

## NAG C Library Function Document

### nag\_pde\_parab\_1d\_cd (d03pfc)

#### 1 Purpose

nag\_pde\_parab\_1d\_cd (d03pfc) integrates a system of linear or nonlinear convection-diffusion equations in one space dimension, with optional source terms. The system must be posed in conservative form. Convection terms are discretized 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 PDEs to a system of ordinary differential equations (ODEs), and the resulting system is solved using a backward differentiation formula (BDF) method.

#### 2 Specification

```
#include <nag.h>
#include <nagd03.h>

void nag_pde_parab_1d_cd (Integer npde, double *ts, double tout,
    void (*pdedef)(Integer npde, double t, double x, const double u[],
        const double ux[], double p[], double c[], double d[], double s[],
        Integer *ires, Nag_Comm *comm),
    void (*numflux)(Integer npde, double t, double x, 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 ibnd, double g[], Integer *ires,
        Nag_Comm *comm),
    double u[], Integer npts, const double x[], const double acc[], double tsmax,
    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 (d03pfc) integrates the system of convection-diffusion equations in conservative form:

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

or the hyperbolic convection-only system:

$$\frac{\partial U_i}{\partial t} + \frac{\partial F_i}{\partial x} = 0, \quad (2)$$

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

$$U(x, t) = \left[ U_1(x, t), \dots, U_{\text{npde}}(x, t) \right]^T.$$

The functions  $P_{ij}$ ,  $F_i$ ,  $C_i$  and  $S_i$  depend on  $x$ ,  $t$  and  $U$ ; and  $D_i$  depends on  $x$ ,  $t$ ,  $U$  and  $U_x$ , where  $U_x$  is the spatial derivative of  $U$ . Note that  $P_{ij}$ ,  $F_i$ ,  $C_i$  and  $S_i$  must not depend on any space derivatives; and none of the functions may depend on time derivatives. In terms of conservation laws,  $F_i$ ,  $\frac{C_i \partial D_i}{\partial x}$  and  $S_i$  are the convective flux, diffusion and source terms respectively.

The integration in time is from  $t_0$  to  $t_{\text{out}}$ , over the space interval  $a \leq x \leq b$ , where  $a = x_1$  and  $b = x_{\text{npts}}$  are the leftmost and rightmost points of a user-defined mesh  $x_1, x_2, \dots, x_{\text{npts}}$ . The initial values of the functions  $U(x, t)$  must be given at  $t = t_0$ .

The PDEs are approximated by a system of ODEs in time for the values of  $U_i$  at mesh points using a spatial discretization 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 vector,  $\hat{F}_i$  say, must be calculated by you 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  $x_{j-1/2} = (x_{j-1} + x_j)/2$ , for  $j = 2, 3, \dots, \text{npts}$ . The left and right values are calculated by `nag_pde_parab_1d_cd` (d03pfc) 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

$$\frac{\partial U_i}{\partial t} + \frac{\partial F_i}{\partial y} = 0, \quad (3)$$

where  $y = x - x_{j-1/2}$ , i.e.,  $y = 0$  corresponds to  $x = x_{j-1/2}$ , 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 (see 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

$$\hat{F} = \frac{1}{2}(F_L + F_R) - \frac{1}{2} \sum_{k=1}^{\text{npde}} \alpha_k |\lambda_k| e_k, \quad (4)$$

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

$$U_R - U_L = \sum_{k=1}^{\text{npde}} \alpha_k e_k. \quad (5)$$

An example is given in Section 9.

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 you. The numerical flux  $\hat{F}_i$  must be supplied in a separate user-supplied function `numflux`. For problems in the form (2), the actual argument d03pfp may be used for `pdedef` (d03pfp is included in the NAG C Library; however, its name may be implementation-dependent: see the Users' Note for your implementation for details). d03pfp sets the matrix with entries  $P_{i,j}$  to the identity matrix, and the functions  $C_i$ ,  $D_i$  and  $S_i$  to zero.

The boundary condition specification has sufficient flexibility to allow for different types of problems. For second-order problems, i.e.,  $D_i$  depending on  $U_x$ , a boundary condition is required for each PDE at both boundaries for the problem to be well-posed. If there are no second-order 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 discretization 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 you, 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 you 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 only linear extrapolation is allowed in this function (for greater flexibility the function `nag_pde_parab_1d_cd_ode` (d03plc) should be used). 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. Examples can be found in Section 9.

The boundary conditions must be specified in a user-supplied function **bndary** in the form

$$G_i^L(x, t, U) = 0 \quad \text{at } x = a, \quad i = 1, 2, \dots, \mathbf{npde}, \quad (6)$$

at the left-hand boundary, and

$$G_i^R(x, t, U) = 0 \quad \text{at } x = b, \quad i = 1, 2, \dots, \mathbf{npde}, \quad (7)$$

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 problem is subject to the following restrictions:

- (i)  $P_{i,j}$ ,  $F_i$ ,  $C_i$  and  $S_i$  must not depend on any space derivatives;
- (ii)  $P_{i,j}$ ,  $F_i$ ,  $C_i$ ,  $D_i$  and  $S_i$  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 mesh points  $x_1, x_2, \dots, x_{\mathbf{npts}}$ ;
- (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.

In total there are  $\mathbf{npde} \times \mathbf{npts}$  ODEs in the time direction. This system is then integrated forwards in time using a BDF method.

For further details of the algorithm, 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

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 Arguments

1: **npde** – Integer *Input*  
*On entry*: the number of PDEs to be solved.  
*Constraint*: **npde**  $\geq 1$ .

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, supplied by the user *External Function*  
**pdedef** must evaluate the functions  $P_{ij}$ ,  $C_i$ ,  $D_i$  and  $S_i$  which partially define the system of PDEs.  $P_{ij}$ ,  $C_i$  and  $S_i$  may depend on  $x$ ,  $t$  and  $U$ ;  $D_i$  may depend on  $x$ ,  $t$ ,  $U$  and  $U_x$ . **pdedef** is called approximately midway between each pair of mesh points in turn by nag\_pde\_parab\_1d\_cd (d03pfc). The actual argument d03ppf may be used for **pdedef** for problems in the form (2) (d03ppf 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[], 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  $i = 1, 2, \dots, \text{npde}$ .

5: **ux[npde]** – const double *Input*  
*On entry*: **ux**[ $i - 1$ ] contains the value of the component  $\frac{\partial U_i(x, t)}{\partial x}$ , for  $i = 1, 2, \dots, \text{npde}$ .

6: **p[npde  $\times$  npde]** – double *Output*  
*On exit*: **p**[ $\text{npde} \times j + i$ ] must be set to the value of  $P_{ij}(x, t, U)$ , for  $i, j = 1, 2, \dots, \text{npde}$ .

7: **c[npde]** – double *Output*  
*On exit*: **c**[ $i - 1$ ] must be set to the value of  $C_i(x, t, U)$ , for  $i = 1, 2, \dots, \text{npde}$ .

8:	<b>d[<b>npde</b>]</b> – double	<i>Output</i>
<i>On exit:</i> <b>d</b> [ <i>i</i> – 1] must be set to the value of $D_i(x, t, U, U_x)$ , for $i = 1, 2, \dots, \text{npde}$ .		
9:	<b>s[<b>npde</b>]</b> – double	<i>Output</i>
<i>On exit:</i> <b>s</b> [ <i>i</i> – 1] must be set to the value of $S_i(x, t, U)$ , for $i = 1, 2, \dots, \text{npde}$ .		
10:	<b>ires</b> – Integer *	<i>Input/Output</i>
<i>On entry:</i> set to –1 or 1.		
<i>On exit:</i> should usually remain unchanged. However, you may set <b>ires</b> to force the integration function to take certain actions as described below:		
<b>ires</b> = 2		
Indicates to the integrator that control should be passed back immediately to the calling function with the error indicator set to <b>fail.code</b> = <b>NE_USER_STOP</b> .		
<b>ires</b> = 3		
Indicates to the integrator that the current time step should be abandoned and a smaller time step used instead. You may wish to set <b>ires</b> = 3 when a physically meaningless input or output value has been generated. If you consecutively set <b>ires</b> = 3, then nag_pde_parab_1d_cd (d03pfc) returns to the calling function with the error indicator set to <b>fail.code</b> = <b>NE_FAILED_DERIV</b> .		
11:	<b>comm</b> – Nag_Comm *	<i>Communication Structure</i>
Pointer to structure of type <b>Nag_Comm</b> ; the following members are relevant to <b>pdedef</b> .		
<b>user</b> – double *		
<b>iuser</b> – Integer *		
<b>p</b> – Pointer		
The type Pointer will be <b>void *</b> . Before calling nag_pde_parab_1d_cd (d03pfc) these pointers may be allocated memory by the user and initialized with various quantities for use by <b>pdedef</b> when called from nag_pde_parab_1d_cd (d03pfc).		

5: **numflx** – function, supplied by the user *External 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 (d03pfc).

Its specification is:

	void numflx (Integer <b>npde</b> , double <b>t</b> , double <b>x</b> , const double <b>uleft</b> [], const double <b>uright</b> [], double <b>flux</b> [], Integer * <b>ires</b> , Nag_Comm * <b>comm</b> , Nag_D03_Save * <b>saved</b> )	
1:	<b>npde</b> – Integer	<i>Input</i>
<i>On entry:</i> the number of PDEs in the system.		
2:	<b>t</b> – double	<i>Input</i>
<i>On entry:</i> the current value of the independent variable <i>t</i> .		
3:	<b>x</b> – double	<i>Input</i>
<i>On entry:</i> the current value of the space variable <i>x</i> .		

4:	<b>uleft</b> [ <b>npde</b> ] – const double	<i>Input</i>
	<i>On entry:</i> <b>uleft</b> [ <i>i</i> – 1] contains the <i>left</i> value of the component $U_i(x)$ , for $i = 1, 2, \dots, \text{npde}$ .	
5:	<b>uright</b> [ <b>npde</b> ] – const double	<i>Input</i>
	<i>On entry:</i> <b>uright</b> [ <i>i</i> – 1] contains the <i>right</i> value of the component $U_i(x)$ , for $i = 1, 2, \dots, \text{npde}$ .	
6:	<b>flux</b> [ <b>npde</b> ] – double	<i>Output</i>
	<i>On exit:</i> <b>flux</b> [ <i>i</i> – 1] must be set to the numerical flux $\hat{F}_i$ , for $i = 1, 2, \dots, \text{npde}$ .	
7:	<b>ires</b> – Integer *	<i>Input/Output</i>
	<i>On entry:</i> set to –1 or 1.	
	<i>On exit:</i> should usually remain unchanged. However, you may set <b>ires</b> to force the integration function to take certain actions as described below:	
	<b>ires</b> = 2	
	Indicates to the integrator that control should be passed back immediately to the calling function with the error indicator set to <b>fail.code</b> = <b>NE_USER_STOP</b> .	
	<b>ires</b> = 3	
	Indicates to the integrator that the current time step should be abandoned and a smaller time step used instead. You may wish to set <b>ires</b> = 3 when a physically meaningless input or output value has been generated. If you consecutively set <b>ires</b> = 3, then <b>nag_pde_parab_1d_cd</b> (d03pfc) returns to the calling function with the error indicator set to <b>fail.code</b> = <b>NE_FAILED_DERIV</b> .	
8:	<b>comm</b> – Nag_Comm *	<i>Communication Structure</i>
	Pointer to structure of type <b>Nag_Comm</b> ; the following members are relevant to <b>numflx</b> .	
	<b>user</b> – double *	
	<b>iuser</b> – Integer *	
	<b>p</b> – Pointer	
	The type Pointer will be <b>void *</b> . Before calling <b>nag_pde_parab_1d_cd</b> (d03pfc) these pointers may be allocated memory by the user and initialized with various quantities for use by <b>numflx</b> when called from <b>nag_pde_parab_1d_cd</b> (d03pfc).	
9:	<b>saved</b> – Nag_D03_Save *	<i>Communication Structure</i>
	If <b>numflx</b> calls one of the approximate Riemann solvers <b>nag_pde_parab_1d_euler_roe</b> (d03puc), <b>nag_pde_parab_1d_euler_osher</b> (d03pvc), <b>nag_pde_parab_1d_euler_hll</b> (d03pwc) or <b>nag_pde_parab_1d_euler_exact</b> (d03pxc) then <b>saved</b> is used to pass data concerning the computation to the solver. You should not change the components of <b>saved</b> .	

6: **bndary** – function, supplied by the user *External Function*

**bndary** must evaluate the functions  $G_i^L$  and  $G_i^R$  which describe the physical and numerical boundary conditions, as given by (6) and (7).

Its specification is:

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

1: <b>npde</b> – Integer	<i>Input</i>
	<i>On entry:</i> the number of PDEs in the system.
2: <b>npts</b> – Integer	<i>Input</i>
	<i>On entry:</i> the number of mesh points in the interval $[a, b]$ .
3: <b>t</b> – double	<i>Input</i>
	<i>On entry:</i> the current value of the independent variable $t$ .
4: <b>x[npts]</b> – const double	<i>Input</i>
	<i>On entry:</i> the mesh points in the spatial direction. $\mathbf{x}[0]$ corresponds to the left-hand boundary, $a$ , and $\mathbf{x}[npts - 1]$ corresponds to the right-hand boundary, $b$ .
5: <b>u[3 × npde]</b> – const double	<i>Input</i>
	<i>On entry:</i> contains the value of solution components in the boundary region.
	If <b>ibnd</b> = 0, $\mathbf{u}[3 \times j + i]$ contains the value of the component $U_i(x, t)$ at $x = \mathbf{x}[j - 1]$ , for $i = 1, 2, \dots, npde$ ; $j = 1, 2, 3$ .
	If <b>ibnd</b> ≠ 0, $\mathbf{u}[3 \times j + i]$ contains the value of the component $U_i(x, t)$ at $x = \mathbf{x}[npts - j]$ , for $i = 1, 2, \dots, npde$ ; $j = 1, 2, 3$ .
6: <b>ibnd</b> – Integer	<i>Input</i>
	<i>On entry:</i> specifies which boundary conditions are to be evaluated.
	<b>ibnd</b> = 0
	<b>bndary</b> must evaluate the left-hand boundary condition at $x = a$ .
	<b>ibnd</b> ≠ 0
	<b>bndary</b> must evaluate the right-hand boundary condition at $x = b$ .
7: <b>g[npde]</b> – double	<i>Output</i>
	<i>On exit:</i> $\mathbf{g}[i - 1]$ must contain the $i$ th component of either $\mathbf{g}^L$ or $\mathbf{g}^R$ in (6) and (7), depending on the value of <b>ibnd</b> , for $i = 1, 2, \dots, npde$ .
8: <b>ires</b> – Integer *	<i>Input/Output</i>
	<i>On entry:</i> set to -1 or 1.
	<i>On exit:</i> should usually remain unchanged. However, you may set <b>ires</b> to force the integration function to take certain actions as described below:
	<b>ires</b> = 2
	Indicates to the integrator that control should be passed back immediately to the calling function with the error indicator set to <b>fail.code</b> = <b>NE_USER_STOP</b> .
	<b>ires</b> = 3
	Indicates to the integrator that the current time step should be abandoned and a smaller time step used instead. You may wish to set <b>ires</b> = 3 when a physically meaningless input or output value has been generated. If you consecutively set <b>ires</b> = 3, then <b>nag_pde_parab_1d_cd</b> (d03pfc) returns to the calling function with the error indicator set to <b>fail.code</b> = <b>NE_FAILED_DERIV</b> .
9: <b>comm</b> – Nag_Comm *	<i>Communication Structure</i>
	Pointer to structure of type <b>Nag_Comm</b> ; the following members are relevant to <b>bndary</b> .

**user** – double \*  
**iuser** – Integer \*  
**p** – Pointer

The type Pointer will be `void *`. Before calling `nag_pde_parab_1d_cd` (d03pfc) these pointers may be allocated memory by the user and initialized with various quantities for use by **bndary** when called from `nag_pde_parab_1d_cd` (d03pfc).

7: **u**[**npde** × **npts**] – double *Input/Output*

*On entry:* **u**[**npde** ×  $j + i$ ] must contain the initial value of  $U_i(x, t)$  at  $x = \mathbf{x}[j - 1]$  and  $t = \mathbf{ts}$ , for  $i = 1, 2, \dots, \mathbf{npde}$ ;  $j = 1, 2, \dots, \mathbf{npts}$ .

*On exit:* **u**[**npde** ×  $j + i$ ] will contain the computed solution  $U_i(x, t)$  at  $x = \mathbf{x}[j - 1]$  and  $t = \mathbf{ts}$ , for  $i = 1, 2, \dots, \mathbf{npde}$ ;  $j = 1, 2, \dots, \mathbf{npts}$ .

8: **npts** – Integer *Input*

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

*Constraint:* **npts**  $\geq 3$ .

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

*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]  $< \mathbf{x}[1] < \dots < \mathbf{x}[\mathbf{npts} - 1]$ .

10: **acc**[2] – const double *Input*

*On entry:* the components of **acc** contain the relative and absolute error tolerances used in the local error test in the time integration.

If  $E(i, j)$  is the estimated error for  $U_i$  at the  $j$ th mesh point, the error test is

$$E(i, j) = \mathbf{acc}[0] \times \mathbf{u}[\mathbf{npde} \times j + i] + \mathbf{acc}[1].$$

*Constraint:* **acc**[0] and **acc**[1]  $\geq 0.0$  (but not both zero).

11: **tsmax** – double *Input*

*On entry:* the maximum absolute step size to be allowed in the time integration. If **tsmax** = 0.0 then no maximum is imposed.

*Constraint:* **tsmax**  $\geq 0.0$ .

12: **rsave**[**lrsave**] – double *Communication Array*

If **ind** = 0, **rsave** need not be set on entry.

If **ind** = 1, **rsave** must be unchanged from the previous call to the function because it contains required information about the iteration.

13: **lrsave** – Integer *Input*

*On entry:* the dimension of the array **rsave** as declared in the function from which `nag_pde_parab_1d_cd` (d03pfc) is called.

*Constraint:* **lrsave**  $\geq (11 + 9 \times \mathbf{npde}) \times \mathbf{npde} \times \mathbf{npts} + (32 + 3 \times \mathbf{npde}) \times \mathbf{npde} + 7 \times \mathbf{npts} + 54$ .

14: **isave**[**lisave**] – Integer *Communication Array*

If **ind** = 0, **isave** need not be set on entry.

If **ind** = 1, **isave** must be unchanged from the previous call to the function because it contains required information about the iteration. In particular:

**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 computing 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 last backward differentiation formula method used.

**isave[4]**

Contains the number of Newton iterations performed by the time integrator. Each iteration involves an ODE residual evaluation followed by a back-substitution using the *LU* decomposition of the Jacobian matrix.

15: **lisave** – Integer*Input*

*On entry:* the dimension of the array **isave** as declared in the function from which **nag\_pde\_parab\_1d\_cd** (d03pfc) is called.

*Constraint:* **lisave**  $\geq \mathbf{npde} \times \mathbf{npts} + 24$ .

16: **itask** – Integer*Input*

*On entry:* the task to be performed by the ODE integrator.

**itask** = 1

Normal computation of output values **u** at  $t = \mathbf{tout}$  (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  $t = \mathbf{tout}$ .

*Constraint:*  $1 \leq \mathbf{itask} \leq 3$ .

17: **itrace** – Integer*Input*

*On entry:* the level of trace information required from **nag\_pde\_parab\_1d\_cd** (d03pfc) and the underlying ODE solver. **itrace** may take the value  $-1, 0, 1, 2$ , or  $3$ .

**itrace** =  $-1$ 

No output is generated.

**itrace** = 0

Only warning messages from the PDE solver are printed .

**itrace**  $> 0$ 

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.

If **itrace**  $< -1$ , then  $-1$  is assumed and similarly if **itrace**  $> 3$ , then  $3$  is assumed.

The advisory messages are given in greater detail as **itrace** increases.

18: <b>outfile</b> – const char *	<i>Input</i>
<i>On entry:</i> the name of a file to which diagnostic output will be directed. If <b>outfile</b> is <b>NULL</b> the diagnostic output will be directed to standard output.	
19: <b>ind</b> – Integer *	<i>Input/Output</i>
<i>On entry:</i> must be set to 0 or 1.	
<b>ind</b> = 0	
Starts or restarts the integration in time.	
<b>ind</b> = 1	
Continues the integration after an earlier exit from the function. In this case, only the arguments <b>tout</b> and <b>fail</b> should be reset between calls to nag_pde_parab_1d_cd (d03pfc).	
<i>Constraint:</i> $0 \leq \text{ind} \leq 1$ .	
<i>On exit:</i> <b>ind</b> = 1.	
20: <b>comm</b> – Nag_Comm *	<i>Communication Structure</i>
The NAG communication argument (see Section 2.2.1.1 of the Essential Introduction).	
21: <b>saved</b> – Nag_D03_Save *	<i>Communication Structure</i>
<b>Note:</b> <b>saved</b> is a NAG defined type (see Section 2.2.1.1 of the Essential Introduction).	
<b>saved</b> must remain unchanged following a previous call to a d03 function and prior to any subsequent call to a d03 function.	
22: <b>fail</b> – NagError *	<i>Input/Output</i>
The NAG error argument (see Section 2.6 of the Essential Introduction).	

## 6 Error Indicators and Warnings

### NE\_ACC\_IN\_DOUBT

Integration completed, but small changes in **acc** are unlikely to result in a changed solution.  
 $\text{acc}[0] = \langle \text{value} \rangle$ ,  $\text{acc}[1] = \langle \text{value} \rangle$ .

### NE\_BAD\_PARAM

On entry, argument  $\langle \text{value} \rangle$  had an illegal value.

### NE\_FAILED\_DERIV

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

### NE\_FAILED\_START

Values in **acc** are too small to start integration:  $\text{acc}[0] = \langle \text{value} \rangle$ ,  $\text{acc}[1] = \langle \text{value} \rangle$ .

### 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**:  $\text{ts} = \langle \text{value} \rangle$ .

Underlying ODE solver cannot make further progress from the point **ts** with the supplied values of **acc**.  $\text{ts} = \langle \text{value} \rangle$ ,  $\text{acc}[0] = \langle \text{value} \rangle$ ,  $\text{acc}[1] = \langle \text{value} \rangle$ .

**NE\_INCOMPAT\_PARAM**

On entry, **acc**[0] and **acc**[1] are both zero.

**NE\_INT**

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

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

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

On entry, **npde** =  $\langle value \rangle$ .

Constraint: **npde**  $\geq 1$ .

On entry, **npts** =  $\langle value \rangle$ .

Constraint: **npts**  $\geq 3$ .

**NE\_INT\_2**

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

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

**NE\_INTERNAL\_ERROR**

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

**NE\_NOT\_CLOSE\_FILE**

Cannot close file  $\langle value \rangle$ .

**NE\_NOT\_STRICTLY\_INCREASING**

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

**NE\_NOT\_WRITE\_FILE**

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

**NE\_REAL**

On entry, **acc**[0]  $< 0.0$ : **acc**[0] =  $\langle value \rangle$ .

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

On entry, **tsmax** =  $\langle value \rangle$ .

Constraint: **tsmax**  $\geq 0.0$ .

**NE\_REAL\_2**

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\_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**, **numflux**, or **bndary**. Integration is successful as far as **ts**: **ts** =  $\langle value \rangle$ .

## 7 Accuracy

nag\_pde\_parab\_1d\_cd (d03pfc) 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. You should therefore test the effect of varying the components of the accuracy argument, **acc**.

## 8 Further Comments

nag\_pde\_parab\_1d\_cd (d03pfc) 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 you are advised to use one of the central-difference schemes for such problems.

You 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 **tsmax**. It is worth experimenting with this argument, 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 and on the accuracy requested.

## 9 Example

For this function two examples are presented. There is a single example program for nag\_pde\_parab\_1d\_cd (d03pfc), with a main program and the code to solve the two example problems is given in the functions ex1 and ex2.

### Example 1 (ex1)

This example is a simple first-order system which illustrates the calculation of the numerical flux using Roe's approximate Riemann solver, and the specification of numerical boundary conditions using extrapolated characteristic variables. The PDEs are

$$\begin{aligned}\frac{\partial U_1}{\partial t} + \frac{\partial U_1}{\partial x} + \frac{\partial U_2}{\partial x} &= 0, \\ \frac{\partial U_2}{\partial t} + 4\frac{\partial U_1}{\partial x} + \frac{\partial U_2}{\partial x} &= 0,\end{aligned}$$

for  $x \in [0, 1]$  and  $t \geq 0$ . The PDEs have an exact solution given by

$$\begin{aligned}U_1(x, t) &= \frac{1}{2}\{\exp(x + t) + \exp(x - 3t)\} + \frac{1}{4}\left\{\sin(2\pi(x - 3t)^2) - \sin(2\pi(x + t)^2)\right\} + 2t^2 - 2xt, \\ U_2(x, t) &= \exp(x - 3t) - \exp(x + t) + \frac{1}{2}\left\{\sin(2\pi(x - 3t)^2) + \sin(2\pi(x - 3t)^2)\right\} + x^2 + 5t^2 - 2xt.\end{aligned}$$

The initial conditions are given by the exact solution. The characteristic variables are  $2U_1 + U_2$  and  $2U_1 - U_2$  corresponding to the characteristics given by  $dx/dt = 3$  and  $dx/dt = -1$  respectively. Hence a physical boundary condition is required for  $2U_1 + U_2$  at the left-hand boundary, and for  $2U_1 - U_2$  at the right-hand boundary (corresponding to the incoming characteristics); and a numerical boundary condition is required for  $2U_1 - U_2$  at the left-hand boundary, and for  $2U_1 + U_2$  at the right-hand boundary (outgoing characteristics). The physical boundary conditions are obtained from the exact solution, and the numerical boundary conditions are calculated by linear extrapolation of the appropriate characteristic variable. The numerical flux is calculated using Roe's approximate Riemann solver: Using the notation in Section 3, the flux vector  $F$  and the Jacobian matrix  $A$  are

$$F = \begin{bmatrix} U_1 + U_2 \\ 4U_1 + U_2 \end{bmatrix} \quad \text{and} \quad A = \begin{bmatrix} 1 & 1 \\ 4 & 1 \end{bmatrix},$$

and the eigenvalues of  $A$  are 3 and  $-1$  with right eigenvectors  $[1 \ 2]^T$  and  $[-1 \ 2]^T$  respectively. Using equation (4) the  $\alpha_k$  are given by

$$\begin{bmatrix} U_{1R} - U_{1L} \\ U_{2R} - U_{2L} \end{bmatrix} = \alpha_1 \begin{bmatrix} 1 \\ 2 \end{bmatrix} + \alpha_2 \begin{bmatrix} -1 \\ 2 \end{bmatrix},$$

that is

$$\alpha_1 = \frac{1}{4}(2U_{1R} - 2U_{1L} + U_{2R} - U_{2L}) \quad \text{and} \quad \alpha_2 = \frac{1}{4}(-2U_{1R} + 2U_{1L} + U_{2R} - U_{2L}).$$

$F_L$  is given by

$$F_L = \begin{bmatrix} U_{1L} + U_{2L} \\ 4U_{1L} + U_{2L} \end{bmatrix},$$

and similarly for  $F_R$ . From equation (4), the numerical flux vector is

$$\hat{F} = \frac{1}{2} \begin{bmatrix} U_{1L} + U_{2L} + U_{1R} + U_{2R} \\ 4U_{1L} + U_{2L} + 4U_{1R} + U_{2R} \end{bmatrix} - \frac{1}{2}\alpha_1|3| \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \frac{1}{2}\alpha_2|-1| \begin{bmatrix} -1 \\ 2 \end{bmatrix},$$

that is

$$\hat{F} = \frac{1}{2} \begin{bmatrix} 3U_{1L} - U_{1R} + \frac{3}{2}U_{2L} + \frac{1}{2}U_{2R} \\ 6U_{1L} + 2U_{1R} + 3U_{2L} - U_{2R} \end{bmatrix}.$$

### Example 2 (ex2)

This example is an advection-diffusion equation in which the flux term depends explicitly on  $x$ :

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

for  $x \in [-1, 1]$  and  $0 \leq t \leq 10$ . The argument  $\epsilon$  is taken to be 0.01. The two physical boundary conditions are  $U(-1, t) = 3.0$  and  $U(1, t) = 5.0$  and the initial condition is  $U(x, 0) = x + 4$ . The integration is run to steady state at which the solution is known to be  $U = 4$  across the domain with a narrow boundary layer at both boundaries. In order to write the PDE in conservative form, a source term must be introduced, i.e.,

$$\frac{\partial U}{\partial t} + \frac{\partial(xU)}{\partial x} = \epsilon \frac{\partial^2 U}{\partial x^2} + U.$$

As in Example 1, the numerical flux is calculated using the Roe approximate Riemann solver. The Riemann problem to solve locally is

$$\frac{\partial U}{\partial t} + \frac{\partial(xU)}{\partial x} = 0.$$

The  $x$  in the flux term is assumed to be constant at a local level, and so using the notation in Section 3,  $F = xU$  and  $A = x$ . The eigenvalue is  $x$  and the eigenvector (a scalar in this case) is 1. The numerical flux is therefore

$$\hat{F} = \begin{cases} xU_L & \text{if } x \geq 0, \\ xU_R & \text{if } x < 0. \end{cases}$$

### 9.1 Program Text

```
/* nag_pde_parab_1d_cd (d03pfc) Example Program.
*
* Copyright 2001 Numerical Algorithms Group.
*
* Mark 7, 2001.
* Mark 7b revised, 2004.
*/
```

```

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

int ex1(void);
int ex2(void);
static void pdedef(Integer, double, double, const double[],
                    const double[], double[], double[], double[],
                    double[], Integer *, Nag_Comm *);
static void bndary1(Integer, Integer, double, const double[],
                     const double[], Integer, double[], Integer *,
                     Nag_Comm *);
static void bndary2(Integer, Integer, double, const double[],
                     const double[], Integer, double[], Integer *,
                     Nag_Comm *);
static void numflux1(Integer, double, double, const double[],
                     const double[], double[], Integer *, Nag_Comm *,
                     Nag_D03_Save *);
static void numflux2(Integer, double, double, const double[],
                     const double[], double[], Integer *, Nag_Comm *,
                     Nag_D03_Save *);
static void exact(double, double *, Integer, const double *, Integer);

int main(void)
{
    Vprintf("nag_pde_parab_1d_cd (d03pfc) Example Program Results\n");
    ex1();
    ex2();
    return 0;
}

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

int ex1(void)
{
    double tout, ts, tsmax;
    const Integer npde=2, npts=101, outpts=7, inter=20, lisave=npde*npts+24,
           lrsave=(11+9*npde)*npde*npts+(32+3*npde)*npde+7*npts+54;
    Integer exit_status, i, ind, it, itask, itrace, j, nop;
    double *acc=0, *rsave=0, *u=0, *ue=0, *x=0, *xout=0;
    Integer *isave=0;
    NagError fail;
    Nag_Comm comm;
    Nag_D03_Save saved;

    /* Allocate memory */

    if ( !(acc = NAG_ALLOC(2, double)) ||
        !(rsave = NAG_ALLOC(lrsave, double)) ||
        !(u = NAG_ALLOC(npde*npts, double)) ||
        !(ue = NAG_ALLOC(npde*outpts, double)) ||
        !(x = NAG_ALLOC(npts, double)) ||
        !(xout = NAG_ALLOC(outpts, double)) ||
        !(isave = NAG_ALLOC(lisave, Integer)) )
    {
        Vprintf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

    Vprintf("\n\nExample 1\n\n\n");
    INIT_FAIL(fail);
    exit_status = 0;

    itrace = 0;

```

```

acc[0] = 1.0e-4;
acc[1] = 1.0e-5;
tsmax = 0.0;

Vprintf(" npts = %4ld acc[0] = %10.3e acc[1] = %10.3e\n\n",
        npts, acc[0], acc[1]);
Vprintf("           x           Approx u     Exact u     Approx v     Exact v\n");

/* Initialise mesh */

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

/* Set initial values */

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

ind = 0;
itask = 1;

for (it = 1; it <= 2; ++it)
{
    tout = 0.1*it;

    /* nag_pde_parab_1d_cd (d03pfc).
     * General system of convection-diffusion PDEs with source
     * terms in conservative form, method of lines, upwind
     * scheme using numerical flux function based on Riemann
     * solver, one space variable
     */
    nag_pde_parab_1d_cd(npde, &ts, tout, d03pfp, numflx1, bndary1, u, npts,
                        x, acc, tsmax, rsave, lrsave, isave, lisave, itask,
                        itrace, 0, &ind, &comm, &saved, &fail);

    if (fail.code != NE_NOERROR)
    {
        Vprintf("Error from nag_pde_parab_1d_cd (d03pfc).\n%s\n",
                fail.message);
        exit_status = 1;
        goto END;
    }

    /* Set output points */

    nop = 0;
    for (i = 0; i < 101; i += inter)
    {
        ++nop;
        xout[nop - 1] = x[i];
    }

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

    /* Check against exact solution */

    exact(tout, ue, npde, xout, nop);

    for (i = 1; i <= nop; ++i)
    {
        j = (i-1)*inter+1;
        Vprintf("      %9.4f %9.4f %9.4f %9.4f %9.4f\n",
                xout[i-1], U(1,j), UE(1,i), U(2,j), UE(2,i));
    }

    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 (acc) NAG_FREE(acc);
    if (rsave) NAG_FREE(rsave);
    if (u) NAG_FREE(u);
    if (ue) NAG_FREE(ue);
    if (x) NAG_FREE(x);
    if (xout) NAG_FREE(xout);
    if (isave) NAG_FREE(isave);

    return exit_status;
}
static void bndary1(Integer npde, Integer npts, double t, const double x[],
                     const double u[], Integer ibnd, double g[], Integer *ires,
                     Nag_Comm *comm)
{
    double c, exu1, exu2;
    double ue[2];

    if (ibnd == 0)
    {
        exact(t, ue, npde, &x[0], 1);
        c = (x[1] - x[0])/(x[2] - x[1]);
        exu1 = (c + 1.0)*U(1, 2) - c*U(1, 3);
        exu2 = (c + 1.0)*U(2, 2) - c*U(2, 3);
        g[0] = 2.0*U(1, 1) + U(2, 1) - 2.0*UE(1, 1) - UE(2, 1);
        g[1] = 2.0*U(1, 1) - U(2, 1) - 2.0*exu1 + exu2;
    } else {
        exact(t, ue, npde, &x[npts-1], 1);
        c = (x[npts-1] - x[npts - 2])/(x[npts - 2] - x[npts - 3]);
        exu1 = (c + 1.0)*U(1, 2) - c*U(1, 3);
        exu2 = (c + 1.0)*U(2, 2) - c*U(2, 3);
        g[0] = 2.0*U(1, 1) - U(2, 1) - 2.0*UE(1, 1) + UE(2, 1);
        g[1] = 2.0*U(1, 1) + U(2, 1) - 2.0*exu1 - exu2;
    }

    return;
}
static void numflx1(Integer npde, double t, double x, const double uleft[],
                     const double uright[], double flux[],
                     Integer *ires, Nag_Comm *comm, Nag_D03_Save *saved)
{
    flux[0] = 0.5*(-uright[0] + 3.0*uleft[0] + 0.5*uright[1] + 1.5*uleft[1]);
    flux[1] = 0.5*( 2.0*uright[0] + 6.0*uleft[0] - uright[1] + uleft[1]*3.);

    return;
}
static void exact(double t, double *u, Integer npde,
                  const double **x, Integer npts)
{
    double x1, x2, pi;
    Integer i;

    pi = nag_pi;

    /* Exact solution (for comparison and b.c. purposes) */

    for (i = 1; i <= npts; ++i)
    {
        x1 = x[i-1] + t;
        x2 = x[i-1] - 3.0*t;

        U(1,i) = 0.5*(exp(x1) + exp(x2))
            + 0.25*(sin(2.0*pi*(x2*x2)) - sin(2.0*pi*(x1*x1)))
            + 2.0*t*t - 2.0*x[i-1]*t;

        U(2,i) = exp(x2) - exp(x1) +
            0.5*(sin(2.0*pi*(x2*x2)) + sin(2.0*pi*(x1*x1))) +
            x[i-1]*x[i-1] + 5.0*t*t - 2.0*x[i-1]*t;
    }
    return;
}

```

```

int ex2(void)
{
    double tout, ts, tsmax;
    const Integer npde=1, npts=151, outpts=7, lisave=npde*npts+24,
           lrsave=(11+9*npde)*npde*npts+(32+3*npde)*npde+7*npts+54;
    Integer exit_status=0, i, ind, it, itask, itrace;
    double *acc=0, *rsave=0, *u=0, *x=0, *xout=0;
    Integer *isave=0;
    NagError fail;
    Nag_Comm comm;
    Nag_D03_Save saved;

    /* Allocate memory */

    if ( !(acc = NAG_ALLOC(2, double)) ||
        !(rsave = NAG_ALLOC(lrsave, double)) ||
        !(u = NAG_ALLOC(npde*npts, double)) ||
        !(x = NAG_ALLOC(npts, double)) ||
        !(xout = NAG_ALLOC(outpts, double)) ||
        !(isave = NAG_ALLOC(lisave, Integer)) )
    {
        Vprintf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

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

    itrace = 0;
    acc[0] = 1e-5;
    acc[1] = 1e-5;

    Vprintf(" npts = %4ld  acc[0] = %10.3e  acc[1] = %10.3e\n\n",
            npts, acc[0], acc[1]);

    /* Initialise mesh */

    for (i = 0; i < npts; ++i) x[i] = -1.0 + 2.0*i/(npts-1.0);

    /* Set initial values */

    for (i = 1; i <= npts; ++i) U(1, i) = x[i-1] + 4.0;

    ind = 0;
    itask = 1;
    tsmax = 0.02;

    /* Set output points */

    xout[0] = x[0];
    xout[1] = x[3];
    xout[2] = x[36];
    xout[3] = x[75];
    xout[4] = x[111];
    xout[5] = x[147];
    xout[6] = x[150];

    Vprintf(" x      ");

    for (i = 0; i < 7; ++i)
    {
        Vprintf("%9.4f", xout[i]);
        Vprintf((i+1)%7 == 0 || i == 6 ? "\n":":");
    }
    Vprintf("\n");

    /* Loop over output value of t */

```

```

ts = 0.0;
tout = 1.0;
for (it = 0; it < 2; ++it)
{
    if (it == 1) tout = 10.0;

    /* nag_pde_parab_1d_cd (d03pfc), see above. */
    nag_pde_parab_1d_cd(npde, &ts, tout, pdedef, numflx2, bndary2, u, npts,
                        x, acc, tsmax, rsave, lrsave, isave, lisave, itask,
                        itrace, 0, &ind, &comm, &saved, &fail);

    if (fail.code != NE_NOERROR)
    {
        Vprintf("Error from nag_pde_parab_1d_cd (d03pfc).\n%s\n",
                fail.message);
        exit_status = 1;
        goto END;
    }

    Vprintf(" t = %6.3f\n", ts);
    Vprintf(" u      %9.4f%9.4f%9.4f%9.4f%9.4f%9.4f\n",
            U(1,1), U(1,4), U(1,37), U(1,76),
            U(1,112), U(1,148), U(1,151));
}

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 (acc) NAG_FREE(acc);
if (rsave) NAG_FREE(rsave);
if (u) NAG_FREE(u);
if (x) NAG_FREE(x);
if (xout) NAG_FREE(xout);
if (isave) NAG_FREE(isave);

return exit_status;
}
static void pdedef(Integer npde, double t, double x, const double u[],
                   const double ux[], double p[], double
                   c[], double d[], double s[], Integer *ires, Nag_Comm *comm)
{
    P(1, 1) = 1.0;
    c[0] = 0.01;
    d[0] = ux[0];
    s[0] = u[0];

    return;
}
static void bndary2(Integer npde, Integer npts, double t,
                    const double x[],
                    const double u[], Integer ibnd,
                    double g[], Integer *ires,
                    Nag_Comm *comm)
{
    if (ibnd == 0)
    {
        g[0] = U(1, 1) - 3.0;
    } else {
        g[0] = U(1, 1) - 5.0;
    }
    return;
}
static void numflx2(Integer npde, double t, double x, const double uleft[],
                     const double uright[], double flux[],

```

```

        Integer *ires, Nag_Comm *comm, Nag_D03_Save *saved)
{
    if (x >= 0.0)
    {
        flux[0] = x * uleft[0];
    } else {
        flux[0] = x * uright[0];
    }
    return;
}

```

## 9.2 Program Data

None.

## 9.3 Program Results

nag\_pde\_parab\_1d\_cd (d03pfc) Example Program Results

Example 1

```

npts = 101 acc[0] = 1.000e-04 acc[1] = 1.000e-05

      x        Approx u      Exact u      Approx v      Exact v
t = 0.100
      0.0000    1.0615    1.0613    -0.0155    -0.0150
      0.2000    0.9892    0.9891    -0.0953    -0.0957
      0.4000    1.0826    1.0826    0.1180     0.1178
      0.6000    1.7001    1.7001    -0.0751    -0.0746
      0.8000    2.3959    2.3966    -0.2453    -0.2458
      1.0000    2.1029    2.1025    0.3760     0.3753

t = 0.200
      0.0000    1.0957    1.0956    0.0368     0.0370
      0.2000    1.0808    1.0811    0.1826     0.1828
      0.4000    1.1102    1.1100    -0.2935    -0.2938
      0.6000    1.6461    1.6454    -1.2921    -1.2908
      0.8000    1.7913    1.7920    -0.8510    -0.8525
      1.0000    2.2050    2.2050    -0.4222    -0.4221

Number of integration steps in time =      56
Number of function evaluations =      229
Number of Jacobian evaluations =        7
Number of iterations =      143

```

Example 2

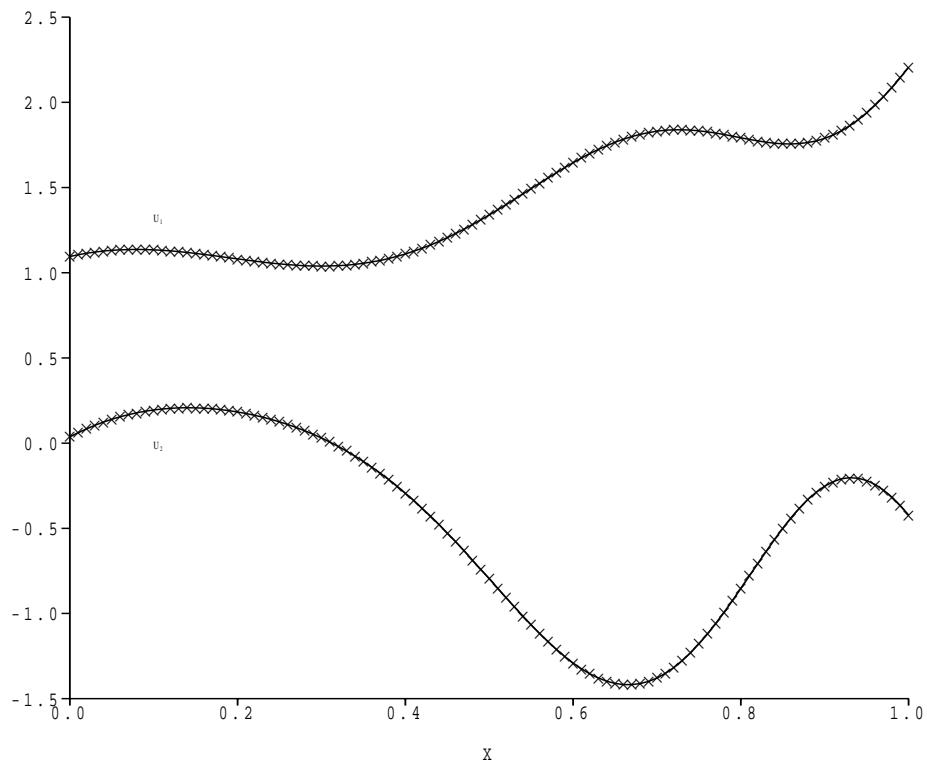
```

npts = 151 acc[0] = 1.000e-05 acc[1] = 1.000e-05

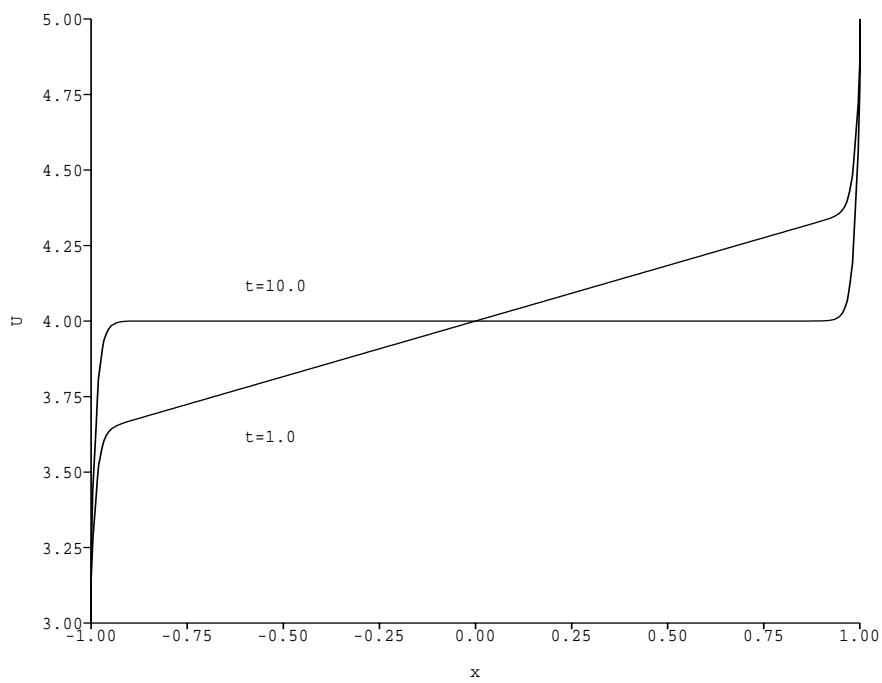
      x        -1.0000    -0.9600    -0.5200     0.0000     0.4800    0.9600    1.0000
t = 1.000
      u        3.0000    3.6221    3.8087     4.0000     4.1766    4.3779    5.0000
t = 10.000
      u        3.0000    3.9592    4.0000     4.0000     4.0000    4.0408    5.0000

Number of integration steps in time =      503
Number of function evaluations =      1190
Number of Jacobian evaluations =        28
Number of iterations =      1035

```



**Figure 1**  
Solution to Example 1



**Figure 2**  
Solution to Example 2