF*(UXX(I,1)+UYY(I,1)) -
                 D*(1.0e0+ALPHA-U(I,1))*EXP(-DELTA/U(I,1))
20 CONTINUE
  RETURN
  END
  SUBROUTINE BNDRY1(NPTS, NPDE, T, X, Y, U, UT, UX, UY, NBPTS, LBND, RES)
   .. Scalar Arguments ..
  real
  INTEGER
                     NBPTS, NPDE, NPTS
   .. Array Arguments ..
                     RES(NPTS, NPDE), U(NPTS, NPDE), UT(NPTS, NPDE),
  real
                     UX(NPTS, NPDE), UY(NPTS, NPDE), X(NPTS), Y(NPTS)
  INTEGER
                     LBND (NBPTS)
  .. Local Scalars ..
  real
                    TOL
  INTEGER
                    I, J
   .. External Functions ..
  real
                    XO2AJF
  EXTERNAL
                     XO2AJF
   .. Intrinsic Functions ..
  INTRINSIC
                     ABS
   .. Executable Statements ..
  TOL = 10.e0*X02AJF()
  DO 20 I = 1, NBPTS
```

D03RAF.16 [NP3086/18/pdf]

```
J = LBND(I)
     IF (ABS(X(J)).LE.TOL) THEN
        RES(J,1) = UX(J,1)
     ELSE IF (ABS(X(J)-1.0e0).LE.TOL) THEN
        RES(J,1) = U(J,1) - 1.0e0
     ELSE IF (ABS(Y(J)).LE.TOL) THEN
        RES(J,1) = UY(J,1)
     ELSE IF (ABS(Y(J)-1.0e0).LE.TOL) THEN
        RES(J,1) = U(J,1) - 1.0e0
     END IF
20 CONTINUE
  RETURN
  END
  SUBROUTINE MONIT1 (NPDE, T, DT, DTNEW, TLAST, NLEV, NGPTS, XPTS, YPTS, LSOL,
                    SOL, IERR)
   .. Parameters ..
  TNTEGER.
                   NOUT
  PARAMETER
                    (NOUT=6)
  .. Scalar Arguments ..
           DT, DTNEW, T
  real
  INTEGER.
                    IERR, NLEV, NPDE
  LOGICAL
                    TLAST
  .. Array Arguments ..
  real
                    SOL(*), XPTS(*), YPTS(*)
  INTEGER LSOL(NLEV), NGPTS(NLEV)
  .. Scalars in Common ..
  INTEGER IOUT
  .. Arrays in Common ..
  real
                   TWANT(2)
  .. Local Scalars ..
  INTEGER I, IPSOL, IPT, LEVEL, NPTS
  .. Common blocks ..
  COMMON
                   /OTIME1/TWANT, IOUT
  .. Save statement ..
                    /OTIME1/
  .. Executable Statements ...
  IF (TLAST) THEN
     Print solution
     IF (IOUT.EQ.2) THEN
        WRITE (NOUT,
 +'('' Solution at every 4th grid point '', ''in level 1 at time
 +'', F8.4,'':'')') T
        WRITE (NOUT,*)
        WRITE (NOUT, '(7X, ''x'', 10X, ''y'', 8X, ''approx u'')')
        WRITE (NOUT,*)
        LEVEL = 1
        NPTS = NGPTS(LEVEL)
        IPSOL = LSOL(LEVEL)
        IPT = 1
        DO 20 I = 1, NPTS, 4
           WRITE (NOUT, '(3(1X,D11.4))') XPTS(IPT+I-1),
             YPTS(IPT+I-1), SOL(IPSOL+I)
20
        CONTINUE
```

```
WRITE (NOUT,*)
             END IF
          END IF
          RETURN
          END
9.1.2 Program Data
None.
9.1.3 Program Results
     DO3RAF Example Program Results
     Example 1
     Statistics:
     Time = 0.2400
     Total number of accepted timesteps =
                                           75
     Total number of rejected timesteps =
                 Total number of
              Residual Jacobian
                                 Newton
                                           Lin sys
                 evals
                          evals
                                    iters
                                             iters
     At level
                  600
                             75
                                      150
                                               159
                Maximum number of
                 Newton iters
                                 Lin sys iters
     At level
                        2
           1
     Solution at every 4th grid point in level 1 at time
                                                         0.2500:
           х
                              approx u
                     У
      0.0000E+00 0.0000E+00 0.2000E+01
      0.2000E+00 0.0000E+00 0.2000E+01
      0.4000E+00 0.0000E+00 0.2000E+01
      0.6000E+00 0.0000E+00 0.2000E+01
      0.8000E+00 0.0000E+00 0.1240E+01
      0.1000E+01 0.0000E+00 0.1000E+01
      0.1500E+00 0.5000E-01 0.2000E+01
      0.3500E+00 0.5000E-01 0.2000E+01
      0.5500E+00 0.5000E-01 0.2000E+01
      0.7500E+00 0.5000E-01 0.1645E+01
      0.9500E+00 0.5000E-01 0.1048E+01
      0.1000E+00 0.1000E+00 0.2000E+01
      0.3000E+00 0.1000E+00 0.2000E+01
      0.5000E+00 0.1000E+00 0.2000E+01
      0.7000E+00 0.1000E+00 0.1999E+01
      0.9000E+00 0.1000E+00 0.1097E+01
      0.5000E-01 0.1500E+00 0.2000E+01
```

D03RAF.18 [NP3086/18/pdf]

0.2500E+00 0.1500E+00 0.2000E+01 0.4500E+00 0.1500E+00 0.2000E+01

```
0.6500E+00 0.1500E+00 0.2000E+01
0.8500E+00 0.1500E+00 0.1154E+01
0.0000E+00 0.2000E+00 0.2000E+01
0.2000E+00 0.2000E+00 0.2000E+01
0.4000E+00 0.2000E+00 0.2000E+01
0.6000E+00 0.2000E+00 0.2000E+01
0.8000E+00 0.2000E+00 0.1240E+01
0.1000E+01 0.2000E+00 0.1000E+01
0.1500E+00 0.2500E+00 0.2000E+01
0.3500E+00 0.2500E+00 0.2000E+01
0.5500E+00 0.2500E+00 0.2000E+01
0.7500E+00 0.2500E+00 0.1635E+01
0.9500E+00 0.2500E+00 0.1048E+01
0.1000E+00 0.3000E+00 0.2000E+01
0.3000E+00 0.3000E+00 0.2000E+01
0.5000E+00 0.3000E+00 0.2000E+01
0.7000E+00 0.3000E+00 0.1999E+01
0.9000E+00 0.3000E+00 0.1097E+01
0.5000E-01 0.3500E+00 0.2000E+01
0.2500E+00 0.3500E+00 0.2000E+01
0.4500E+00 0.3500E+00 0.2000E+01
0.6500E+00 0.3500E+00 0.2000E+01
0.8500E+00 0.3500E+00 0.1153E+01
0.0000E+00 0.4000E+00 0.2000E+01
0.2000E+00 0.4000E+00 0.2000E+01
0.4000E+00 0.4000E+00 0.2000E+01
0.6000E+00 0.4000E+00 0.2000E+01
0.8000E+00 0.4000E+00 0.1234E+01
0.1000E+01 0.4000E+00 0.1000E+01
0.1500E+00 0.4500E+00 0.2000E+01
0.3500E+00 0.4500E+00 0.2000E+01
0.5500E+00 0.4500E+00 0.2000E+01
0.7500E+00 0.4500E+00 0.1508E+01
0.9500E+00 0.4500E+00 0.1048E+01
0.1000E+00 0.5000E+00 0.2000E+01
0.3000E+00 0.5000E+00 0.2000E+01
0.5000E+00 0.5000E+00 0.2000E+01
0.7000E+00 0.5000E+00 0.1993E+01
0.9000E+00 0.5000E+00 0.1095E+01
0.5000E-01 0.5500E+00 0.2000E+01
0.2500E+00 0.5500E+00 0.2000E+01
0.4500E+00 0.5500E+00 0.2000E+01
0.6500E+00 0.5500E+00 0.2000E+01
0.8500E+00 0.5500E+00
                      0.1145E+01
0.0000E+00 0.6000E+00 0.2000E+01
0.2000E+00 0.6000E+00 0.2000E+01
0.4000E+00 0.6000E+00 0.2000E+01
0.6000E+00 0.6000E+00 0.2000E+01
0.8000E+00 0.6000E+00 0.1200E+01
0.1000E+01 0.6000E+00 0.1000E+01
0.1500E+00 0.6500E+00 0.2000E+01
0.3500E+00 0.6500E+00 0.2000E+01
0.5500E+00 0.6500E+00 0.2000E+01
0.7500E+00 0.6500E+00 0.1253E+01
0.9500E+00 0.6500E+00 0.1044E+01
0.1000E+00 0.7000E+00 0.1999E+01
0.3000E+00 0.7000E+00 0.1999E+01
0.5000E+00 0.7000E+00 0.1993E+01
```

At level

1

2

3

4

4

2

```
0.7000E+00 0.7000E+00 0.1279E+01
 0.9000E+00 0.7000E+00 0.1082E+01
 0.5000E-01 0.7500E+00 0.1645E+01
 0.2500E+00 0.7500E+00 0.1635E+01
 0.4500E+00 0.7500E+00 0.1508E+01
 0.6500E+00 0.7500E+00 0.1253E+01
 0.8500E+00 0.7500E+00 0.1109E+01
 0.0000E+00 0.8000E+00 0.1240E+01
0.2000E+00 0.8000E+00 0.1240E+01
 0.4000E+00 0.8000E+00 0.1234E+01
 0.6000E+00 0.8000E+00 0.1200E+01
 0.8000E+00 0.8000E+00 0.1119E+01
0.1500E+00 0.8500E+00 0.1154E+01
0.3500E+00 0.8500E+00 0.1153E+01
0.5500E+00 0.8500E+00 0.1145E+01
0.7500E+00 0.8500E+00 0.1109E+01
 0.9500E+00 0.8500E+00 0.1029E+01
 0.1000E+00 0.9000E+00 0.1097E+01
 0.3000E+00 0.9000E+00 0.1097E+01
 0.5000E+00 0.9000E+00 0.1095E+01
 0.7000E+00 0.9000E+00 0.1082E+01
 0.9000E+00 0.9000E+00 0.1039E+01
 0.5000E-01 0.9500E+00 0.1048E+01
 0.2500E+00 0.9500E+00 0.1048E+01
 0.4500E+00 0.9500E+00 0.1048E+01
 0.6500E+00 0.9500E+00 0.1044E+01
 0.8500E+00 0.9500E+00 0.1029E+01
 0.0000E+00 0.1000E+01 0.1000E+01
 0.2000E+00 0.1000E+01 0.1000E+01
0.4000E+00 0.1000E+01 0.1000E+01
0.6000E+00 0.1000E+01 0.1000E+01
 0.8000E+00 0.1000E+01 0.1000E+01
 0.1000E+01 0.1000E+01 0.1000E+01
Statistics:
Time = 0.2500
Total number of accepted timesteps =
                                   180
Total number of rejected timesteps =
           Total number of
        Residual Jacobian Newton
                                    Lin sys
           evals
                    evals
                            iters
                                      iters
At level
           1468
                               382
                                        391
     1
                      181
     2
            662
                      82
                               170
                                        170
     3
            176
                       22
                                44
                                         44
           Maximum number of
           Newton iters Lin sys iters
```

D03RAF.20 [NP3086/18/pdf]

2

1

1

9.2 Example 2

This example is taken from a multispecies food web model, in which predator-prey relationships in a spatial domain are simulated [6]. In this example there is just one species each of prey and predator, and the two PDEs for the concentrations c_1 and c_2 of the prey and the predator respectively are

$$\frac{\partial c_1}{\partial t} = c_1(b_1 + a_{11}c_1 + a_{12}c_2) + d_1\left(\frac{\partial^2 c_1}{\partial x^2} + \frac{\partial^2 c_1}{\partial y^2}\right),$$

$$0 = c_2(b_2 + a_{21}c_1 + a_{22}c_2) + d_2\left(\frac{\partial^2 c_2}{\partial x^2} + \frac{\partial^2 c_2}{\partial y^2}\right),$$

with $a_{11}=a_{22}=-1,\,a_{12}=-0.5\times 10^{-6},\,{\rm and}\,\,a_{21}=10^4,\,{\rm and}\,\,$

$$b_1 = 1 + \alpha xy + \beta \sin(4\pi x)\sin(4\pi y),$$

where $\alpha = 50$ and $\beta = 300$, and $b_2 = -b_1$.

The initial conditions are taken to be simple peaked functions which satisfy the boundary conditions and very nearly satisfy the PDEs:

$$c_1 = 10 + (16x(1-x)y(1-y))^2,$$

$$c_2 = b_2 + a_{21}c_1,$$

and the boundary conditions are of Neumann type, i.e., zero normal derivatives everywhere.

During the solution a number of peaks and troughs develop across the domain, and so the number of levels required increases with time. Since the solution varies rapidly in space across the whole of the domain, refinement at intermediate levels tends to occur at all points of the domain.

9.2.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
SUBROUTINE EX2
.. Parameters ..
                 NOUT
INTEGER
PARAMETER
                  (NOUT=6)
INTEGER
                 MXLEV, NPDE, NPTS
PARAMETER
                  (MXLEV=4, NPDE=2, NPTS=8000)
                 LENIWK, LENRWK, LENLWK
INTEGER
PARAMETER
                  (LENIWK=NPTS*(5*MXLEV+14)+2+7*MXLEV,
                 LENRWK=NPTS*NPDE*(5*MXLEV+9+18*NPDE)+NPTS*2,
                 LENLWK=NPTS+1)
.. Scalars in Common ..
                 ALPHA, BETA, PI
real
INTEGER
                 IOUT
.. Arrays in Common ..
                 TWANT(2)
.. Local Scalars ..
real
                 TOLS, TOLT, TOUT, TS, XMAX, XMIN, XX, YMAX, YMIN
                 I, IFAIL, IND, ITRACE, J, MAXLEV, NX, NY
INTEGER
.. Local Arrays ..
real
                 DT(3), OPTR(3, NPDE), RWK(LENRWK)
INTEGER
                 IWK(LENIWK), OPTI(4)
LOGICAL
                 LWK (LENLWK)
.. External Functions ..
real
                 XO1AAF
EXTERNAL
                 X01AAF
```

[NP3086/18/pdf] D03RAF.21

.. External Subroutines ..

```
EXTERNAL
                    BNDRY2, DO3RAF, MONIT2, PDEF2, PDEIV2
   .. Common blocks ..
   COMMON
                    /OTIME2/TWANT, IOUT
  COMMON
                    /PARAM2/ALPHA, BETA, PI
   .. Save statement ..
                    /OTIME2/, /PARAM2/
   .. Executable Statements ..
  WRITE (NOUT,*)
  WRITE (NOUT,*)
  WRITE (NOUT,*) 'Example 2'
  WRITE (NOUT,*)
  XX = 0.0e0
  PI = XO1AAF(XX)
  ALPHA = 50.0e0
  BETA = 300.0e0
  IND = 0
  ITRACE = 0
  TS = 0.0e0
  TWANT(1) = 0.01e0
  TWANT(2) = 0.025e0
  DT(1) = 0.5e-3
  DT(2) = 1.0e-6
  DT(3) = 0.0e0
  XMIN = 0.0e0
  XMAX = 1.0e0
  YMIN = 0.0e0
  YMAX = 1.0e0
  TOLS = 0.075e0
  TOLT = 0.1e0
  NX = 11
  NY = 11
  OPTI(1) = 4
  DO 20 I = 2, 4
      OPTI(I) = 0
20 CONTINUE
  OPTR(1,1) = 250.0e0
  OPTR(1,2) = 1.5e6
  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 DO3RAF(NPDE,TS,TOUT,DT,XMIN,XMAX,YMIN,YMAX,NX,NY,TOLS,
                  TOLT, 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)')
```

D03RAF.22 [NP3086/18/pdf]

```
IWK(1)
      WRITE (NOUT, '('' Total number of rejected timesteps ='', I5)')
      WRITE (NOUT,*)
      WRITE (NOUT,
        ,(\,,\,,
                        Total number of '')')
      WRITE (NOUT,
  + '(''
            Residual Jacobian Newton '' , '' Lin sys'')'
       )
      WRITE (NOUT,
                                      iters '' , ''
                    evals
                             evals
                                                          iters',),
       )
      WRITE (NOUT,'('' At level '')')
      MAXLEV = OPTI(1)
      DO 80 J = 1, MAXLEV
         IF (IWK(J+2).NE.O) WRITE (NOUT, '(16,4I10)') 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
   RETURN
   END
   SUBROUTINE PDEIV2(NPTS, NPDE, T, X, Y, U)
   .. Scalar Arguments ..
   real
   INTEGER
                   NPDE, NPTS
   .. Array Arguments ..
                    U(NPTS, NPDE), X(NPTS), Y(NPTS)
   real
   .. Scalars in Common ..
   real
                    ALPHA, BETA, PI
   .. Local Scalars ..
                   B2, FP
   real
   INTEGER
                    Т
   .. Intrinsic Functions ..
   INTRINSIC SIN
   .. Common blocks ..
   COMMON
                    /PARAM2/ALPHA, BETA, PI
   .. Save statement ..
                    /PARAM2/
   .. Executable Statements ..
   FP = 4.0e0*PI
   DO 20 I = 1, NPTS
```

```
B2 = -1.0e0 - ALPHA*X(I)*Y(I) - BETA*SIN(FP*X(I))*SIN(FP*Y(I))
      U(I,1) = 1.0e1 + (16.0e0*X(I)*(1.0e0-X(I))*Y(I)*(1.0e0-Y(I)))
               **2
      U(I,2) = B2 + 1.0e4*U(I,1)
20 CONTINUE
  RETURN
  END
  SUBROUTINE PDEF2(NPTS, NPDE, T, X, Y, U, UT, UX, UY, UXX, UXY, UYY, RES)
   .. Scalar Arguments ..
  real
                    Т
  INTEGER
                    NPDE, NPTS
   .. Array Arguments ..
                    RES(NPTS,NPDE), U(NPTS,NPDE), UT(NPTS,NPDE),
  real
                    UX(NPTS,NPDE), UXX(NPTS,NPDE), UXY(NPTS,NPDE),
                    UY(NPTS, NPDE), UYY(NPTS, NPDE), X(NPTS), Y(NPTS)
   .. Scalars in Common ..
                   ALPHA, BETA, PI
  real
   .. Local Scalars ..
  real
            B1, B2, FP
  INTEGER
   .. Intrinsic Functions ..
  INTRINSIC
                   SIN
   .. Common blocks ..
  COMMON
                   /PARAM2/ALPHA, BETA, PI
   .. Save statement ..
  SAVE
                   /PARAM2/
   .. Executable Statements ..
  FP = 4.0e0*PI
  DO 20 I = 1, NPTS
      B1 = 1.0e0 + ALPHA*X(I)*Y(I) + BETA*SIN(FP*X(I))*SIN(FP*Y(I))
      B2 = -B1
      RES(I,1) = UT(I,1) - (UXX(I,1)+UYY(I,1)) - U(I,1)*(B1-U(I,1)
                 -0.5e-6*U(I,2)
      RES(I,2) = -0.05e0*(UXX(I,2)+UYY(I,2)) - U(I,2)
                 *(B2+1.0e4*U(I,1)-U(I,2))
20 CONTINUE
  RETURN
  END
   SUBROUTINE BNDRY2(NPTS, NPDE, T, X, Y, U, UT, UX, UY, NBPTS, LBND, RES)
   .. Scalar Arguments ..
  real
                     Τ
   INTEGER
                     NBPTS, NPDE, NPTS
   .. Array Arguments ..
                     RES(NPTS, NPDE), U(NPTS, NPDE), UT(NPTS, NPDE),
  real
                     UX(NPTS, NPDE), UY(NPTS, NPDE), X(NPTS), Y(NPTS)
  INTEGER
                     LBND(NBPTS)
   .. Local Scalars ..
  real
  INTEGER.
                     I, J
   .. External Functions ..
  real
                    X02AJF
  EXTERNAL
                    XO2AJF
   .. Intrinsic Functions ..
```

D03RAF.24 [NP3086/18/pdf]

```
INTRINSIC
                    ABS
   .. Executable Statements ..
  TOL = 10.e0*X02AJF()
  DO 20 I = 1, NBPTS
     J = LBND(I)
     IF (ABS(X(J)).LE.TOL.OR.ABS(X(J)-1.0e0).LE.TOL) THEN
        RES(J,1) = UX(J,1)
        RES(J,2) = UX(J,2)
     ELSE IF (ABS(Y(J)).LE.TOL.OR.ABS(Y(J)-1.0e0).LE.TOL) THEN
        RES(J,1) = UY(J,1)
        RES(J,2) = UY(J,2)
     END IF
20 CONTINUE
  RETURN
  END
  SUBROUTINE MONIT2(NPDE, T, DT, DTNEW, TLAST, NLEV, NGPTS, XPTS, YPTS, LSOL,
                    SOL, IERR)
   .. Parameters ..
  INTEGER
                   NOUT
                   (NOUT=6)
  PARAMETER
  .. Scalar Arguments ..
  real
                 DT, DTNEW, T
                  IERR, NLEV, NPDE
  INTEGER
  LOGICAL TLAST
  .. Array Arguments ..
           SOL(*), XPTS(*), YPTS(*)
  real
  INTEGER
                  LSOL(NLEV), NGPTS(NLEV)
  .. Scalars in Common ..
  INTEGER IOUT
  .. Arrays in Common ..
  real
                   TWANT(2)
   .. Local Scalars ..
  INTEGER
                  I, IPSOL, IPT, LEVEL, NPTS
  .. Common blocks ..
  COMMON
                  /OTIME2/TWANT, IOUT
  .. Save statement ..
  SAVE
                   /OTIME2/
  .. Executable Statements ..
  IF (TLAST) THEN
     Print solution
     IF (IOUT.EQ.2) THEN
        WRITE (NOUT,
 +'('' Solution at every 2nd grid point '', ''in level 1 at time
 +'', F8.4,'':'')') T
        WRITE (NOUT, *)
        WRITE (NOUT.
          '(7X,''x'',10X,''y'',9X,''approx c1'',3X,''approx c2'')')
        WRITE (NOUT,*)
        LEVEL = 1
        NPTS = NGPTS(LEVEL)
        IPSOL = LSOL(LEVEL)
```

9.2.2 Program Data

None.

9.2.3 Program Results

DO3RAF Example Program Results

```
Example 2
```

```
Statistics:
Time = 0.0100
Total number of accepted timesteps = 14
Total number of rejected timesteps = 0
```

	T o t	al numb	er of		
	Residual	Jacobian	Newton	Lin sys	
	evals	evals	iters	iters	
At level					
1	196	14	28	42	
2	168	12	24	34	
3	70	5	10	16	
Morimum mumbom of					

Maximum number of
Newton iters Lin sys iters
At level

1 2 2 2 2 2 3 2 3

Solution at every 2nd grid point in level 1 at time 0.0250:

х	У	approx c1	approx c2
0.0000E+00	0.0000E+00	0.6615E+02	0.6615E+06
0.2000E+00	0.0000E+00	0.5138E+02	0.5137E+06
0.4000E+00	0.0000E+00	0.1274E+02	0.1275E+06
0.6000E+00	0.0000E+00	0.5217E+02	0.5217E+06
0.8000E+00	0.0000E+00	0.1684E+02	0.1684E+06
0.1000E+01	0.0000E+00	0.4618E+01	0.4619E+05
0.1000E+00	0.1000E+00	0.8832E+02	0.8829E+06
0.3000E+00	0.1000E+00	0.1897E+02	0.1898E+06
0.5000E+00	0.1000E+00	0.3109E+02	0.3109E+06
0.7000E+00	0.1000E+00	0.5115E+02	0.5114E+06

D03RAF.26 [NP3086/18/pdf]

```
0.9000E+00 0.1000E+00
                        0.6498E+01
                                     0.6526E+05
0.0000E+00 0.2000E+00
                        0.5138E+02
                                     0.5137E+06
0.2000E+00 0.2000E+00
                        0.4480E+02
                                     0.4479E+06
0.4000E+00 0.2000E+00
                        0.1763E+02
                                     0.1764E+06
0.6000E+00 0.2000E+00
                        0.4849E+02
                                     0.4848E+06
0.8000E+00 0.2000E+00
                        0.2308E+02
                                     0.2309E+06
0.1000E+01 0.2000E+00
                        0.1998E+02
                                     0.1998E+06
0.1000E+00 0.3000E+00
                        0.1897E+02
                                     0.1898E+06
0.3000E+00 0.3000E+00
                        0.3745E+02
                                    0.3744E+06
0.5000E+00 0.3000E+00
                        0.2815E+02
                                     0.2815E+06
0.7000E+00 0.3000E+00
                        0.2379E+02
                                     0.2380E+06
                                     0.6074E+06
0.9000E+00 0.3000E+00
                        0.6076E+02
0.0000E+00 0.4000E+00
                        0.1274E+02
                                     0.1275E+06
0.2000E+00 0.4000E+00
                        0.1763E+02
                                     0.1764E+06
0.4000E+00 0.4000E+00
                        0.5816E+02
                                     0.5813E+06
0.6000E+00 0.4000E+00
                        0.1425E+02
                                     0.1428E+06
0.8000E+00 0.4000E+00
                        0.5783E+02
                                     0.5782E+06
0.1000E+01 0.4000E+00
                        0.6492E+02
                                     0.6492E+06
                                     0.3109E+06
0.1000E+00 0.5000E+00
                        0.3109E+02
0.3000E+00 0.5000E+00
                        0.2815E+02
                                     0.2815E+06
0.5000E+00 0.5000E+00
                        0.2966E+02
                                     0.2966E+06
0.7000E+00 0.5000E+00
                        0.3422E+02
                                     0.3422E+06
                                     0.4003E+06
0.9000E+00 0.5000E+00
                        0.4004E+02
0.0000E+00 0.6000E+00
                        0.5217E+02
                                     0.5217E+06
0.2000E+00 0.6000E+00
                        0.4849E+02
                                     0.4848E+06
                                     0.1428E+06
0.4000E+00 0.6000E+00
                        0.1425E+02
                        0.7001E+02
                                     0.6998E+06
0.6000E+00 0.6000E+00
0.8000E+00 0.6000E+00
                        0.2397E+02
                                     0.2398E+06
0.1000E+01 0.6000E+00
                        0.1981E+02
                                     0.1981E+06
0.1000E+00 0.7000E+00
                        0.5115E+02
                                     0.5114E+06
0.3000E+00 0.7000E+00
                        0.2379E+02
                                     0.2380E+06
0.5000E+00 0.7000E+00
                        0.3422E+02
                                     0.3422E+06
0.7000E+00 0.7000E+00
                        0.5069E+02
                                     0.5067E+06
0.9000E+00 0.7000E+00
                        0.3143E+02
                                     0.3145E+06
                        0.1684E+02
                                     0.1684E+06
0.0000E+00 0.8000E+00
0.2000E+00 0.8000E+00
                        0.2308E+02
                                     0.2309E+06
0.4000E+00 0.8000E+00
                        0.5783E+02
                                     0.5781E+06
0.6000E+00 0.8000E+00
                        0.2397E+02
                                     0.2398E+06
0.8000E+00 0.8000E+00
                        0.7164E+02
                                     0.7162E+06
0.1000E+01 0.8000E+00
                        0.8397E+02
                                     0.8397E+06
0.1000E+00 0.9000E+00
                        0.6498E+01
                                     0.6526E+05
0.3000E+00 0.9000E+00
                        0.6076E+02
                                     0.6074E+06
0.5000E+00 0.9000E+00
                        0.4004E+02
                                     0.4003E+06
0.7000E+00
           0.9000E+00
                        0.3143E+02
                                     0.3145E+06
0.9000E+00
           0.9000E+00
                        0.1403E+03
                                     0.1403E+07
0.0000E+00 0.1000E+01
                        0.4618E+01
                                     0.4619E+05
0.2000E+00 0.1000E+01
                        0.1998E+02
                                     0.1998E+06
0.4000E+00 0.1000E+01
                        0.6492E+02
                                     0.6491E+06
0.6000E+00 0.1000E+01
                        0.1980E+02
                                     0.1980E+06
0.8000E+00 0.1000E+01
                        0.8397E+02
                                     0.8396E+06
0.1000E+01 0.1000E+01
                        0.1075E+03
                                     0.1075E+07
```

Statistics:

```
Time = 0.0250
```

Total number of accepted timesteps = 29
Total number of rejected timesteps = 0

Total number of

	Residual	Jacobian	Newton	Lin sys
	evals	evals	iters	iters
At level				
1	406	29	58	87
2	378	27	54	79
3	280	20	40	61
4	98	7	14	27
	Махі	i mum r	number	o f
	Newtor	n iters	Lin sys it	ers
At level				
1	2	2	2	
2	2	2	2	
3	2	2	3	
4	2	2	3	

 $D03RAF.28 \; (last)$ [NP3086/18/pdf]