NAG C Library Function Document

nag_pde_parab_1d_cd_ode_remesh (d03psc)

1 Purpose

nag_pde_parab_1d_cd_ode_remesh (d03psc) integrates a system of linear or nonlinear convection-diffusion equations in one space dimension, with optional source terms and scope for coupled ordinary differential equations (ODEs). The system must be posed in conservative form. This function also includes the option of automatic adaptive spatial remeshing. Convection terms are discretised using a sophisticated upwind scheme involving a user-supplied numerical flux function based on the solution of a Riemann problem at each mesh point. The method of lines is employed to reduce the partial differential equations (PDEs) to a system of ODEs, and the resulting system is solved using a backward differentiation formula (BDF) method or a Theta method.

2 Specification

```
void nag_pde_parab_1d_cd_ode_remesh (Integer npde, double *ts, double tout,
     void (*pdedef)(Integer npde, double t, double x, const double u[],
          const double ux[], Integer ncode, const double v[], const double vdot[],
          double p[], double c[], double d[], double s[], Integer *ires,
          Nag_Comm *comm),
     void (*numflx)(Integer npde, double t, double x, Integer ncode,
          const double v[], const double uleft[], const double uright[],
          double flux[], Integer *ires, Nag_Comm *comm, Nag_D03_Save *saved),
     void (*bndary)(Integer npde, Integer npts, double t, const double x[],
          const double u[], Integer ncode, const double v[], const double vdot[],
          Integer ibnd, double g[], Integer *ires, Nag_Comm *comm),
     void (*uvinit)(Integer npde, Integer npts, Integer nxi, const double x[],
          const double xi[], double u[], Integer ncode, double v[],
          Nag_Comm *comm),
     double u[], Integer npts, double x[], Integer ncode,
     void (*odedef)(Integer npde, double t, Integer ncode, const double v[],
          const double vdot[], Integer nxi, const double xi[], const double ucp[],
          const double ucpx[], const double ucpt[], double r[], Integer *ires,
          Nag_Comm *comm),
     Integer nxi, const double xi[], Integer neqn, const double rtol[],
     const double atol[], Integer itol, Nag_NormType norm, Nag_LinAlgOption laopt,
     const double algopt[], Boolean remesh, Integer nxfix, const double xfix[],
     Integer nrmesh, double dxmesh, double trmesh, Integer ipminf, double xratio,
     double con,
     void (*monitf)(double t, Integer npts, Integer npde, const double x[],
          const double u[], double fmon[], Nag_Comm *comm),
     double rsave[], Integer lrsave, Integer isave[], Integer lisave, Integer itask,
     Integer itrace, const char *outfile, Integer *ind, Nag_Comm *comm,
     Nag_D03_Save *saved, NagError *fail)
```

3 Description

nag_pde_parab_1d_cd_ode_remesh (d03psc) integrates the system of convection-diffusion equations in conservative form:

$$\sum_{j=1}^{\mathbf{npde}} P_{i,j} \frac{\partial U_j}{\partial t} + \frac{\partial F_i}{\partial x} = C_i \frac{\partial D_i}{\partial x} + S_i, \qquad (1)$$

or the hyperbolic convection-only system:

$$\frac{\partial U_i}{\partial t} + \frac{\partial F_i}{\partial x} = 0, \tag{2}$$

for $i = 1, 2, \ldots, \textbf{npde}$, $a \leq x \leq b$, $t \geq t_0$, where the vector U is the set of PDE solution values

$$U(x,t) = [U_1(x,t), \ldots, U_{\textbf{npde}}(x,t)]^{\mathrm{T}}.$$

The optional coupled ODEs are of the general form

$$R_i(t, V, \dot{V}, \xi, U^*, U_x^*, U_t^*) = 0, \quad i = 1, 2, \ldots, \textbf{ncode}, \tag{3}$$

where the vector V is the set of ODE solution values

$$V(t) = [V_1(t), \ldots, V_{\textbf{ncode}}(t)]^{\mathrm{T}},$$

$\dot{V}$ denotes its derivative with respect to time, and U_x is the spatial derivative of U.

In (2), $P_{i,j}$, F_i and C_i depend on x, t, U and V; D_i depends on x, t, U, U_x and V; and S_i depends on x, t, U, V and **linearly** on $\dot{V}$. Note that $P_{i,j}$, F_i, C_i and S_i must not depend on any space derivatives, and $P_{i,j}$, F_i, C_i and D_i must not depend on any time derivatives. In terms of conservation laws, F_i, $C_i \partial D_i / \partial x$ and S_i are the convective flux, diffusion and source terms respectively.

In (3), ξ represents a vector of n_ξ spatial coupling points at which the ODEs are coupled to the PDEs. These points may or may not be equal to PDE spatial mesh points. U^*, U_x^* and U_t^* are the functions U, U_x and U_t evaluated at these coupling points. Each R_i may depend only linearly on time derivatives. Hence (3) may be written more precisely as

$$R = L - M\dot{V} - NU_t^*, \tag{4}$$

where $R = [R_1, \ldots, R_{\textbf{ncode}}]^T$, L is a vector of length **ncode**, M is an **ncode** by **ncode** matrix, N is an **ncode** by $(n_\xi \times \textbf{npde})$ matrix and the entries in L, M and N may depend on t, ξ, U^*, U_x^* and V. In practice the user only needs to supply a vector of information to define the ODEs and not the matrices L, M and N. (See Section 5 for the specification of the user-supplied procedure **odedef**.)

The integration in time is from t_0 to t_{out}, over the space interval $a \leq x \leq b$, where $a = x_1$ and $b = x_{\textbf{npts}}$ are the leftmost and rightmost points of a user-defined mesh $x_1, x_2, \ldots, x_{\textbf{npts}}$ defined initially by the user and (possibly) adapted automatically during the integration according to user-specified criteria.

The initial $(t = t_0)$ values of the functions $U(x,t)$ and $V(t)$ must be specified in a function **uvinit** supplied by the user. Note that **uvinit** will be called again following any initial remeshing, and so $U(x, t_0)$ should be specified for **all** values of x in the interval $a \leq x \leq b$, and not just the initial mesh points.

The PDEs are approximated by a system of ODEs in time for the values of U_i at mesh points using a spatial discretisation method similar to the central-difference scheme used in nag_pde_parab_1d_fd (d03pcc), nag_pde_parab_1d_fd_ode (d03phc) and nag_pde_parab_1d_fd_ode_remesh (d03ppc), but with the flux F_i replaced by a *numerical flux*, which is a representation of the flux taking into account the direction of the flow of information at that point (i.e., the direction of the characteristics). Simple central differencing of the numerical flux then becomes a sophisticated upwind scheme in which the correct direction of upwinding is automatically achieved.

The numerical flux, $\hat{F}_i$ say, must be calculated by the user in terms of the *left* and *right* values of the solution vector U (denoted by U_L and U_R respectively), at each mid-point of the mesh $x_{j-\frac{1}{2}} = (x_{j-1} + x_j)/2$ for $j = 2, 3, \ldots, \textbf{npts}$. The left and right values are calculated by nag_pde_parab_1d_cd_ode_remesh (d03psc) from two adjacent mesh points using a standard upwind technique combined with a Van Leer slope-limiter (see LeVeque (1990)). The physically correct value for $\hat{F}_i$ is derived from the solution of the Riemann problem given by

$$\frac{\partial U_i}{\partial t} + \frac{\partial F_i}{\partial y} = 0, \tag{5}$$

where $y = x - x_{j-\frac{1}{2}}$, i.e., $y = 0$ corresponds to $x = x_{j-\frac{1}{2}}$, with discontinuous initial values $U = U_L$ for $y < 0$ and $U = U_R$ for $y > 0$, using an *approximate Riemann solver*. This applies for either of the systems (1) or (2); the numerical flux is independent of the functions $P_{i,j}$, C_i, D_i and S_i. A description of several approximate Riemann solvers can be found in LeVeque (1990) and Berzins *et al.* (1989). Roe's scheme (Roe (1981)) is perhaps the easiest to understand and use, and a brief summary follows. Consider the system of PDEs $U_t + F_x = 0$ or equivalently $U_t + AU_x = 0$. Provided the system is linear in U, i.e., the Jacobian matrix A does not depend on U, the numerical flux $\hat{F}$ is given by

$$\hat{F} = \tfrac{1}{2}(F_L + F_R) - \tfrac{1}{2}\sum_{k=1}^{\mathbf{npde}} \alpha_k |\lambda_k| e_k, \qquad (6)$$

where F_L (F_R) is the flux F calculated at the left (right) value of U, denoted by U_L (U_R); the λ_k are the eigenvalues of A; the e_k are the right eigenvectors of A; and the α_k are defined by

$$U_R - U_L = \sum_{k=1}^{\mathbf{npde}} \alpha_k e_k. \qquad (7)$$

Examples are given in the documents for nag_pde_parab_1d_cd (d03pfc) and nag_pde_parab_1d_cd_ode (d03plc).

If the system is nonlinear, Roe's scheme requires that a linearized Jacobian is found (see Roe (1981)).

The functions $P_{i,j}$, C_i, D_i and S_i (but **not** F_i) must be specified in a function **pdedef** supplied by the user. The numerical flux $\hat{F}_i$ must be supplied in a separate user-supplied function **numflx**. For problems in the form (2), the actual argument d03plp may be used for **pdedef** (d03plp is included in the NAG C Library; however, its name may be implementation-dependent: see the Users' Note for your implementation for details). d03plp sets the matrix with entries $P_{i,j}$ to the identity matrix, and the functions C_i, D_i and S_i to zero.

For second-order problems i.e., diffusion terms present, a boundary condition is required for each PDE at both boundaries for the problem to be well-posed. If there are no diffusion terms present, then the continuous PDE problem generally requires exactly one boundary condition for each PDE, that is **npde** boundary conditions in total. However, in common with most discretisation schemes for first-order problems, a *numerical boundary condition* is required at the other boundary for each PDE. In order to be consistent with the characteristic directions of the PDE system, the numerical boundary conditions must be derived from the solution inside the domain in some manner (see below). Both types of boundary conditions must be supplied by the user, i.e., a total of **npde** conditions at each boundary point.

The position of each boundary condition should be chosen with care. In simple terms, if information is flowing into the domain then a physical boundary condition is required at that boundary, and a numerical boundary condition is required at the other boundary. In many cases the boundary conditions are simple, e.g., for the linear advection equation. In general the user should calculate the characteristics of the PDE system and specify a physical boundary condition for each of the characteristic variables associated with incoming characteristics, and a numerical boundary condition for each outgoing characteristic.

A common way of providing numerical boundary conditions is to extrapolate the characteristic variables from the inside of the domain (note that when using banded matrix algebra the fixed bandwidth means that only linear extrapolation is allowed, i.e., using information at just two interior points adjacent to the boundary). For problems in which the solution is known to be uniform (in space) towards a boundary during the period of integration then extrapolation is unnecessary; the numerical boundary condition can be supplied as the known solution at the boundary. Another method of supplying numerical boundary conditions involves the solution of the characteristic equations associated with the outgoing characteristics. Examples of both methods can be found in the documents for nag_pde_parab_1d_cd (d03pfc) and nag_pde_parab_1d_cd_ode (d03plc).

The boundary conditions must be specified in a function **bndary** (provided by the user) in the form

$$G_i^L(x,t,U,V,\dot{V}) = 0 \quad \text{at} \quad x = a, \quad i = 1,2,\ldots,\mathbf{npde}, \qquad (8)$$

at the left-hand boundary, and

$$G_i^R(x,t,U,V,\dot{V}) = 0 \quad \text{at} \quad x = b, \quad i = 1,2,\ldots,\mathbf{npde}, \qquad (9)$$

at the right-hand boundary.

Note that spatial derivatives at the boundary are not passed explicitly to the function **bndary**, but they can be calculated using values of U at and adjacent to the boundaries if required. However, it should be noted that instabilities may occur if such one-sided differencing opposes the characteristic direction at the boundary.

The algebraic-differential equation system which is defined by the functions R_i must be specified in a function **odedef** supplied by the user. The user must also specify the coupling points ξ (if any) in the array **xi**.

In total there are **npde** $\times$ **npts** $+$ **ncode** ODEs in the time direction. This system is then integrated forwards in time using a BDF or Theta method, optionally switching between Newton's method and functional iteration (see Berzins *et al.* (1989) and the references therein).

The adaptive space remeshing can be used to generate meshes that automatically follow the changing time-dependent nature of the solution, generally resulting in a more efficient and accurate solution using fewer mesh points than may be necessary with a fixed uniform or non-uniform mesh. Problems with travelling wavefronts or variable-width boundary layers for example will benefit from using a moving adaptive mesh. The discrete time-step method used here (developed by Furzeland (1984)) automatically creates a new mesh based on the current solution profile at certain time-steps, and the solution is then interpolated onto the new mesh and the integration continues.

The method requires the user to supply a function **monitf** which specifies in an analytical or numerical form the particular aspect of the solution behaviour the user wishes to track. This so-called monitor function is used by the functions to choose a mesh which equally distributes the integral of the monitor function over the domain. A typical choice of monitor function is the second space derivative of the solution value at each point (or some combination of the second space derivatives if there is more than one solution component), which results in refinement in regions where the solution gradient is changing most rapidly.

The user specifies the frequency of mesh updates together with certain other criteria such as adjacent mesh ratios. Remeshing can be expensive and the user is encouraged to experiment with the different options in order to achieve an efficient solution which adequately tracks the desired features of the solution.

Note that unless the monitor function for the initial solution values is zero at all user-specified initial mesh points, a new initial mesh is calculated and adopted according to the user-specified remeshing criteria. The function **uvinit** will then be called again to determine the initial solution values at the new mesh points (there is no interpolation at this stage) and the integration proceeds.

The problem is subject to the following restrictions:

(i) In (1), $\dot{V}_j(t)$, for $j = 1, 2, \ldots,$ **ncode**, may only appear **linearly** in the functions S_i, for $i = 1, 2, \ldots,$ **npde**, with a similar restriction for G_i^L and G_i^R;

(ii) $P_{i,j}$, F_i, C_i and S_i must not depend on any space derivatives; and $P_{i,j}$, C_i, D_i and F_i must not depend on any time derivatives;

(iii) $t_0 < t_{\text{out}}$, so that integration is in the forward direction;

(iv) The evaluation of the terms $P_{i,j}$, C_i, D_i and S_i is done by calling the function **pdedef** at a point approximately midway between each pair of mesh points in turn. Any discontinuities in these functions **must** therefore be at one or more of the **fixed** mesh points specified by **xfix**;

(v) At least one of the functions $P_{i,j}$ must be non-zero so that there is a time derivative present in the PDE problem.

For further details of the scheme, see Pennington and Berzins (1994) and the references therein.

4 References

Berzins M, Dew P M and Furzeland R M (1989) Developing software for time-dependent problems using the method of lines and differential-algebraic integrators *Appl. Numer. Math.* **5** 375–397

Furzeland R M (1984) The construction of adaptive space meshes *TNER.85.022* Thornton Research Centre, Chester

Hirsch C (1990) *Numerical Computation of Internal and External Flows, Volume 2: Computational Methods for Inviscid and Viscous Flows* John Wiley

LeVeque R J (1990) *Numerical Methods for Conservation Laws* Birkhäuser Verlag

Pennington S V and Berzins M (1994) New NAG Library software for first-order partial differential equations *ACM Trans. Math. Softw.* **20** 63–99

Roe P L (1981) Approximate Riemann solvers, parameter vectors, and difference schemes *J. Comput. Phys.* **43** 357–372

5 Parameters

1: **npde** – Integer *Input*

On entry: the number of PDEs to be solved.

Constraint: **npde** ≥ 1.

2: **ts** – double * *Input/Output*

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

On exit: the value of t corresponding to the solution values in **u**. Normally **ts** = **tout**.

Constraint: **ts** < **tout**.

3: **tout** – double *Input*

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

4: **pdedef** *Function*

pdedef must evaluate the functions $P_{i,j}$, C_i, D_i and S_i which partially define the system of PDEs. $P_{i,j}$ and C_i may depend on x, t, U and V; D_i may depend on x, t, U, U_x and V; and S_i may depend on x, t, U, V and linearly on $\dot{V}$. **pdedef** is called approximately midway between each pair of mesh points in turn by nag_pde_parab_1d_cd_ode_remesh (d03psc). The actual argument d03plp may be used for **pdedef** for problems in the form (2) (d03plp is included in the NAG C Library; however, its name may be implementation-dependent: see the Users' Note for your implementation for details).

Its specification is:

```
void pdedef (Integer npde, double t, double x, const double u[],
     const double ux[], Integer ncode, const double v[], const double vdot[],
     double p[], double c[], double d[], double s[], Integer *ires,
     Nag_Comm *comm)
```

1: **npde** – Integer *Input*

On entry: the number of PDEs in the system.

2: **t** – double *Input*

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

3: **x** – double *Input*

On entry: the current value of the space variable x.

4: **u**[**npde**] – const double *Input*

On entry: **u**$[i-1]$ contains the value of the component $U_i(x,t)$, for $i = 1, \ldots,$ **npde**.

5: **ux**[**npde**] – const double *Input*

On entry: **ux**[$i-1$] contains the value of the component $\partial U_i(x,t)/\partial x$, for $i = 1,2,\ldots,$ **npde**.

6: **ncode** – Integer *Input*

On entry: the number of coupled ODEs in the system.

7: **v**[**ncode**] – const double *Input*

On entry: **v**[$i-1$] contains the value of component $V_i(t)$, for $i = 1,2,\ldots,$ **ncode**.

8: **vdot**[**ncode**] – const double *Input*

On entry: **vdot**[$i-1$] contains the value of component $\dot{V}_i(t)$, for $i = 1,2,\ldots,$ **ncode**.

Note: $\dot{V}_i(t)$, for $i = 1,2,\ldots,$ **ncode**, may only appear linearly in S_j, for $j = 1,2,\ldots,$ **npde**.

9: **p**[**npde** $\times$ **npde**] – double *Output*

Note: where $\mathbf{P}(i,j)$ appears in this document it refers to the array element **p**[**npde** $\times (j-1)+i-1$]. We recommend using a #define to make the same definition in your calling program.

On exit: $\mathbf{P}(i,j)$ must be set to the value of $P_{i,j}(x,t,U,V)$, for $i,j = 1,2,\ldots,$ **npde**.

10: **c**[**npde**] – double *Output*

On exit: **c**[$i-1$] must be set to the value of $C_i(x,t,U,V)$, for $i = 1,2,\ldots,$ **npde**.

11: **d**[**npde**] – double *Output*

On exit: **d**[$i-1$] must be set to the value of $D_i(x,t,U,U_x,V)$, for $i = 1,2,\ldots,$ **npde**.

12: **s**[**npde**] – double *Output*

On exit: **s**[$i-1$] must be set to the value of $S_i(x,t,U,V,\dot{V})$, for $i = 1,2,\ldots,$ **npde**.

13: **ires** – Integer * *Input/Output*

On entry: set to -1 or 1.

On exit: should usually remain unchanged. However, the user may set **ires** to force the integration function to take certain actions as described below:

ires $= 2$

Indicates to the integrator that control should be passed back immediately to the calling function with the error indicator set to **fail.code** = **NE_USER_STOP**.

ires $= 3$

Indicates to the integrator that the current time step should be abandoned and a smaller time step used instead. The user may wish to set **ires** $= 3$ when a physically meaningless input or output value has been generated. If the user consecutively sets **ires** $= 3$, then nag_pde_parab_1d_cd_ode_remesh (d03psc) returns to the calling function with the error indicator set to **fail.code** = **NE_FAILED_DERIV**.

14: **comm** – NAG_Comm * *Input/Output*

The NAG communication parameter (see the Essential Introduction).

5: **numflx** *Function*

numflx must supply the numerical flux for each PDE given the *left* and *right* values of the solution vector **u**. **numflx** is called approximately midway between each pair of mesh points in turn by nag_pde_parab_1d_cd_ode_remesh (d03psc).

Its specification is:

```
void numflx (Integer npde, double t, double x, Integer ncode, const double v[],
     const double uleft[], const double uright[], double flux[], Integer *ires,
     Nag_Comm *comm, Nag_D03_Save *saved)
```

1: **npde** – Integer *Input*

On entry: the number of PDEs in the system.

2: **t** – double *Input*

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

3: **x** – double *Input*

On entry: the current value of the space variable x.

4: **ncode** – Integer *Input*

On entry: the number of coupled ODEs in the system.

5: **v**[**ncode**] – const double *Input*

On entry: **v**$[i-1]$ contains the value of the component $V_i(t)$, for $i = 1, 2, \ldots,$ **ncode**.

6: **uleft**[**npde**] – const double *Input*

On entry: **uleft**$[i-1]$ contains the *left* value of the component $U_i(x)$, for $i = 1, 2, \ldots,$ **npde**.

7: **uright**[**npde**] – const double *Input*

On entry: **uright**$[i-1]$ contains the *right* value of the component $U_i(x)$, for $i = 1, 2, \ldots,$ **npde**.

8: **flux**[**npde**] – double *Output*

On exit: **flux**$[i-1]$ must be set to the numerical flux $\hat{F}_i$, for $i = 1, 2, \ldots,$ **npde**.

9: **ires** – Integer * *Input/Output*

On entry: set to -1 or 1.

On exit: should usually remain unchanged. However, the user may set **ires** to force the integration function to take certain actions as described below:

ires $= 2$

Indicates to the integrator that control should be passed back immediately to the calling function with the error indicator set to **fail.code** = **NE_USER_STOP**.

ires $= 3$

Indicates to the integrator that the current time step should be abandoned and a smaller time step used instead. The user may wish to set **ires** $= 3$ when a physically meaningless input or output value has been generated. If the user consecutively sets **ires** $= 3$, then nag_pde_parab_1d_cd_ode_remesh (d03psc) returns to the calling function with the error indicator set to **fail.code** = **NE_FAILED_DERIV**.

10: **comm** – NAG_Comm * *Input/Output*

The NAG communication parameter (see the Essential Introduction).

11: **saved** – Nag_D03_Save * *Input/Output*

On entry: contains the current state of saved data concerning the computation. If **numflx** calls one of the approximate Riemann solvers nag_pde_parab_1d_euler_roe (d03puc), nag_pde_parab_1d_euler_osher (d03pvc), nag_pde_parab_1d_euler_hll (d03pwc), or nag_pde_parab_1d_euler_exact (d03pxc) then **saved** should be passed through unchanged to that function.

On exit: the user should not change the components of **saved**.

6: **bndary** *Function*

bndary must evaluate the functions G_i^L and G_i^R which describe the physical and numerical boundary conditions, as given by (8) and (9).

Its specification is:

```
void bndary (Integer npde, Integer npts, double t, const double x[],
     const double u[], Integer ncode, const double v[], const double vdot[],
     Integer ibnd, double g[], Integer *ires, Nag_Comm *comm)
```

1: **npde** – Integer *Input*

On entry: the number of PDEs in the system.

2: **npts** – Integer *Input*

On entry: the number of mesh points in the interval $[a, b]$.

3: **t** – double *Input*

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

4: **x**[**npts**] – const double *Input*

On entry: the mesh points in the spatial direction. **x**[0] corresponds to the left-hand boundary, a, and **x**[**npts** $-$ 1] corresponds to the right-hand boundary, b.

5: **u**[**npde** $\times$ **npts**] – const double *Input*

Note: where $\mathbf{U}(i, j)$ appears in this document it refers to the array element **u**[**npde** $\times (j-1)+i-1$]. We recommend using a #define to make the same definition in your calling program.

On entry: $\mathbf{U}(i, j)$ contains the value of the component $U_i(x, t)$ at $x =$ **x**[$j-1$] for $i = 1, 2, \ldots,$ **npde**; $j = 1, 2, \ldots,$ **npts**.

Note: if banded matrix algebra is to be used then the functions G_i^L and G_i^R may depend on the value of $U_i(x, t)$ at the boundary point and the two adjacent points only.

6: **ncode** – Integer *Input*

On entry: the number of coupled ODEs in the system.

7: **v**[**ncode**] – const double *Input*

On entry: **v**[$i-1$] contains the value of component $V_i(t)$, for $i = 1, 2, \ldots,$ **ncode**.

8: **vdot**[**ncode**] – const double *Input*

On entry: **vdot**[$i-1$] contains the value of component $\dot{V}_i(t)$, for $i = 1, 2, \ldots,$ **ncode**.

Note: $\dot{V}_i(t)$, for $i = 1, 2, \ldots,$ **ncode**, may only appear linearly in G^L_j and G^R_j, for $j = 1, 2, \ldots,$ **npde**.

9: **ibnd** – Integer *Input*

On entry: specifies which boundary conditions are to be evaluated. If **ibnd** $= 0$, then **bndary** must evaluate the left-hand boundary condition at $x = a$. If **ibnd** $\neq 0$, then **bndary** must evaluate the right-hand boundary condition at $x = b$.

10: **g**[**npde**] – double *Output*

On exit: **g**$[i-1]$ must contain the ith component of either G^L_i or G^R_i in (8) and (9), depending on the value of **ibnd**, for $i = 1, 2, \ldots,$ **npde**.

11: **ires** – Integer * *Input/Output*

On entry: set to -1 or 1.

On exit: should usually remain unchanged. However, the user may set **ires** to force the integration function to take certain actions as described below:

ires $= 2$

Indicates to the integrator that control should be passed back immediately to the calling function with the error indicator set to **fail.code** = **NE_USER_STOP**.

ires $= 3$

Indicates to the integrator that the current time step should be abandoned and a smaller time step used instead. The user may wish to set **ires** $= 3$ when a physically meaningless input or output value has been generated. If the user consecutively sets **ires** $= 3$, then nag_pde_parab_1d_cd_ode_remesh (d03psc) returns to the calling function with the error indicator set to **fail.code** = **NE_FAILED_DERIV**.

12: **comm** – NAG_Comm * *Input/Output*

The NAG communication parameter (see the Essential Introduction).

7: **uvinit** *Function*

uvinit must supply the initial $(t = t_0)$ values of $U(x,t)$ and $V(t)$ for all values of x in the interval $a \leq x \leq b$.

Its specification is:

```
void uvinit (Integer npde, Integer npts, Integer nxi, const double x[],
      const double xi[], double u[], Integer ncode, double v[], Nag_Comm *comm)
```

1: **npde** – Integer *Input*

On entry: the number of PDEs in the system.

2: **npts** – Integer *Input*

On entry: the number of mesh points in the interval $[a, b]$.

3: **nxi** – Integer *Input*

On entry: the number of ODE/PDE coupling points.

4: **x**[**npts**] – const double *Input*

On entry: the current mesh. **x**$[i-1]$ contains the value of x_i for $i = 1, 2, \ldots,$ **npts**.

5: **xi**[**nxi**] – const double *Input*

On entry: **xi**$[i-1]$ contains the ODE/PDE coupling point, ξ_i, for $i = 1, 2, \ldots,$ **nxi**.

6: **u**[**npde** × **npts**] – double *Output*

Note: where $\mathbf{U}(i, j)$ appears in this document it refers to the array element **u**[**npde** $\times (j-1) + i - 1$]. We recommend using a #define to make the same definition in your calling program.

On exit: $\mathbf{U}(i, j)$ contains the value of the component $U_i(x_j, t_0)$, for $i = 1, 2, \ldots,$ **npde**; $j = 1, 2, \ldots,$ **npts**.

7: **ncode** – Integer *Input*

On entry: the number of coupled ODEs in the system.

8: **v**[**ncode**] – double *Output*

On exit: **v**$[i-1]$ must contain the value of component $V_i(t_0)$ for $i = 1, 2, \ldots,$ **ncode**.

9: **comm** – NAG_Comm * *Input/Output*

The NAG communication parameter (see the Essential Introduction).

8: **u**[**neqn**] – double *Input/Output*

On entry: if **ind** $= 1$ the value of **u** must be unchanged from the previous call.

On exit: **u**[**npde** $\times (j-1) + i - 1$] contains the computed solution $U_i(x_j, t)$, for $i = 1, 2, \ldots,$ **npde**; $j = 1, 2, \ldots,$ **npts**, and **u**[**npts** × **npde** $+ k - 1$] contains $V_k(t)$, for $k = 1, 2, \ldots,$ **ncode**, all evaluated at $t =$ **ts**.

9: **npts** – Integer *Input*

On entry: the number of mesh points in the interval $[a, b]$.

Constraint: **npts** ≥ 3.

10: **x**[**npts**] – double *Input/Output*

On entry: the mesh points in the space direction. **x**[0] must specify the left-hand boundary, a, and **x**[**npts** $- 1$] must specify the right-hand boundary, b.

Constraint: **x**$[0] <$ **x**$[1] < \ldots <$ **x**[**npts** $- 1$].

On exit: the final values of the mesh points.

11: **ncode** – Integer *Input*

On entry: the number of coupled ODE components.

Constraint: **ncode** ≥ 0.

12: **odedef** *Function*

odedef must evaluate the functions R, which define the system of ODEs, as given in (4). If the user wishes to compute the solution of a system of PDEs only (i.e., **ncode** $= 0$), **odedef** must be the dummy function d03pek. (d03pek is included in the NAG C Library; however, its name may be implementation-dependent: see the Users' Note for your implementation for details.)

Its specification is:

```
void odedef (Integer npde, double t, Integer ncode, const double v[],
     const double vdot[], Integer nxi, const double xi[], const double ucp[],
     const double ucpx[], const double ucpt[], double r[], Integer *ires,
     Nag_Comm *comm)
```

1: **npde** – Integer *Input*

On entry: the number of PDEs in the system.

2: **t** – double *Input*

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

3: **ncode** – Integer *Input*

On entry: the number of coupled ODEs in the system.

4: **v**[**ncode**] – const double *Input*

On entry: **v**$[i-1]$ contains the value of component $V_i(t)$, for $i = 1, 2, \ldots,$ **ncode**.

5: **vdot**[**ncode**] – const double *Input*

On entry: **vdot**$[i-1]$ contains the value of component $\dot{V}_i(t)$, for $i = 1, 2, \ldots,$ **ncode**.

6: **nxi** – Integer *Input*

On entry: the number of ODE/PDE coupling points.

7: **xi**[**nxi**] – const double *Input*

On entry: **xi**$[i-1]$ contains the ODE/PDE coupling point, ξ_i, for $i = 1, 2, \ldots,$ **nxi**.

8: **ucp**[**npde** × **nxi**] – const double *Input*

Note: where **UCP**(i,j) appears in this document it refers to the array element **ucp**[**npde** $\times (j-1)+i-1]$. We recommend using a #define to make the same definition in your calling program.

On entry: **UCP**(i,j) contains the value of $U_i(x,t)$ at the coupling point $x = \xi_j$, for $i = 1, 2, \ldots,$ **npde**; $j = 1, 2, \ldots,$ **nxi**.

9: **ucpx**[**npde** × **nxi**] – const double *Input*

Note: where **UCPX**(i,j) appears in this document it refers to the array element **ucpx**[**npde** $\times (j-1)+i-1]$. We recommend using a #define to make the same definition in your calling program.

On entry: **UCPX**(i,j) contains the value of $(\partial U_i(x,t))/(\partial x)$ at the coupling point $x = \xi_j$, for $i = 1, 2, \ldots,$ **npde**; $j = 1, 2, \ldots,$ **nxi**.

10: **ucpt**[**npde** × **nxi**] – const double *Input*

Note: where **UCPT**(i,j) appears in this document it refers to the array element **ucpt**[**npde** $\times (j-1)+i-1]$. We recommend using a #define to make the same definition in your calling program.

On entry: **UCPT**(i,j) contains the value of $(\partial U_i)/(\partial t)$ at the coupling point $x = \xi_j$, for $i = 1, 2, \ldots,$ **npde**; $j = 1, 2, \ldots,$ **nxi**.

11: **r**[**ncode**] – double *Output*

On exit: **r**$[i-1]$ must contain the ith component of R, for $i = 1, 2, \ldots,$ **ncode**, where R is defined as

$$R = L - M\dot{V} - NU_t^*, \tag{10}$$

or

$$R = -M\dot{V} - NU_t^*. \tag{11}$$

The definition of **r** is determined by the input value of **ires**.

12: **ires** – Integer * *Input/Output*

On entry: the form of R that must be returned in the array R. If **ires** $= 1$, then the equation (10) above must be used. If **ires** $= -1$, then the equation (11) above must be used.

On exit: should usually remain unchanged. However, the user may reset **ires** to force the integration function to take certain actions as described below:

ires $= 2$

Indicates to the integrator that control should be passed back immediately to the calling function with the error indicator set to **fail.code** = **NE_USER_STOP**.

ires $= 3$

Indicates to the integrator that the current time step should be abandoned and a smaller time step used instead. The user may wish to set **ires** $= 3$ when a physically meaningless input or output value has been generated. If the user consecutively sets **ires** $= 3$, then nag_pde_parab_1d_cd_ode_remesh (d03psc) returns to the calling function with the error indicator set to **fail.code** = **NE_FAILED_DERIV**.

13: **comm** – NAG_Comm * *Input/Output*

The NAG communication parameter (see the Essential Introduction).

13: **nxi** – Integer *Input*

On entry: the number of ODE/PDE coupling points.

Constraints:

if **ncode** $= 0$, **nxi** $= 0$;
if **ncode** > 0, **nxi** ≥ 0.

14: **xi**[dim] – const double *Input*

Note: the dimension, dim, of the array **xi** must be at least **nxi**.

On entry: **xi**[$i-1$], $i = 1, 2, \ldots,$ **nxi**, must be set to the ODE/PDE coupling points.

Constraint: **x**[0] $\leq$ **xi**[0] $<$ **xi**[1] $< \ldots <$ **xi**[**nxi** -1] $\leq$ **x**[**npts** -1].

15: **neqn** – Integer *Input*

On entry: the number of ODEs in the time direction.

Constraint: **neqn** = **npde** $\times$ **npts** $+$ **ncode**.

16: **rtol**[dim] – const double *Input*

Note: the dimension, dim, of the array **rtol** must be at least 1 when **itol** $= 1$ or 2 and at least **neqn** when **itol** $= 3$ or 4.

On entry: the relative local error tolerance.

Constraint: **rtol**[$i-1$] ≥ 0 for all relevant i.

17: **atol**[dim] – const double *Input*

Note: the dimension, dim, of the array **atol** must be at least 1 when **itol** $= 1$ or 3 and at least **neqn** when **itol** $= 2$ or 4.

On entry: the absolute local error tolerance.

Constraint: **atol**$[i-1] \geq 0$ for all relevant i.

18: **itol** – Integer *Input*

On entry: a value to indicate the form of the local error test. If e_i is the estimated local error for $\mathbf{u}[i-1]$, $i = 1, 2, \ldots, \mathbf{neqn}$, and $\| \quad \|$ denotes the norm, then the error test to be satisfied is $\|e_i\| < 1.0$. **itol** indicates to nag_pde_parab_1d_cd_ode_remesh (d03psc) whether to interpret either or both of **rtol** and **atol** as a vector or scalar in the formation of the weights w_i used in the calculation of the norm (see the description of the parameter **norm** below):

itol	**rtol**	**atol**	w_i
1	scalar	scalar	$\mathbf{rtol}[0] \times \lvert\mathbf{u}[i-1]\rvert + \mathbf{atol}[0]$
2	scalar	vector	$\mathbf{rtol}[0] \times \lvert\mathbf{u}[i-1]\rvert + \mathbf{atol}[i-1]$
3	vector	scalar	$\mathbf{rtol}[i-1] \times \lvert\mathbf{u}[i-1]\rvert + \mathbf{atol}[0]$
4	vector	vector	$\mathbf{rtol}[i-1] \times \lvert\mathbf{u}[i-1]\rvert + \mathbf{atol}[i-1]$

Constraint: $1 \leq$ **itol** ≤ 4.

19: **norm** – Nag_NormType *Input*

On entry: the type of norm to be used. Two options are available:

norm = **Nag_OneNorm**

Averaged L_1 norm.

norm = **Nag_TwoNorm**

Averaged L_2 norm.

If U_{norm} denotes the norm of the vector **u** of length **neqn**, then for the averaged L_1 norm

$$U_{norm} = \frac{1}{\mathbf{neqn}} \sum_{i=1}^{\mathbf{neqn}} \mathbf{u}[i-1]/w_i,$$

and for the averaged L_2 norm

$$U_{norm} = \sqrt{\frac{1}{\mathbf{neqn}} \sum_{i=1}^{\mathbf{neqn}} (\mathbf{u}[i-1]/w_i)^2},$$

See the description of parameter **itol** for the formulation of the weight vector w.

Constraint: **norm** = **Nag_OneNorm** or **Nag_TwoNorm**.

20: **laopt** – Nag_LinAlgOption *Input*

On entry: the type of matrix algebra required. The possible choices are:

laopt = **Nag_LinAlgFull**

Full matrix methods to be used.

laopt = **Nag_LinAlgBand**

Banded matrix methods to be used.

laopt = **Nag_LinAlgSparse**

Sparse matrix methods to be used.

Constraint: **laopt** = **Nag_LinAlgFull**, **Nag_LinAlgBand** or **Nag_LinAlgSparse**.

Note: the user is recommended to use the banded option when no coupled ODEs are present (**ncode** $= 0$). Also, the banded option should not be used if the boundary conditions involve solution components at points other than the boundary and the immediately adjacent two points

21: **algopt**[30] – const double *Input*

On entry: **algopt** may be set to control various options available in the integrator. If the user wishes to employ all the default options, then **algopt**[0] should be set to 0.0. Default values will also be used for any other elements of **algopt** set to zero. The permissible values, default values, and meanings are as follows:

algopt[0] selects the ODE integration method to be used. If **algopt**[0] $= 1.0$, a BDF method is used and if **algopt**[0] $= 2.0$, a Theta method is used. The default is **algopt**[0] $= 1.0$.

If **algopt**[0] $= 2.0$, then **algopt**[i], for $i = 1, 2, 3$ are not used.

algopt[1] specifies the maximum order of the BDF integration formula to be used. **algopt**[1] may be 1.0, 2.0, 3.0, 4.0 or 5.0. The default value is **algopt**[1] $= 5.0$.

algopt[2] specifies what method is to be used to solve the system of nonlinear equations arising on each step of the BDF method. If **algopt**[2] $= 1.0$ a modified Newton iteration is used and if **algopt**[2] $= 2.0$ a functional iteration method is used. If functional iteration is selected and the integrator encounters difficulty, then there is an automatic switch to the modified Newton iteration. The default value is **algopt**[2] $= 1.0$.

algopt[3] specifies whether or not the Petzold error test is to be employed. The Petzold error test results in extra overhead but is more suitable when algebraic equations are present, such as $P_{i,j} = 0.0$, for $j = 1, 2, \ldots,$ **npde** for some i or when there is no $\dot{V}_i(t)$ dependence in the coupled ODE system. If **algopt**[3] $= 1.0$, then the Petzold test is used. If **algopt**[3] $= 2.0$, then the Petzold test is not used. The default value is **algopt**[3] $= 1.0$.

If **algopt**[0] $= 1.0$, then **algopt**[i], for $i = 4, 5, 6$ are not used.

algopt[4], specifies the value of Theta to be used in the Theta integration method.

$0.51 \leq$ **algopt**[4] ≤ 0.99. The default value is **algopt**[4] $= 0.55$.

algopt[5] specifies what method is to be used to solve the system of nonlinear equations arising on each step of the Theta method. If **algopt**[5] $= 1.0$, a modified Newton iteration is used and if **algopt**[5] $= 2.0$, a functional iteration method is used. The default value is **algopt**[5] $= 1.0$.

algopt[6] specifies whether or not the integrator is allowed to switch automatically between modified Newton and functional iteration methods in order to be more efficient. If **algopt**[6] $= 1.0$, then switching is allowed and if **algopt**[6] $= 2.0$, then switching is not allowed. The default value is **algopt**[6] $= 1.0$.

algopt[10] specifies a point in the time direction, t_{crit}, beyond which integration must not be attempted. The use of t_{crit} is described under the parameter **itask**. If **algopt**[0] $\neq 0.0$, a value of 0.0 for **algopt**[10], say, should be specified even if **itask** subsequently specifies that t_{crit} will not be used.

algopt[11] specifies the minimum absolute step size to be allowed in the time integration. If this option is not required, **algopt**[11] should be set to 0.0.

algopt[12] specifies the maximum absolute step size to be allowed in the time integration. If this option is not required, **algopt**[12] should be set to 0.0.

algopt[13] specifies the initial step size to be attempted by the integrator. If **algopt**[13] $= 0.0$, then the initial step size is calculated internally.

algopt[14] specifies the maximum number of steps to be attempted by the integrator in any one call. If **algopt**[14] $= 0.0$, then no limit is imposed.

algopt[22] specifies what method is to be used to solve the nonlinear equations at the initial point to initialise the values of U, U_t, V and $\dot{V}$. If **algopt**[22] $= 1.0$, a modified Newton iteration is used and if **algopt**[22] $= 2.0$, functional iteration is used. The default value is **algopt**[22] $= 1.0$.

algopt[28] and **algopt**[29] are used only for the sparse matrix algebra option, i.e., **laopt** = **Nag_LinAlgSparse**.

algopt[28] governs the choice of pivots during the decomposition of the first Jacobian matrix. It should lie in the range $0.0 <$ **algopt**[28] < 1.0, with smaller values biasing the algorithm towards maintaining sparsity at the expense of numerical stability. If **algopt**[28] lies outside the range then the default value is used. If the functions regard the Jacobian matrix as numerically singular, then increasing **algopt**[28] towards 1.0 may help, but at the cost of increased fill-in. The default value is **algopt**[28] $= 0.1$.

algopt[29] is used as the relative pivot threshold during subsequent Jacobian decompositions (see **algopt**[28]) below which an internal error is invoked. **algopt**[29] must be greater than zero, otherwise the default value is used. If **algopt**[29] is greater than 1.0 no check is made on the pivot size, and this may be a necessary option if the Jacobian matrix is found to be numerically singular (see **algopt**[28]). The default value is **algopt**[29] $= 0.0001$.

22: **remesh** – Boolean *Input*

On entry: indicates whether or not spatial remeshing should be performed.

remesh = **TRUE**

Indicates that spatial remeshing should be performed as specified.

remesh = **FALSE**

Indicates that spatial remeshing should be suppressed.

Note: **remesh** should **not** be changed between consecutive calls to nag_pde_parab_1d_cd_ode_remesh (d03psc). Remeshing can be switched off or on at specified times by using appropriate values for the parameters **nrmesh** and **trmesh** at each call.

23: **nxfix** – Integer *Input*

On entry: the number of fixed mesh points.

Constraint: $0 \leq$ **nxfix** $\leq$ **npts** $- 2$.

Note: the end-points **x**[0] and **x**[**npts** $- 1$] are fixed automatically and hence should not be specified as fixed points..

24: **xfix**[dim] – const double *Input*

Note: the dimension, dim, of the array **xfix** must be at least max(1, **nxfix**).

On entry: **xfix**[$i-1$], $i = 1, 2, \ldots,$ **nxfix**, must contain the value of the x coordinate at the ith fixed mesh point.

Constraint: **xfix**[$i-1$] $<$ **xfix**[i], $i = 1, 2, \ldots,$ **nxfix** $- 1$, and each fixed mesh point must coincide with a user-supplied initial mesh point, that is **xfix**[$i-1$] $=$ **x**[$j-1$] for some j, $2 \leq j \leq$ **npts** $- 1$.

Note: the positions of the fixed mesh points in the array **x**[**npts** $- 1$] remain fixed during remeshing, and so the number of mesh points between adjacent fixed points (or between fixed points and end-points) does not change. The user should take this into account when choosing the initial mesh distribution.

25: **nrmesh** – Integer *Input*

On entry: specifies the spatial remeshing frequency and criteria for the calculation and adoption of a new mesh.

nrmesh < 0

Indicates that a new mesh is adopted according to the parameter **dxmesh** below. The mesh is tested every |**nrmesh**| timesteps.

nrmesh $= 0$

Indicates that remeshing should take place just once at the end of the first time step reached when $t >$ **trmesh** (see below).

nrmesh > 0

Indicates that remeshing will take place every **nrmesh** time steps, with no testing using **dxmesh**.

Note: nrmesh may be changed between consecutive calls to nag_pde_parab_1d_cd_ode_remesh (d03psc) to give greater flexibility over the times of remeshing.

26: **dxmesh** – double *Input*

On entry: determines whether a new mesh is adopted when **nrmesh** is set less than zero. A possible new mesh is calculated at the end of every |**nrmesh**| time steps, but is adopted only if

$$x_i^{new} > x_i^{old} + \mathbf{dxmesh} \times (x_{i+1}^{old} - x_i^{old})$$

or

$$x_i^{new} < x_i^{old} - \mathbf{dxmesh} \times (x_i^{old} - x_{i-1}^{old})$$

dxmesh thus imposes a lower limit on the difference between one mesh and the next.

Constraint: **dxmesh** ≥ 0.0.

27: **trmesh** – double *Input*

On entry: specifies when remeshing will take place when **nrmesh** is set to zero. Remeshing will occur just once at the end of the first time step reached when t is greater than **trmesh**.

Note: trmesh may be changed between consecutive calls to nag_pde_parab_1d_cd_ode_remesh (d03psc) to force remeshing at several specified times.

28: **ipminf** – Integer *Input*

On entry: the level of trace information regarding the adaptive remeshing.

ipminf $= 0$

No trace information.

ipminf $= 1$

Brief summary of mesh characteristics.

ipminf $= 2$

More detailed information, including old and new mesh points, mesh sizes and monitor function values.

Constraint: $0 \leq$ **ipminf** ≤ 2.

29: **xratio** – double *Input*

On entry: an input bound on the adjacent mesh ratio (greater than 1.0 and typically in the range 1.5 to 3.0). The remeshing functions will attempt to ensure that

$$(x_i - x_{i-1})/\mathbf{xratio} < x_{i+1} - x_i < \mathbf{xratio} \times (x_i - x_{i-1})$$

Suggested value: **xratio** $= 1.5$.

Constraint: **xratio** > 1.0.

30: **con** – double *Input*

On entry: an input bound on the sub-integral of the monitor function $F^{mon}(x)$ over each space step. The remeshing functions will attempt to ensure that

$$\int_{x_i}^{x_{i+1}} F^{mon}(x)dx \leq \textbf{con} \int_{x_1}^{x_{\textbf{npts}}} F^{mon}(x)dx,$$

(see Furzeland (1984)). **con** gives the user more control over the mesh distribution e.g., decreasing **con** allows more clustering. A typical value is 2/(**npts** $-$ 1), but the user is encouraged to experiment with different values. Its value is not critical and the mesh should be qualitatively correct for all values in the range given below.

Suggested value: **con** $= 2.0/($**npts** $- 1)$.

Constraint: $0.1/($**npts** $- 1) \leq$ **con** $\leq 10.0/($**npts** $- 1)$.

31: **monitf** *Function*

monitf must supply and evaluate a remesh monitor function to indicate the solution behaviour of interest.

If the user specifies **remesh** = **FALSE**, i.e., no remeshing, then **monitf** will not be called and the dummy function d03pel may be used for **monitf**. (d03pel is included in the NAG C Library; however, its name may be implementation-dependent: see the Users' Note for your implementation for details.)

Its specification is:

```
void monitf (double t, Integer npts, Integer npde, const double x[],
     const double u[], double fmon[], Nag_Comm *comm)
```

1: **t** – double *Input*

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

2: **npts** – Integer *Input*

On entry: the number of mesh points in the interval $[a, b]$.

3: **npde** – Integer *Input*

On entry: the number of PDEs in the system.

4: **x**[**npts**] – const double *Input*

On entry: the current mesh. **x**$[i-1]$ contains the value of x_i for $i = 1, 2, \ldots,$ **npts**.

5: **u**[**npde** $\times$ **npts**] – const double *Input*

Note: where **U**(i, j) appears in this document it refers to the array element **u**[**npde** $\times (j-1) + i - 1$]. We recommend using a #define to make the same definition in your calling program.

On entry: **U**(i, j) contains the value of $U_i(x, t)$ at $x =$ **x**$[j-1]$ and time t, for $i = 1, 2, \ldots,$ **npde**, $j = 1, 2, \ldots,$ **npts**.

6: **fmon**[**npts**] – double *Output*

On exit: **fmon**$[i-1]$ must contain the value of the monitor function $F^{mon}(x)$ at mesh point $x =$ **x**$[i-1]$.

Constraint: **fmon**$[i] \geq 0$.

7: **comm** – NAG_Comm * *Input/Output*

The NAG communication parameter (see the Essential Introduction).

32: **rsave**[**lrsave**] – double *Input/Output*

On entry: if **ind** $= 0$, **rsave** need not be set. If **ind** $= 1$ then it must be unchanged from the previous call to the function.

On exit: contains information about the iteration required for subsequent calls.

33: **lrsave** – Integer *Input*

On entry: the dimension of the array **rsave** as declared in the function from which nag_pde_parab_1d_cd_ode_remesh (d03psc) is called. Its size depends on the type of matrix algebra selected:

if **laopt** = **Nag_LinAlgFull**, **lrsave** $\geq$ **neqn** $\times$ **neqn** $+$ **neqn** $+ \, nwkres + lenode$;

if **laopt** = **Nag_LinAlgBand**, **lrsave** $\geq (3 \times mlu + 1) \times$ **neqn** $+ \, nwkres + lenode$;

if **laopt** = **Nag_LinAlgSparse**, **lrsave** $\geq 4 \times$ **neqn** $+ 11 \times$ **neqn**$/2 + 1 + nwkres + lenode$,

where $mlu =$ the lower or upper half bandwidths, and
$mlu = 3 \times$ **npde** $- 1$, for PDE problems only, and
$mlu =$ **neqn** $- 1$, for coupled PDE/ODE problems.

$nwkres =$ **npde** $\times (2 \times$ **npts** $+ 6 \times$ **nxi** $+ 3 \times$ **npde** $+ 26) +$ **nxi** $+$ **ncode** $+ 7 \times$ **npts** $+$ **nxfix** $+ 1$, when **ncode** > 0 and **nxi** > 0, and
$nwkres =$ **npde** $\times (2 \times$ **npts** $+ 3 \times$ **npde** $+ 32) +$ **ncode** $+ 7 \times$ **npts** $+$ **nxfix** $+ 2$, when **ncode** > 0 and **nxi** $= 0$, and
$nwkres =$ **npde** $\times (2 \times$ **npts** $+ 3 \times$ **npde** $+ 32) + 7 \times$ **npts** $+$ **nxfix** $+ 3$, when **ncode** $= 0$.

$lenode = (6 + \mathrm{int}($**algopt**$[1])) \times$ **neqn** $+ 50$, when the BDF method is used, and
$lenode = 9 \times$ **neqn** $+ 50$, when the Theta method is used.

Note: when **laopt** = **Nag_LinAlgSparse**, the value of **lrsave** may be too small when supplied to the integrator. An estimate of the minimum size of **lrsave** is printed on the current error message unit if **itrace** > 0 and the function returns with **fail.code** = **NE_INT_2**.

34: **isave**[**lisave**] – Integer *Input/Output*

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

isave[0] contains the number of steps taken in time.

isave[1] contains the number of residual evaluations of the resulting ODE system used. One such evaluation involves evaluating the PDE functions at all the mesh points, as well as one evaluation of the functions in the boundary conditions.

isave[2] contains the number of Jacobian evaluations performed by the time integrator.

isave[3] contains the order of the BDF method last used in the time integration, if applicable. When the Theta method is used **isave**[3] contains no useful information.

isave[4] contains the number of Newton iterations performed by the time integrator. Each iteration involves residual evaluation of the resulting ODE system followed by a back-substitution using the LU decomposition of the Jacobian matrix.

35: **lisave** – Integer *Input*

On entry: the dimension of the array **isave**. Its size depends on the type of matrix algebra selected:

if **laopt** = **Nag_LinAlgFull**, **lisave** ≥ 25

if **laopt** = **Nag_LinAlgBand**, **lisave** $\geq$ **neqn** $+$ **nxfix** $+ 25$

if **laopt** = **Nag_LinAlgSparse**, **lisave** $\geq 25 \times$ **neqn** $+$ **nxfix** $+ 25$

Note: when **laopt** = **Nag_LinAlgSparse**, the value of **lisave** may be too small when supplied to the integrator. An estimate of the minimum size of **lisave** is printed on the current error message unit if **itrace** > 0 and the function returns with **fail.code** = **NE_INT_2**.

36: **itask** – Integer *Input*

On entry: the task to be performed by the ODE integrator. The permitted values of **itask** and their meanings are detailed below:

itask = 1

Normal computation of output values **u** at $t =$ **tout** (by overshooting and interpolating).

itask = 2

Take one step in the time direction and return.

itask = 3

Stop at first internal integration point at or beyond $t =$ **tout**.

itask = 4

Normal computation of output values **u** at $t =$ **tout** but without overshooting $t = t_{\mathrm{crit}}$ where t_{crit} is described under the parameter **algopt**.

itask = 5

Take one step in the time direction and return, without passing t_{crit}, where t_{crit} is described under the parameter **algopt**.

Constraint: $1 \leq$ **itask** ≤ 5.

37: **itrace** – Integer *Input*

On entry: the level of trace information required from nag_pde_parab_1d_cd_ode_remesh (d03psc) and the underlying ODE solver. **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 from the PDE solver are printed. If **itrace** > 0, then output from the underlying ODE solver is printed. This output contains details of Jacobian entries, the nonlinear iteration and the time integration during the computation of the ODE system. The advisory messages are given in greater detail as **itrace** increases.

38: **outfile** – char * *Input*

On entry: the name of a file to which diagnostic output will be directed. If **outfile** is NULL the diagnostic output will be directed to standard output.

39: **ind** – Integer * *Input/Output*

On entry: **ind** must be set to 0 or 1.

ind = 0

Starts or restarts the integration in time.

ind = 1

Continues the integration after an earlier exit from the function. In this case, only the parameters **tout**, **fail**, **nrmesh** and **trmesh** may be reset between calls to nag_pde_parab_1d_cd_ode_remesh (d03psc).

Constraint: $0 \leq$ **ind** ≤ 1.

On exit: **ind** = 1.

40: **comm** – NAG_Comm * *Input/Output*

The NAG communication parameter (see the Essential Introduction).

41: **saved** – Nag_D03_Save * *Input/Output*

Note: saved is a NAG defined structure. See Section 2.2.1.1 of the Essential Introduction.

On entry: if the current call to nag_pde_parab_1d_cd_ode_remesh (d03psc) follows a previous call to a Chapter d03 function then **saved** must contain the unchanged value output from that previous call.

On exit: data to be passed unchanged to any subsequent call to a Chapter d03 function.

42: **fail** – NagError * *Input/Output*

The NAG error parameter (see the Essential Introduction).

6 Error Indicators and Warnings

NE_INT

On entry, **nxi** $= \langle value \rangle$.
Constraint: **nxi** ≥ 0.

On entry, **npde** $= \langle value \rangle$.
Constraint: **npde** ≥ 1.

On entry, **npts** $= \langle value \rangle$.
Constraint: **npts** ≥ 3.

On entry, **ind** is not equal to 0 or 1: **ind** $= \langle value \rangle$.

On entry, **itask** is not equal to 1, 2, 3, 4 or 5: **itask** $= \langle value \rangle$.

On entry, **itol** is not equal to 1, 2, 3, or 4: **itol** $= \langle value \rangle$.

On entry, **ncode** $= \langle value \rangle$.
Constraint: **ncode** ≥ 0.

ires set to an invalid value in call to **pdedef**, **numflx**, **bndary**, or **odedef**.

On entry, **ipminf** is not equal to 0, 1, or 2: **ipminf** $= \langle value \rangle$.

On entry, **nxfix** $= \langle value \rangle$.
Constraint: **nxfix** ≥ 0.

On entry, **ncode** $= 0$, but **nxi** is not equal to 0: **nxi** $= \langle value \rangle$.

NE_INT_2

On entry, **lrsave** is too small: **lrsave** $= \langle value \rangle$. Minimum possible dimension: $\langle value \rangle$.

On entry, **lisave** is too small: **lisave** $= \langle value \rangle$. Minimum possible dimension: $\langle value \rangle$.

When using the sparse option **lisave** or **lrsave** is too small: **lisave** $= \langle value \rangle$, **lrsave** $= \langle value \rangle$.

On entry, corresponding elements **atol**$[i-1]$ and **rtol**$[j-1]$ are both zero. $i = \langle value \rangle$, $j = \langle value \rangle$.

On entry, **nxfix** $>$ **npts** $- 2$: **nxfix** $= \langle value \rangle$, **npts** $= \langle value \rangle$.

NE_INT_4

On entry, **neqn** is not equal to **npde** $\times$ **npts** $+$ **ncode**: **neqn** $= \langle value \rangle$, **npde** $= \langle value \rangle$, **npts** $= \langle value \rangle$, **ncode** $= \langle value \rangle$.

NE_ENUM_INT

On entry, **laopt** $= \langle value \rangle$, **ncode** $= \langle value \rangle$.
Constraint: **laopt** $=$ **Nag_LinAlgFull**, **Nag_LinAlgBand** or **Nag_LinAlgSparse**.

NE_ACC_IN_DOUBT

Integration completed, but small changes in **atol** or **rtol** are unlikely to result in a changed solution.

NE_BAD_MONIT

fmon is negative at one or more mesh points, or zero mesh spacing has been obtained due to a poor monitor function.

NE_FAILED_DERIV

In setting up the ODE system an internal auxiliary was unable to initialize the derivative. This could be due to user setting **ires** $= 3$ in **pdedef**, **numflx**, **bndary**, or **odedef**.

NE_FAILED_START

atol and **rtol** were too small to start integration.

NE_FAILED_STEP

Error during Jacobian formulation for ODE system. Increase **itrace** for further details.

Repeated errors in an attempted step of underlying ODE solver. Integration was successful as far as **ts**: **ts** $= \langle value \rangle$.

Underlying ODE solver cannot make further progress from the point **ts** with the supplied values of **atol** and **rtol**. **ts** $= \langle value \rangle$.

NE_INCOMPAT_PARAM

On entry, the point **xfix**$[i-1]$ does not coincide with any **x**$[j-1]$: $i = \langle value \rangle$, **xfix**$[i-1] = \langle value \rangle$.

On entry, **con** $> 10.0/($**npts** $- 1)$: **con** $= \langle value \rangle$, **npts** $= \langle value \rangle$.

On entry, **con** $< 0.1/($**npts** $- 1)$: **con** $= \langle value \rangle$, **npts** $= \langle value \rangle$.

NE_INTERNAL_ERROR

Serious error in internal call to an auxiliary. Increase **itrace** for further details.

NE_ITER_FAIL

In solving ODE system, the maximum number of steps **algopt**$[14]$ has been exceeded. **algopt**$[14] = \langle value \rangle$.

NE_NOT_STRICTLY_INCREASING

On entry **xfix**$[i] \leq$ **xfix**$[i-1]$: $i = \langle value \rangle$, **xfix**$[i] = \langle value \rangle$, **xfix**$[i-1] = \langle value \rangle$.

On entry **xi**$[i] \leq$ **xi**$[i-1]$: $i = \langle value \rangle$, **xi**$[i] = \langle value \rangle$, **xi**$[i-1] = \langle value \rangle$.

On entry, mesh points **x** appear to be badly ordered: $i = \langle value \rangle$, **x**$[i-1] = \langle value \rangle$ $j = \langle value \rangle$, **x**$[j-1] = \langle value \rangle$.

NE_REAL

On entry, **xratio** $= \langle value \rangle$.
Constraint: **xratio** > 1.0.

On entry, **dxmesh** $= \langle value \rangle$.
Constraint: **dxmesh** ≥ 0.0.

NE_REAL_2

On entry, at least one point in **xi** lies outside $[$**x**$[0]$, **x**$[$**npts** $- 1]]$: **x**$[0] = \langle value \rangle$, **x**$[$**npts** $- 1] = \langle value \rangle$.

On entry, **tout** $-$ **ts** is too small: **tout** $= \langle value \rangle$, **ts** $= \langle value \rangle$.

On entry, **tout** $\leq$ **ts**: **tout** $= \langle value \rangle$, **ts** $= \langle value \rangle$.

NE_REAL_ARRAY

On entry, **rtol**$[i-1] < 0.0$: $i = \langle value\rangle$, **rtol**$[i-1] = \langle value\rangle$.

On entry, **atol**$[i-1] < 0.0$: $i = \langle value\rangle$, **atol**$[i-1] = \langle value\rangle$.

NE_REMESH_CHANGED

remesh has been changed between calls to nag_pde_parab_1d_fd_ode_remesh (d03ppc).

NE_SING_JAC

Singular Jacobian of ODE system. Check problem formulation.

NE_TIME_DERIV_DEP

The functions P, D, or C appear to depend on time derivatives.

NE_USER_STOP

In evaluating residual of ODE system, **ires** $= 2$ has been set in **pdedef**, **numflx**, **bndary**, or **odedef**. Integration is successful as far as **ts**: **ts** $= \langle value\rangle$.

NE_ZERO_WTS

Zero error weights encountered during time integration.

NE_ALLOC_FAIL

Memory allocation failed.

NE_BAD_PARAM

On entry, parameter $\langle value\rangle$ had an illegal value.

NE_NOT_WRITE_FILE

Cannot open file $\langle value\rangle$ for writing.

NE_NOT_CLOSE_FILE

Cannot close file $\langle value\rangle$.

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please consult NAG for assistance.

7 Accuracy

The function controls the accuracy of the integration in the time direction but not the accuracy of the approximation in space. The spatial accuracy depends on both the number of mesh points and on their distribution in space. In the time integration only the local error over a single step is controlled and so the accuracy over a number of steps cannot be guaranteed. The user should therefore test the effect of varying the accuracy parameters, **atol** and **rtol**.

8 Further Comments

The function is designed to solve systems of PDEs in conservative form, with optional source terms which are independent of space derivatives, and optional second-order diffusion terms. The use of the function to solve systems which are not naturally in this form is discouraged, and users are advised to use one of the central-difference scheme functions for such problems.

Users should be aware of the stability limitations for hyperbolic PDEs. For most problems with small error tolerances the ODE integrator does not attempt unstable time steps, but in some cases a maximum time step should be imposed using **algopt**[12]. It is worth experimenting with this parameter, particularly if the integration appears to progress unrealistically fast (with large time steps). Setting the maximum time step to the minimum mesh size is a safe measure, although in some cases this may be too restrictive.

Problems with source terms should be treated with caution, as it is known that for large source terms stable and reasonable looking solutions can be obtained which are in fact incorrect, exhibiting non-physical speeds of propagation of discontinuities (typically one spatial mesh point per time step). It is essential to employ a very fine mesh for problems with source terms and discontinuities, and to check for non-physical propagation speeds by comparing results for different mesh sizes. Further details and an example can be found in Pennington and Berzins (1994).

The time taken depends on the complexity of the system, the accuracy requested, and the frequency of the mesh updates. For a given system with fixed accuracy and mesh-update frequency it is approximately proportional to **neqn**.

9 Example

For this function two examples are presented, with a main program and two example problems given in the functions $ex1$ and $ex2$.

Example 1 ($ex1$)

This example is a simple model of the advection and diffusion of a cloud of material:

$$\frac{\partial U}{\partial t} + W\frac{\partial U}{\partial x} = C\frac{\partial^2 U}{\partial x^2},$$

for $x \in [0, 1]$ and $t \leq 0 \leq 0.3$. In this example the constant wind speed $W = 1$ and the diffusion coefficient $C = 0.002$.

The cloud does not reach the boundaries during the time of integration, and so the two (physical) boundary conditions are simply $U(0, t) = U(1, t) = 0.0$, and the initial condition is

$$U(x, 0) = \sin\left(\pi\frac{x - a}{b - a}\right), \text{for} \quad a \leq x \leq b,$$

and $U(x, 0) = 0$ elsewhere, where $a = 0.2$ and $b = 0.4$.

The numerical flux is simply $\hat{F} = WU_L$.

The monitor function for remeshing is taken to be the absolute value of the second derivative of U.

Example 2 ($ex2$)

This example is a linear advection equation with a non-linear source term and discontinuous initial profile:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = -pu(u - 1)(u - \tfrac{1}{2}),$$

for $0 \leq x \leq 1$ and $t \geq 0$. The discontinuity is modelled by a ramp function of width 0.01 and gradient 100, so that the exact solution at any time $t \geq 0$ is

$$u(x, t) = 1.0 + \max(\min(\delta, 0), -1),$$

where $\delta = 100(0.1 - x + t)$. The initial profile is given by the exact solution. The characteristic points into the domain at $x = 0$ and out of the domain at $x = 1$, and so a physical boundary condition $u(0, t) = 1$ is imposed at $x = 0$, with a numerical boundary condition at $x = 1$ which can be specified as $u(1, t) = 0$ since the discontinuity does not reach $x = 1$ during the time of integration.

The numerical flux is simply $\hat{F} = U_L$ at all times.

The remeshing monitor function (described below) is chosen to create an increasingly fine mesh towards the discontinuity in order to ensure good resolution of the discontinuity, but without loss of efficiency in the surrounding regions. However, refinement must be limited so that the time step required for stability does not become unrealistically small. The region of refinement must also keep up with the discontinuity as it moves across the domain, and hence it cannot be so small that the discontinuity moves out of the refined region between remeshing.

The above requirements mean that the use of the first or second spatial derivative of U for the monitor function is inappropriate; the large relative size of either derivative in the region of the discontinuity leads to extremely small mesh-spacing in a very limited region, and the solution is then far more expensive than for a very fine fixed mesh.

An alternative monitor function based on a cosine function proves very successful. It is only semi-automatic as it requires some knowledge of the solution (for problems without an exact solution an initial approximate solution can be obtained using a coarse fixed mesh). On each call to the user-supplied **monitf** function the discontinuity is located by finding the maximum spatial derivative of the solution. On the first call the desired width of the region of non-zero monitor function is set (this can be changed at a later time if desired). Then on each call the monitor function is assigned using a cosine function so that it has a value of one at the discontinuity down to zero at the edges of the predetermined region of refinement, and zero outside the region. Thus the monitor function and the subsequent refinement are limited, and the region is large enough to ensure that there is always sufficient refinement at the discontinuity.

9.1 Program Text

```
/* nag_pde_parab_1d_cd_ode_remesh (d03psc) Example Program.
 *
 * Copyright 2001 Numerical Algorithms Group.
 *
 * Mark 7, 2001.
 */

#include <stdio.h>
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagd03.h>
#include <nagx01.h>

int ex1(void), ex2(void);

static void uvin1(Integer, Integer, Integer, const double[],
                  const double[], double[],Integer, double[],
                  Nag_Comm *);

static void uvin2(Integer, Integer, Integer, const double[],
                  const double[], double[],Integer, double[],
                  Nag_Comm *);

static void pdef1(Integer, double, double, const double[],
                  const double[], Integer, const double[],
                  const double[], double[], double[], double[],
                  double[], Integer *, Nag_Comm *);

static void pdef2(Integer, double, double, const double[],
                  const double[], Integer, const double[],
                  const double[], double[], double[], double[],
                  double[], Integer *, Nag_Comm *);

static void bndry1(Integer, Integer, double, const double[],
                   const double[], Integer, const double[],
                   const double[], Integer, double[],
                   Integer *, Nag_Comm *);

static void bndry2(Integer, Integer, double, const double[],
                   const double[], Integer, const double[],
                   const double[], Integer, double[],
                   Integer *, Nag_Comm *);

static void monit1(double, Integer, Integer, const double[],
                   const double[], double[], Nag_Comm *);

static void monit2(double, Integer, Integer, const double[],
                   const double[], double[], Nag_Comm *);

static void nmflx1(Integer, double, double, Integer,
                   const double[], const double[],
                   const double[], double[], Integer *,
                   Nag_Comm *, Nag_D03_Save *);

static void nmflx2(Integer, double, double, Integer,
                   const double[], const double[],
                   const double[], double[], Integer *,
                   Nag_Comm *, Nag_D03_Save *);

static void exact(double, double *, const double *, Integer,
                  Integer);

#define P(I,J) p[npde*((J)-1)+(I)-1]
#define UE(I,J) ue[npde*((J)-1)+(I)-1]
#define U(I,J) u[npde*((J)-1)+(I)-1]
#define UOUT(I,J,K) uout[npde*(intpts*((K)-1)+(J)-1)+(I)-1]

int main(void)
{
  Vprintf("d03psc Example Program Results\n");
  ex1();
  ex2();
  return 0;
}

int ex1(void)
{
  const Integer npde=1, npts=61, ncode=0, nxi=0, nxfix=0, itype=1,
    neqn=npde*npts+ncode, intpts=7, lisave=25+nxfix+neqn,
    nwkres=npde*(3*npts+3*npde+32)+7*npts+3, lenode=11*neqn+50,
    mlu=3*npde-1, lrsave=(3*mlu+1)*neqn+nwkres+lenode;
  static double xout[7] = { .2,.3,.4,.5,.6,.7,.8 };
  double con, dxmesh, tout, trmesh, ts, xratio;
  Integer exit_status, i, ind, ipminf, it, itask, itol,
    itrace, m, nrmesh;
  Boolean remesh;
  double *algopt=0, *atol=0, *rsave=0, *rtol=0,
    *u=0, *uout=0, *x=0, *xfix=0, *xi=0;
  Integer *isave=0;
  NagError fail;
  Nag_Comm comm;
  Nag_D03_Save saved;

  INIT_FAIL(fail);
  exit_status = 0;

  /* Allocate memory */

  if ( !(algopt = NAG_ALLOC(30, double)) ||
       !(atol = NAG_ALLOC(1, double)) ||
       !(rsave = NAG_ALLOC(lrsave, double)) ||
       !(rtol = NAG_ALLOC(1, double)) ||
       !(u = NAG_ALLOC(npde*npts, double)) ||
       !(uout = NAG_ALLOC(npde*intpts*itype, double)) ||
       !(x = NAG_ALLOC(npts, double)) ||
       !(xfix = NAG_ALLOC(1, double)) ||
       !(xi = NAG_ALLOC(1, double)) ||
       !(isave = NAG_ALLOC(lisave, Integer)) )
    {
      Vprintf("Allocation failure\n");
      exit_status = 1;
      goto END;
    }

  Vprintf("\n\nExample 1\n\n");

  itrace = 0;
  itol = 1;
```

```
atol[0] = 1.0e-4;
rtol[0] = 1.0e-4;

Vprintf("  npts = %4ld", npts);
Vprintf(" atol = %10.3e", atol[0]);
Vprintf(" rtol = %10.3e\n\n", rtol[0]);

/* Initialise mesh */

for (i = 0; i < npts; ++i) x[i] = i/(npts-1.0);
xfix[0] = 0.0;

/* Set remesh parameters */

remesh = 1;
nrmesh = 3;
dxmesh = 0.0;
trmesh = 0.0;
con = 2.0/(npts-1.0);
xratio = 1.5;
ipminf = 0;

xi[0] = 0.0;
ind = 0;
itask = 1;

for (i = 0; i < 30; ++i) algopt[i] = 0.0;

/* b.d.f. integration */

algopt[0] = 1.0;
algopt[12] = 0.005;

/* Loop over output value of t */

ts = 0.0;
tout = 0.0;
for (it = 0; it < 3; ++it)
  {
    tout = 0.1*(it+1);

    d03psc(npde, &ts, tout, pdef1, nmflx1, bndry1, uvin1, u,
           npts, x, ncode, d03pek, nxi, xi, neqn, rtol, atol,
           itol, Nag_OneNorm, Nag_LinAlgBand, algopt, remesh,
           nxfix, xfix, nrmesh, dxmesh, trmesh, ipminf, xratio,
           con, monit1, rsave, lrsave, isave, lisave, itask,
           itrace, 0, &ind, &comm, &saved, &fail);

    if (fail.code != NE_NOERROR)
      {
        Vprintf("Error from d03psc.\n%s\n", fail.message);
        exit_status = 1;
        goto END;
      }

    Vprintf(" t = %6.3f\n", ts);
    Vprintf(" x         ");

    for (i = 1; i <= intpts; ++i)
      {
        Vprintf("%9.4f", xout[i-1]);
        Vprintf(i%7 == 0 || i == 7 ?"\n":"");
      }

    /* Interpolate at output points */

    m = 0;
    d03pzc(npde, m, u, npts, x, xout, intpts, itype, uout, &fail);

    if (fail.code != NE_NOERROR)
      {
          Vprintf("Error from d03pzc.\n%s\n", fail.message);
          exit_status = 1;
          goto END;
        }

      Vprintf(" Approx u ");

      for (i = 1; i <= intpts; ++i)
        {
          Vprintf("%9.4f", UOUT(1,i,1));
          Vprintf(i%7 == 0 || i == 7 ?"\n":"");
        }
      Vprintf("\n");
    }

  Vprintf(" Number of integration steps in time = %6ld\n", isave[0]);
  Vprintf(" Number of function evaluations = %6ld\n", isave[1]);
  Vprintf(" Number of Jacobian evaluations =%6ld\n", isave[2]);
  Vprintf(" Number of iterations = %6ld\n\n", isave[4]);
 END:

  if (algopt) NAG_FREE(algopt);
  if (atol) NAG_FREE(atol);
  if (rsave) NAG_FREE(rsave);
  if (rtol) NAG_FREE(rtol);
  if (u) NAG_FREE(u);
  if (uout) NAG_FREE(uout);
  if (x) NAG_FREE(x);
  if (xfix) NAG_FREE(xfix);
  if (xi) NAG_FREE(xi);
  if (isave) NAG_FREE(isave);

  return exit_status;

}

static void uvin1(Integer npde, Integer npts, Integer nxi, const double x[],
                  const double xi[], double u[],Integer ncode, double v[],
                  Nag_Comm *comm)
{
  Integer i;

  for (i = 1; i <= npts; ++i)
    {
      if (x[i-1] > 0.2 && x[i-1] <= 0.4)
        {
          U(1, i) = sin(nag_pi*(5.0*x[i-1]-1.0));
        } else {
          U(1, i) = 0.0;
        }
    }
  return;
}

static void pdef1(Integer npde, double t, double x, const double u[],
                  const double ux[], Integer ncode, const double v[],
                  const double vdot[], double p[], double c[], double d[],
                  double s[], Integer *ires, Nag_Comm *comm)
{
  P(1, 1) = 1.0;
  c[0] = 0.002;
  d[0] = ux[0];
  s[0] = 0.0;

  return;
}

static void bndry1(Integer npde, Integer npts, double t, const double x[],
                   const double u[], Integer ncode, const double v[],
                   const double vdot[], Integer ibnd, double g[],
                   Integer *ires, Nag_Comm *comm)
```

```
{
  /* Zero solution at both boundaries */

  if (ibnd == 0)
    {
      g[0] = U(1, 1);
    } else {
      g[0] = U(1, npts);
    }
  return;
}

static void monit1(double t, Integer npts, Integer npde, const double x[],
                   const double u[], double fmon[], Nag_Comm *comm)
{
  double h1, h2, h3;
  Integer i;

  for (i = 2; i <= npts-1; ++i)
    {
      h1 = x[i - 1] - x[i - 2];
      h2 = x[i] - x[i - 1];
      h3 = 0.5*(x[i] - x[i - 2]);

      /* Second derivatives */

      fmon[i-1] = fabs(((U(1,i+1) - U(1,i))/h2 - (U(1,i) - U(1,i-1))/h1)/h3);
    }
  fmon[0] = fmon[1];
  fmon[npts-1] = fmon[npts-2];

  return;
}

static void nmflx1(Integer npde, double t, double x, Integer ncode,
                   const double v[], const double uleft[],
                   const double uright[], double flux[], Integer *ires,
                   Nag_Comm *comm, Nag_D03_Save *saved)
{
  flux[0] = uleft[0];

  return;
}

int ex2(void)
{
  const Integer npde=1, npts=61, ncode=0, nxi=0, nxfix=0, itype=1,
    neqn=npde*npts+ncode, intpts=7, lisave=25+nxfix+neqn,
    nwkres=npde*(3*npts+3*npde+32)+7*npts+3, lenode=11*neqn+50,
    mlu=3*npde-1, lrsave=(3*mlu+1)*neqn+nwkres+lenode;
  static double xout[7] = { 0.,.3,.4,.5,.6,.7,1. };
  double con, dxmesh, tout, trmesh, ts, xratio;
  Integer exit_status, i, ind, ipminf, it, itask, itol, itrace, m,
    nrmesh;
  Boolean remesh;
  double *algopt=0, *atol=0, *rsave=0, *rtol=0,
    *u=0, *ue=0, *uout=0, *x=0, *xfix=0, *xi=0;
  Integer *isave=0;
  NagError fail;
  Nag_Comm comm;
  Nag_D03_Save saved;

  INIT_FAIL(fail);
  exit_status = 0;

  /* Allocate memory */

  if ( !(algopt = NAG_ALLOC(30, double)) ||
       !(atol = NAG_ALLOC(1, double)) ||
       !(rsave = NAG_ALLOC(lrsave, double)) ||
       !(rtol = NAG_ALLOC(1, double)) ||
        !(u = NAG_ALLOC(npts, double)) ||
        !(ue = NAG_ALLOC(npde*intpts, double)) ||
        !(uout = NAG_ALLOC(npde*intpts*itype, double)) ||
        !(x = NAG_ALLOC(npts, double)) ||
        !(xfix = NAG_ALLOC(1, double)) ||
        !(xi = NAG_ALLOC(1, double)) ||
        !(isave = NAG_ALLOC(lisave, Integer)) )
    {
      Vprintf("Allocation failure\n");
      exit_status = 1;
      goto END;
    }

  Vprintf("\n\nExample 2\n\n");

  itrace = 0;
  itol = 1;
  atol[0] = 5e-4;
  rtol[0] = 0.05;

  Vprintf(" npts = %4ld", npts);
  Vprintf(" atol = %10.3e", atol[0]);
  Vprintf(" rtol = %10.3e\n\n", rtol[0]);

  /* Initialise mesh */

  for (i = 0; i < npts; ++i) x[i] = i/(npts-1.0);
  xfix[0] = 0.0;

  /* Set remesh parameters */

  remesh = TRUE;
  nrmesh = 5;
  dxmesh = 0.0;
  trmesh = 0.0;
  con = 1.0/(npts-1.0);
  xratio = 1.5;
  ipminf = 0;

  xi[0] = 0.0;
  ind = 0;
  itask = 1;

  for (i = 0; i < 30; ++i) algopt[i] = 0.0;

  /* Theta integration */

  algopt[0] = 2.0;
  algopt[5] = 2.0;
  algopt[6] = 2.0;

  /* Max. time step */

  algopt[12] = 0.0025;

  ts = 0.0;
  tout = 0.0;
  for (it = 0; it < 2; ++it)
    {
      tout = 0.2*(it+1);

      d03psc(npde, &ts, tout, pdef2, nmflx2, bndry2, uvin2, u,
             npts, x, ncode, d03pek, nxi, xi, neqn, rtol, atol,
             itol, Nag_OneNorm, Nag_LinAlgBand, algopt, remesh,
             nxfix, xfix, nrmesh, dxmesh, trmesh, ipminf, xratio,
             con, monit2, rsave, lrsave, isave, lisave, itask,
             itrace, 0, &ind, &comm, &saved, &fail);

      if (fail.code != NE_NOERROR)
        {
          Vprintf("Error from d03psc.\n%s\n", fail.message);
          exit_status = 1;
          goto END;
        }

      Vprintf(" t = %6.3f\n", ts);
      Vprintf("        x        Approx u    Exact u\n\n");

      /* Interpolate at output points */

      m = 0;
      d03pzc(npde, m, u, npts, x, xout, intpts, itype, uout, &fail);

      if (fail.code != NE_NOERROR)
        {
          Vprintf("Error from d03pzc.\n%s\n", fail.message);
          exit_status = 1;
          goto END;
        }

      /* Check against exact solution */

      exact(tout, ue, xout, npde, intpts);
      for (i = 1; i <= intpts; ++i)
        {
          Vprintf("   %9.4f", xout[i-1]);
          Vprintf("   %9.4f", UOUT(1,i,1));
          Vprintf("   %9.4f\n", UE(1,i));
        }
    }

  Vprintf(" Number of integration steps in time = %6ld\n", isave[0]);
  Vprintf(" Number of function evaluations = %6ld\n", isave[1]);
  Vprintf(" Number of Jacobian evaluations =%6ld\n", isave[2]);
  Vprintf(" Number of iterations = %6ld\n\n", isave[4]);
 END:

  if (algopt) NAG_FREE(algopt);
  if (atol) NAG_FREE(atol);
  if (rsave) NAG_FREE(rsave);
  if (rtol) NAG_FREE(rtol);
  if (u) NAG_FREE(u);
  if (ue) NAG_FREE(ue);
  if (uout) NAG_FREE(uout);
  if (x) NAG_FREE(x);
  if (xfix) NAG_FREE(xfix);
  if (xi) NAG_FREE(xi);
  if (isave) NAG_FREE(isave);

  return exit_status;
}

static void uvin2(Integer npde, Integer npts, Integer nxi, const double x[],
                  const double xi[], double u[],Integer ncode, double v[],
                  Nag_Comm *comm)
{
  double t;

  t = 0.0;
  exact(t, u, x, npde, npts);

  return;
}

static void pdef2(Integer npde, double t, double x, const double u[],
                  const double ux[], Integer ncode, const double v[],
                  const double vdot[], double p[], double c[], double d[],
                  double s[], Integer *ires, Nag_Comm *comm)
{
  P(1, 1) = 1.0;
  c[0] = 0.0;
  d[0] = 0.0;
  s[0] = -100.0*u[0]*(u[0]-1.0)*(u[0]-0.5);

  return;
}

static void bndry2(Integer npde, Integer npts, double t, const double x[],
                   const double u[], Integer ncode, const double v[],
                   const double vdot[], Integer ibnd, double g[],
                   Integer *ires, Nag_Comm *comm)
{
  /* Solution known to be constant at both boundaries */

  double ue[1];

  if (ibnd == 0)
    {
      exact(t, ue, &x[0], npde, 1);
      g[0] = UE(1, 1) - U(1, 1);
    } else {
      exact(t, ue, &x[npts-1], npde, 1);
      g[0] = UE(1, 1) - U(1,npts);
    }

  return;
}

static void nmflx2(Integer npde, double t, double x, Integer ncode,
                   const double v[], const double uleft[],
                   const double uright[], double flux[], Integer *ires,
                   Nag_Comm *comm, Nag_D03_Save *saved)
{
  flux[0] = uleft[0];

  return;
}

static void monit2(double t, Integer npts, Integer npde, const double x[],
                   const double u[], double fmon[], Nag_Comm *comm)
{
  static double xa = 0.0;
  static Integer icount = 0;
  double h1, ux, uxmax, xl, xleft, xmax, xr, xright;
  Integer i;

  /* Locate shock */

  uxmax = 0.0;
  xmax = 0.0;
  for (i = 2; i <= npts-1; ++i)
    {
      h1 = x[i - 1] - x[i - 2];
      ux = fabs((U(1, i) - U(1, i-1))/h1);
      if (ux > uxmax)
        {
          uxmax = ux;
          xmax = x[i - 1];
        }
    }

  /* Assign width (on first call only) */

  if (icount == 0)
    {
      icount = 1;
      xleft = xmax - x[0];
      xright = x[npts-1] - xmax;
      if (xleft > xright)
        {
          xa = xright;
        } else {
          xa = xleft;
        }
    }
  xl = xmax - xa;
  xr = xmax + xa;

  /* Assign monitor function */

  for (i = 0; i < npts; ++i)
    {
      if (x[i] > xl && x[i] < xr)
        {
          fmon[i] = 1.0 + cos(nag_pi*(x[i] - xmax)/xa);
        } else {
          fmon[i] = 0.0;
        }
    }
  return;
}

static void exact(double t, double *u, const double *x, Integer npde,
                  Integer npts)
{
  /* Exact solution (for comparison and b.c. purposes) */

  double del, psi, rm, rn, s;
  Integer i;

  s = 0.1;
  del = 0.01;
  rm = -1.0/del;
  rn = s/del + 1.0;

  for (i = 1; i <= npts; ++i)
    {
      psi = x[i - 1] - t;
      if (psi < s)
        {
          U(1, i) = 1.0;
        } else if (psi > del + s) {
          U(1, i) = 0.0;
        } else {
          U(1, i) = rm*psi + rn;
        }
    }
  return;
}
```

9.2 Program Data

None.

9.3 Program Results

```
d03psc Example Program Results

Example 1

  npts =   61 atol =  1.000e-04 rtol =  1.000e-04

 t =  0.100
 x           0.2000   0.3000   0.4000   0.5000   0.6000   0.7000   0.8000
 Approx u    0.0000   0.1198   0.9461   0.1182   0.0000   0.0000   0.0000

 t =  0.200
 x           0.2000   0.3000   0.4000   0.5000   0.6000   0.7000   0.8000
 Approx u    0.0000   0.0007   0.1631   0.9015   0.1629   0.0001   0.0000

 t =  0.300
 x           0.2000   0.3000   0.4000   0.5000   0.6000   0.7000   0.8000
 Approx u    0.0000   0.0000   0.0025   0.1924   0.8596   0.1946   0.0002
 Number of integration steps in time =     92
 Number of function evaluations =    443
 Number of Jacobian evaluations =    39
 Number of iterations =    231

Example 2

 npts =   61 atol =  5.000e-04 rtol =  5.000e-02

 t =  0.200
        x        Approx u    Exact u

     0.0000      1.0000      1.0000
     0.3000      0.9507      1.0000
     0.4000      0.0000      0.0000
     0.5000      0.0000      0.0000
     0.6000      0.0000      0.0000
     0.7000     -0.0000      0.0000
     1.0000     -0.0000      0.0000
 t =  0.400
        x        Approx u    Exact u

     0.0000      1.0000      1.0000
     0.3000      1.0000      1.0000
     0.4000      1.0000      1.0000
     0.5000      0.9694      1.0000
     0.6000     -0.0000      0.0000
     0.7000     -0.0000      0.0000
     1.0000      0.0000      0.0000
 Number of integration steps in time =    468
 Number of function evaluations =   1059
 Number of Jacobian evaluations =     1
 Number of iterations =      2
```

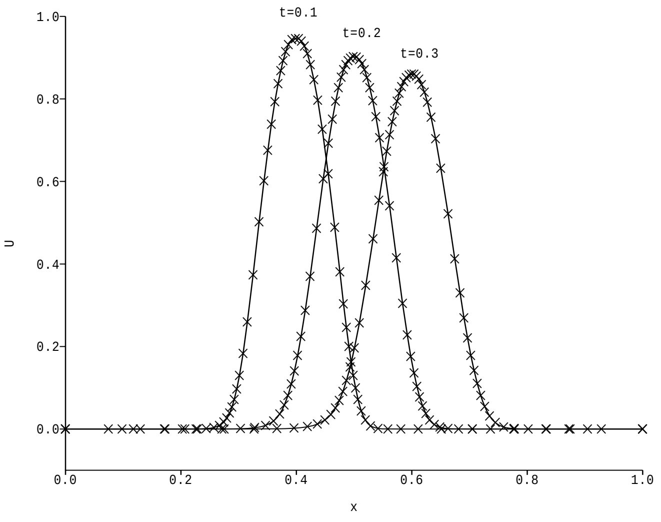

Figure 1
Solution to Example 1

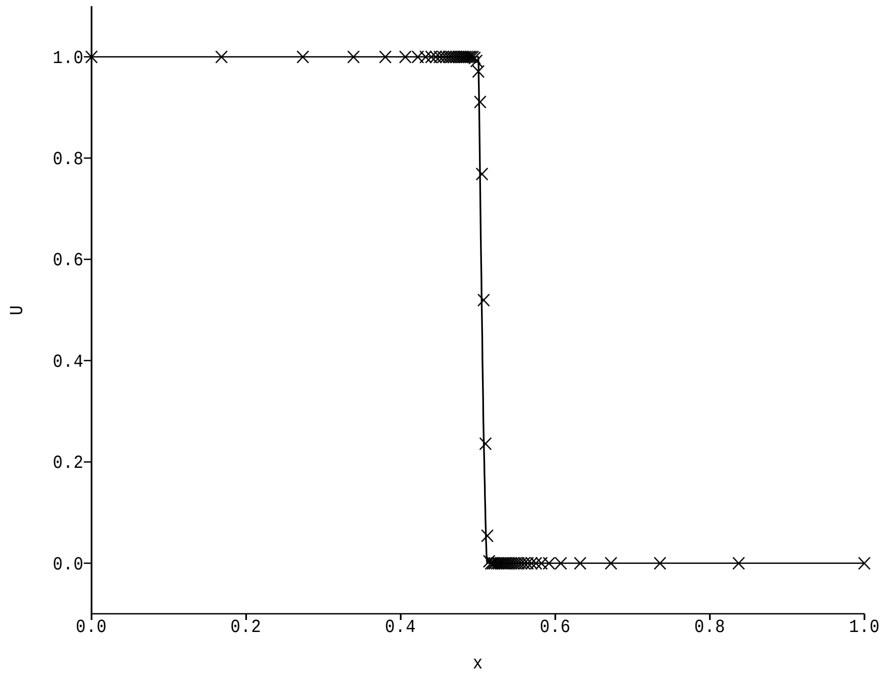

Figure 2
Solution to Example 2