

NAG C Library Function Document

nag_pde_parab_1d_coll (d03pdc)

1 Purpose

nag_pde_parab_1d_coll (d03pdc) integrates a system of linear or nonlinear parabolic partial differential equations (PDEs) in one space variable. The spatial discretization is performed using a Chebyshev C^0 collocation method, and the method of lines is employed to reduce the PDEs to a system of ordinary differential equations (ODEs). The resulting system is solved using a backward differentiation formula method.

2 Specification

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

void nag_pde_parab_1d_coll (Integer npde, Integer m, double *ts, double tout,
    void (*pdedef)(Integer npde, double t, const double x[], Integer nptl,
        const double u[], const double ux[], double p[], double q[], double r[],
        Integer *ires, Nag_Comm *comm),
    void (*bndary)(Integer npde, double t, const double u[], const double ux[],
        Integer ibnd, double beta[], double gamma[], Integer *ires,
        Nag_Comm *comm),
    double u[], Integer nbkpts, const double xbkpts[], Integer npoly,
    Integer npts, double x[],
    void (*uinit)(Integer npde, Integer npts, const double x[], double u[],
        Nag_Comm *comm),
    double acc, 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_coll (d03pdc) integrates the system of parabolic equations:

$$\sum_{j=1}^{\text{npde}} P_{i,j} \frac{\partial U_j}{\partial t} + Q_i = x^{-m} \frac{\partial}{\partial x} (x^m R_i), \quad i = 1, 2, \dots, \text{npde}, \quad a \leq x \leq b, t \geq t_0, \quad (1)$$

where $P_{i,j}$, Q_i and R_i depend on x , t , U , U_x and the vector U is the set of solution values

$$U(x, t) = \left[U_1(x, t), \dots, U_{\text{npde}}(x, t) \right]^T, \quad (2)$$

and the vector U_x is its partial derivative with respect to x . Note that $P_{i,j}$, Q_i and R_i must not depend on $\frac{\partial U}{\partial t}$.

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 $b = x_{\text{nbkpts}}$ are the leftmost and rightmost of a user-defined set of break points $x_1, x_2, \dots, x_{\text{nbkpts}}$. The co-ordinate system in space is defined by the value of m ; $m = 0$ for Cartesian co-ordinates, $m = 1$ for cylindrical polar co-ordinates and $m = 2$ for spherical polar co-ordinates.

The system is defined by the functions $P_{i,j}$, Q_i and R_i which must be specified in a function **pdedef** supplied by you.

The initial values of the functions $U(x, t)$ must be given at $t = t_0$, and must be specified in a function **uinit**.

The functions R_i , for $i = 1, 2, \dots, \mathbf{npde}$, which may be thought of as fluxes, are also used in the definition of the boundary conditions for each equation. The boundary conditions must have the form

$$\beta_i(x, t)R_i(x, t, U, U_x) = \gamma_i(x, t, U, U_x), \quad i = 1, 2, \dots, \mathbf{npde}, \quad (3)$$

where $x = a$ or $x = b$.

The boundary conditions must be specified in a function **boundary** provided by you. Thus, the problem is subject to the following restrictions:

- (i) $t_0 < t_{\text{out}}$, so that integration is in the forward direction;
- (ii) $P_{i,j}$, Q_i and the flux R_i must not depend on any time derivatives;
- (iii) the evaluation of the functions $P_{i,j}$, Q_i and R_i is done at both the break points and internally selected points for each element in turn, that is $P_{i,j}$, Q_i and R_i are evaluated twice at each break point. Any discontinuities in these functions **must** therefore be at one or more of the break points $x_1, x_2, \dots, x_{\mathbf{nbkpts}}$;
- (iv) at least one of the functions $P_{i,j}$ must be non-zero so that there is a time derivative present in the problem;
- (v) if $m > 0$ and $x_1 = 0.0$, which is the left boundary point, then it must be ensured that the PDE solution is bounded at this point. This can be done by either specifying the solution at $x = 0.0$ or by specifying a zero flux there, that is $\beta_i = 1.0$ and $\gamma_i = 0.0$. See also Section 8 below.

The parabolic equations are approximated by a system of ODEs in time for the values of U_i at the mesh points. This ODE system is obtained by approximating the PDE solution between each pair of break points by a Chebyshev polynomial of degree **npoly**. The interval between each pair of break points is treated by nag_pde_parab_1d_coll (d03pdc) as an element, and on this element, a polynomial and its space and time derivatives are made to satisfy the system of PDEs at **npoly** – 1 spatial points, which are chosen internally by the code and the break points. In the case of just one element, the break points are the boundaries. The user-defined break points and the internally selected points together define the mesh. The smallest value that **npoly** can take is one, in which case, the solution is approximated by piecewise linear polynomials between consecutive break points and the method is similar to an ordinary finite element method.

In total there are $(\mathbf{nbkpts} - 1) \times \mathbf{npoly} + 1$ mesh points in the spatial direction, and $\mathbf{npde} \times ((\mathbf{nbkpts} - 1) \times \mathbf{npoly} + 1)$ ODEs in the time direction; one ODE at each break point for each PDE component and $(\mathbf{npoly} - 1)$ ODEs for each PDE component between each pair of break points. The system is then integrated forwards in time using a backward differentiation formula method.

4 References

Berzins M (1990) Developments in the NAG Library software for parabolic equations *Scientific Software Systems* (ed J C Mason and M G Cox) 59–72 Chapman and Hall

Berzins M and Dew P M (1991) Algorithm 690: Chebyshev polynomial software for elliptic-parabolic systems of PDEs *ACM Trans. Math. Software* **17** 178–206

Zaturska N B, Drazin P G and Banks W H H (1988) On the flow of a viscous fluid driven along a channel by a suction at porous walls *Fluid Dynamics Research* **4**

5 Arguments

1: **npde** – Integer *Input*

On entry: the number of PDEs in the system to be solved.

Constraint: **npde** ≥ 1 .

2: **m** – Integer *Input*

On entry: the co-ordinate system used:

m = 0

Indicates Cartesian co-ordinates.

m = 1

Indicates cylindrical polar co-ordinates.

m = 2

Indicates spherical polar co-ordinates.

Constraint: $0 \leq \mathbf{m} \leq 2$.3: **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**.4: **tout** – double*Input**On entry:* the final value of t to which the integration is to be carried out.5: **pdedef** – function, supplied by the user*External Function***pdedef** must compute the values of the functions $P_{i,j}$, Q_i and R_i which define the system of PDEs. The functions may depend on x , t , U and U_x and must be evaluated at a set of points.

Its specification is:

```
void pdedef (Integer npde, double t, const double x[], Integer nptl,
             const double u[], const double ux[], double p[], double q[], 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: **x[nptl]** – const double*Input**On entry:* contains a set of mesh points at which $P_{i,j}$, Q_i and R_i are to be evaluated. $\mathbf{x}[0]$ and $\mathbf{x}[nptl - 1]$ contain successive user-supplied break points and the elements of the array will satisfy $\mathbf{x}[0] < \mathbf{x}[1] < \dots < \mathbf{x}[nptl - 1]$.4: **nptl** – Integer*Input**On entry:* the number of points at which evaluations are required (the value of **npoly** + 1).5: **u[npde × nptl]** – const double*Input**On entry:* $\mathbf{u}[\mathbf{npde} \times j + i]$ contains the value of the component $U_i(x, t)$ where $x = \mathbf{x}[j - 1]$, for $i = 1, 2, \dots, \mathbf{npde}$; $j = 1, 2, \dots, \mathbf{nptl}$.6: **ux[npde × nptl]** – const double*Input**On entry:* $\mathbf{ux}[\mathbf{npde} \times j + i]$ contains the value of the component $\frac{\partial U_i(x, t)}{\partial x}$ where $x = \mathbf{x}[j - 1]$, for $i = 1, 2, \dots, \mathbf{npde}$; $j = 1, 2, \dots, \mathbf{nptl}$.

7:	p [npde × npde × nptl] – double	<i>Output</i>
<i>On exit:</i> p [npde × npde × j + i] must be set to the value of $P_{i,j}(x, t, U, U_x)$ where $x = \mathbf{x}[k - 1]$, for $i, j = 1, 2, \dots, \mathbf{npde}$; $k = 1, 2, \dots, \mathbf{nptl}$.		
8:	q [npde × nptl] – double	<i>Output</i>
<i>On exit:</i> q [npde × j + i] must be set to the value of $Q_i(x, t, U, U_x)$ where $x = \mathbf{x}[j - 1]$, for $i = 1, 2, \dots, \mathbf{npde}$; $j = 1, 2, \dots, \mathbf{nptl}$.		
9:	r [npde × nptl] – double	<i>Output</i>
<i>On exit:</i> r [npde × j + i] must be set to the value of $R_i(x, t, U, U_x)$ where $x = \mathbf{x}[j - 1]$, for $i = 1, 2, \dots, \mathbf{npde}$; $j = 1, 2, \dots, \mathbf{nptl}$.		
10:	ires – 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 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. You may wish to set ires = 3 when a physically meaningless input or output value has been generated. If you consecutively set ires = 3 , then nag_pde_parab_1d_coll (d03pdc) returns to the calling function with the error indicator set to fail.code = NE_FAILED_DERIV .		
11:	comm – Nag_Comm *	<i>Communication Structure</i>
Pointer to structure of type Nag_Comm ; the following members are relevant to pdedef .		
user – double *		
iuser – Integer *		
p – Pointer		
The type Pointer will be void * . Before calling nag_pde_parab_1d_coll (d03pdc) these pointers may be allocated memory by the user and initialized with various quantities for use by pdedef when called from nag_pde_parab_1d_coll (d03pdc).		

6: **bndary** – function, supplied by the user *External Function*
bndary must compute the functions β_i and γ_i which define the boundary conditions as in equation (3).

Its specification is:

	void bndary (Integer npde , double t , const double u [], const double ux [], Integer ibnd , double beta [], double gamma [], Integer * ires , Nag_Comm * comm)	
1:	npde – Integer	<i>Input</i>
<i>On entry:</i> the number of PDEs in the system.		
2:	t – double	<i>Input</i>
<i>On entry:</i> the current value of the independent variable t .		

3:	u[npde] – const double	<i>Input</i>
<i>On entry:</i> u [<i>i</i> – 1] contains the value of the component $U_i(x, t)$ at the boundary specified by ibnd , for $i = 1, 2, \dots, \text{npde}$.		
4:	ux[npde] – const double	<i>Input</i>
<i>On entry:</i> ux [<i>i</i> – 1] contains the value of the component $\frac{\partial U_i(x, t)}{\partial x}$ at the boundary specified by ibnd , for $i = 1, 2, \dots, \text{npde}$.		
5:	ibnd – Integer	<i>Input</i>
<i>On entry:</i> specifies which boundary conditions are to be evaluated.		
ibnd = 0		
bndary must set up the coefficients of the left-hand boundary, $x = a$.		
ibnd ≠ 0		
bndary must set up the coefficients of the right-hand boundary, $x = b$.		
6:	beta[npde] – double	<i>Output</i>
<i>On exit:</i> beta [<i>i</i> – 1] must be set to the value of $\beta_i(x, t)$ at the boundary specified by ibnd , for $i = 1, 2, \dots, \text{npde}$.		
7:	gamma[npde] – double	<i>Output</i>
<i>On exit:</i> gamma [<i>i</i> – 1] must be set to the value of $\gamma_i(x, t, U, U_x)$ at the boundary specified by ibnd , for $i = 1, 2, \dots, \text{npde}$.		
8:	ires – 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 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. You may wish to set ires = 3 when a physically meaningless input or output value has been generated. If you consecutively set ires = 3, then nag_pde_parab_1d_coll (d03pdc) returns to the calling function with the error indicator set to fail.code = NE_FAILED_DERIV .		
9:	comm – Nag_Comm *	<i>Communication Structure</i>
Pointer to structure of type Nag_Comm ; the following members are relevant to bndary .		
user – double *		
iuser – Integer *		
p – Pointer		
The type Pointer will be void * . Before calling nag_pde_parab_1d_coll (d03pdc) 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_coll (d03pdc).		

7: **u[**npde** × **npts**]** – double *Input/Output*
On entry: if **ind** = 1 the value of **u** must be unchanged from the previous call.

On exit: $\mathbf{u}[\mathbf{npde} \times j + i]$ will contain the computed solution at $t = \mathbf{ts}$.

8: **nbkpts** – Integer *Input*

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

Constraint: $\mathbf{nbkpts} \geq 2$.

9: **xbkpts[nbkpts]** – const double *Input*

On entry: the values of the break points in the space direction. $\mathbf{xbkpts}[0]$ must specify the left-hand boundary, a , and $\mathbf{xbkpts}[nbkpts - 1]$ must specify the right-hand boundary, b .

Constraint: $\mathbf{xbkpts}[0] < \mathbf{xbkpts}[1] < \dots < \mathbf{xbkpts}[nbkpts - 1]$.

10: **npoly** – Integer *Input*

On entry: the degree of the Chebyshev polynomial to be used in approximating the PDE solution between each pair of break points.

Constraint: $1 \leq \mathbf{npoly} \leq 49$.

11: **npts** – Integer *Input*

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

Constraint: $\mathbf{npts} = (\mathbf{nbkpts} - 1) \times \mathbf{npoly} + 1$.

12: **x[npts]** – double *Output*

On exit: the mesh points chosen by `nag_pde_parab_1d_coll` (d03pdc) in the spatial direction. The values of \mathbf{x} will satisfy $\mathbf{x}[0] < \mathbf{x}[1] < \dots < \mathbf{x}[\mathbf{npts} - 1]$.

13: **uinit** – function, supplied by the user *External Function*

uinit must compute the initial values of the PDE components $U_i(x_j, t_0)$, for $i = 1, 2, \dots, \mathbf{npde}$; $j = 1, 2, \dots, \mathbf{npts}$.

Its specification is:

```
void uinit (Integer npde, Integer npts, const double x[], double u[],
           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: **x[npts]** – const double *Input*

On entry: $\mathbf{x}[j - 1]$, contains the values of the j th mesh point, for $j = 1, 2, \dots, \mathbf{npts}$.

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

On exit: $\mathbf{u}[\mathbf{npde} \times j + i]$ must be set to the initial value $U_i(x_j, t_0)$, for $i = 1, 2, \dots, \mathbf{npde}$; $j = 1, 2, \dots, \mathbf{npts}$.

5: **comm** – Nag_Comm * *Communication Structure*

Pointer to structure of type **Nag_Comm**; the following members are relevant to **uinit**.

user – double *
iuser – Integer *
p – Pointer

The type Pointer will be `void *`. Before calling `nag_pde_parab_1d_coll (d03pdc)` these pointers may be allocated memory by the user and initialized with various quantities for use by **uinit** when called from `nag_pde_parab_1d_coll (d03pdc)`.

14: **acc** – double*Input*

On entry: a positive quantity for controlling the local error estimate 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:

$$|E(i,j)| = \mathbf{acc} \times (1.0 + |\mathbf{u}[\mathbf{npde} \times j + i]|).$$

Constraint: $\mathbf{acc} > 0.0$.

15: **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.

16: **lrsave** – Integer*Input*

On entry: the dimension of the array **rsave** as declared in the function from which `nag_pde_parab_1d_coll (d03pdc)` is called.

Constraint: $\mathbf{lrsave} \geq 11 \times \mathbf{npde} \times \mathbf{npts} + 50 + \mathbf{nwkres} + \mathbf{lenode}$, where $\mathbf{nwkres} = 3 \times (\mathbf{npoly} + 1)^2 + (\mathbf{npoly} + 1) \times (\mathbf{npde}^2 + 6 \times \mathbf{npde} + \mathbf{nbkpts} + 1) + 13 \times \mathbf{npde} + 5$, and $\mathbf{lenode} = \mathbf{npde} \times \mathbf{npts} \times (3 \times \mathbf{npde} \times (\mathbf{npoly} + 1) - 2)$.

17: **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.

18: **lisave** – Integer *Input*

On entry: the dimension of the array **isave** as declared in the function from which nag_pde_parab_1d_coll (d03pdc) is called.

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

19: **itask** – Integer *Input*

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

itask = 1

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

itask = 2

One step and return.

itask = 3

Stop at first internal integration point at or beyond $t = \mathbf{tout}$.

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

20: **itrace** – Integer *Input*

On entry: the level of trace information required from nag_pde_parab_1d_coll (d03pdc) 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.

21: **outfile** – const 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.

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

On entry: 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 arguments **tout** and **fail** should be reset between calls to nag_pde_parab_1d_coll (d03pdc).

Constraint: $0 \leq \mathbf{ind} \leq 1$.

On exit: **ind** = 1.

23: **comm** – Nag_Comm * *Communication Structure*

The NAG communication argument (see Section 2.2.1.1 of the Essential Introduction).

24: **saved** – Nag_D03_Save **Communication Structure***Note:** **saved** is a NAG defined type (see Section 2.2.1.1 of the Essential Introduction).**saved** must remain unchanged following a previous call to a d03 function and prior to any subsequent call to a d03 function.25: **fail** – NagError **Input/Output*

The NAG error argument (see Section 2.6 of the Essential Introduction).

6 Error Indicators and Warnings

NE_ACC_IN_DOUBT

Integration completed, but a small change in **acc** is unlikely to result in a changed solution.
acc = $\langle\text{value}\rangle$.

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** or **bndary**.

NE_FAILED_START

acc was too small to start integration: **acc** = $\langle\text{value}\rangle$.

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

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

NE_INCOMPAT_PARAM

On entry, **m** > 0 and **xbkpts**[0] < 0.0: **m** = $\langle\text{value}\rangle$, **xbkpts**[0] = $\langle\text{value}\rangle$.

NE_INT

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

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

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

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

On entry, **nbkpts** = $\langle\text{value}\rangle$.

Constraint: **nbkpts** \geq 2.

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

Constraint: **npde** \geq 1.

On entry, **npoly** = $\langle\text{value}\rangle$.

Constraint: $1 \leq \text{npoly} \leq 49$.

NE_INT_2

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

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

NE_INT_3

On entry, **npts** = $\langle value \rangle$, **nbkpts** = $\langle value \rangle$, **npoly** = $\langle value \rangle$.
 Constraint: **npts** = $(\text{nbkpts} - 1) \times \text{npoly} + 1$.

On entry, **npts** is not equal to $(\text{nbkpts} - 1) \times \text{npoly} + 1$: **npts** = $\langle value \rangle$, **nbkpts** = $\langle value \rangle$, **npoly** = $\langle value \rangle$.

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, break points **xbkpts** are badly ordered: $i = \langle value \rangle$, **xbkpts**[$i - 1$] = $\langle value \rangle$, $j = \langle value \rangle$, **xbkpts**[$j - 1$] = $\langle value \rangle$.

NE_NOT_WRITE_FILE

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

NE_REAL

On entry, **acc** = $\langle value \rangle$.
 Constraint: **acc** > 0.0.

NE_REAL_2

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

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

NE_SING_JAC

Singular Jacobian of ODE system. Check problem formulation.

NE_TIME_DERIV_DEP

Flux function appears to depend on time derivatives.

NE_USER_STOP

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

7 Accuracy

`nag_pde_parab_1d_coll` (d03pdc) controls the accuracy of the integration in the time direction but not the accuracy of the approximation in space. The spatial accuracy depends on the degree of the polynomial approximation **npoly**, and on both the number of break 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 accuracy argument, **acc**.

8 Further Comments

`nag_pde_parab_1d_coll` (d03pdc) is designed to solve parabolic systems (possibly including elliptic equations) with second-order derivatives in space. The argument specification allows you to include equations with only first-order derivatives in the space direction but there is no guarantee that the method

of integration will be satisfactory for such systems. The position and nature of the boundary conditions in particular are critical in defining a stable problem.

The time taken depends on the complexity of the parabolic system and on the accuracy requested.

9 Example

The problem consists of a fourth-order PDE which can be written as a pair of second-order elliptic-parabolic PDEs for $U_1(x, t)$ and $U_2(x, t)$,

$$0 = \frac{\partial^2 U_1}{\partial x^2} - U_2 \quad (4)$$

$$\frac{\partial U_2}{\partial t} = \frac{\partial^2 U_2}{\partial x^2} + U_2 \frac{\partial U_1}{\partial x} - U_1 \frac{\partial U_2}{\partial x} \quad (5)$$

where $-1 \leq x \leq 1$ and $t \geq 0$. The boundary conditions are given by

$$\frac{\partial U_1}{\partial x} = 0 \quad \text{and} \quad U_1 = 1 \quad \text{at } x = -1, \quad \text{and}$$

$$\frac{\partial U_1}{\partial x} = 0 \quad \text{and} \quad U_1 = -1 \quad \text{at } x = 1.$$

The initial conditions at $t = 0$ are given by

$$U_1 = -\sin \frac{\pi x}{2} \quad \text{and} \quad U_2 = \frac{\pi^2}{4} \sin \frac{\pi x}{2}.$$

The absence of boundary conditions for $U_2(x, t)$ does not pose any difficulties provided that the derivative flux boundary conditions are assigned to the first PDE (4) which has the correct flux, $\frac{\partial U_1}{\partial x}$. The conditions on $U_1(x, t)$ at the boundaries are assigned to the second PDE by setting $\beta_2 = 0.0$ in equation (3) and placing the Dirichlet boundary conditions on $U_1(x, t)$ in the function γ_2 .

9.1 Program Text

```
/* nag_pde_parab_1d_coll (d03pdc) Example Program.
*
* Copyright 2001 Numerical Algorithms Group.
*
* Mark 7, 2001.
* Mark 7b revised, 2004.
*/
#include <stdio.h>
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagd03.h>
#include <nagx01.h>
static void uinit(Integer, Integer, const double[], double[], Nag_Comm *);
static void pdedef(Integer, double, const double[], Integer, const double[],
                  const double[], double[], double[], double[],
                  Integer *, Nag_Comm *);
static void bndary(Integer, double, const double[], const double[], Integer,
                  double[], double[], Integer *, Nag_Comm *);
#define U(I,J) u[npde*((J)-1)+(I)-1]
#define UOUT(I,J,K) uout[npde*(intpts*((K)-1)+(J)-1)+(I)-1]
#define P(I,J,K) p[npde*(npde*((K)-1)+(J)-1)+(I)-1]
#define Q(I,J) q[npde*((J)-1)+(I)-1]
#define R(I,J) r[npde*((J)-1)+(I)-1]
#define UX(I,J) ux[npde*((J)-1)+(I)-1]
int main(void)
{
```

```

const Integer nbkpts=10, nelts=nbkpts-1, npde=2, npoly=3,
  m=0, itype=1, npts=nelts*npoly+1, neqn=npde*npts,
  intpts=6, np11=npoly+1, lisave=neqn+24,
  mu=npde*(npoly+1)-1, lenode=(3*mu+1)*neqn,
  nwkres=3*np11*np11+np11*(npde*npde+6*npde+nbkpts+1)
  +13*npde+5, lrsave=11*neqn+50+nwkres+lenode;

static double xout[6] = { -1.,-.6,-.2,.2,.6,1. };
double acc, tout, ts;
Integer exit_status, i, ind, it, itask, itrace;

double *rsave=0, *u=0, *uout=0, *x=0, *xbkpts=0;
Integer *isave=0;
NagError fail;
Nag_Comm comm;
Nag_D03_Save saved;

/* Allocate memory */

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

INIT_FAIL(fail);
exit_status = 0;

Vprintf("nag_pde_parab_1d_coll (d03pdc) Example Program Results\n\n");

acc = 1e-4;
itrace = 0;

/* Set the break-points */

for (i = 0; i < 10; ++i)
{
    xbkpts[i] = i*2.0/9.0- 1.0;
}

ind = 0;
itask = 1;
ts = 0.0;
tout = 1e-5;
Vprintf(" Polynomial degree =%4ld", npoly);
Vprintf(" No. of elements = %4ld\n\n", nelts);
Vprintf(" Accuracy requirement = %9.3e", acc);
Vprintf(" Number of points = %5ld\n\n", npts);
Vprintf(" t / x ");

for (i = 0; i < 6; ++i)
{
    Vprintf("%8.4f", xout[i]);
    Vprintf((i+1)%6 == 0 || i == 5 ?"\n":"");
}
Vprintf("\n");

/* Loop over output values of t */

for (it = 0; it < 5; ++it)
{
    tout *= 10.0;

    /* nag_pde_parab_1d_coll (d03pdc).
     * General system of parabolic PDEs, method of lines,

```

```

* Chebyshev C^0 collocation, one space variable
*/
nag_pde_parab_1d_coll(npde, m, &ts, tout, pdedef, bndary, u, nbkpts,
                      xbkpts, npoly, npts, x, uinit, acc, rsave, lrsave,
                      isave, lisave, itask, itrace, 0, &ind, &comm,
                      &saved, &fail);

if (fail.code != NE_NOERROR)
{
    Vprintf("Error from nag_pde_parab_1d_coll (d03pdc).\n%s\n",
            fail.message);
    exit_status = 1;
    goto END;
}

/* Interpolate at required spatial points */

/* nag_pde_interp_1d_coll (d03pyc).
 * PDEs, spatial interpolation with nag_pde_parab_1d_coll
 * (d03pdc) or nag_pde_parab_1d_coll_ode (d03pjc)
 */
nag_pde_interp_1d_coll(npde, u, nbkpts, xbkpts, npoly, npts, xout, intpts,
                      itype, uout, rsave, lrsave, &fail);

if (fail.code != NE_NOERROR)
{
    Vprintf("Error from nag_pde_interp_1d_coll (d03pyc).\n%s\n",
            fail.message);
    exit_status = 1;
    goto END;
}

Vprintf("\n %6.4f u(1)", tout);

for (i = 1; i <= 6; ++i)
{
    Vprintf("%8.4f", UOUT(1,i,1));
    Vprintf(i%6 == 0 || i == 6 ? "\n": "");
}

Vprintf("      u(2)");

for (i = 1; i <= 6; ++i)
{
    Vprintf("%8.4f", UOUT(2,i,1));
    Vprintf(i%6 == 0 || i == 6 ? "\n": "");
}
}

/* Print integration statistics */

Vprintf("\n");
Vprintf(" Number of integration steps in time           ");
Vprintf("%4ld\n", isave[0]);
Vprintf(" Number of residual evaluations of resulting ODE system ");
Vprintf("%4ld\n", isave[1]);
Vprintf(" Number of Jacobian evaluations           ");
Vprintf("%4ld\n", isave[2]);
Vprintf(" Number of iterations of nonlinear solver      ");
Vprintf("%4ld\n", isave[4]);

END:
if (rsave) NAG_FREE(rsave);
if (u) NAG_FREE(u);
if (uout) NAG_FREE(uout);
if (x) NAG_FREE(x);
if (xbkpts) NAG_FREE(xbkpts);
if (isave) NAG_FREE(isave);

return exit_status;
}

```

```

static void uinit(Integer npde, Integer npts, const double x[],
                  double u[], Nag_Comm *comm)
{
    Integer i;
    double piby2;

    piby2 = 0.5*nag_pi;
    for (i = 1; i <= npts; ++i)
    {
        U(1, i) = -sin(piby2*x[i-1]);
        U(2, i) = -piby2*piby2*U(1, i);
    }
    return;
}
static void pdedef(Integer npde, double t, const double x[], Integer nptl,
                   const double u[], const double ux[], double p[],
                   double q[], double r[], Integer *ires,
                   Nag_Comm *comm)
{
    Integer i;

    for (i = 1; i <= nptl; ++i)
    {
        Q(1, i) = U(2, i);
        Q(2, i) = U(1, i)*UX(2, i) - UX(1, i)*U(2, i);
        R(1, i) = UX(1, i);
        R(2, i) = UX(2, i);
        P(1, 1, i) = 0.0;
        P(1, 2, i) = 0.0;
        P(2, 1, i) = 0.0;
        P(2, 2, i) = 1.0;
    }
    return;
}
static void bndary(Integer npde, double t, const double u[],
                   const double ux[], Integer ibnd, double beta[],
                   double gamma[], Integer *ires, Nag_Comm *comm)
{
    if (ibnd == 0)
    {
        beta[0] = 1.0;
        gamma[0] = 0.0;
        beta[1] = 0.0;
        gamma[1] = u[0] - 1.0;
    }
    else
    {
        beta[0] = 1.0;
        gamma[0] = 0.0;
        beta[1] = 0.0;
        gamma[1] = u[0] + 1.0;
    }
    return;
}

```

9.2 Program Data

None.

9.3 Program Results

```

nag_pde_parab_1d_coll (d03pdc) Example Program Results

Polynomial degree =    3    No. of elements =      9

Accuracy requirement = 1.000e-04  Number of points =      28

t / x      -1.0000 -0.6000 -0.2000  0.2000  0.6000  1.0000

```

```
0.0001 u(1) 1.0000 0.8090 0.3090 -0.3090 -0.8090 -1.0000
      u(2) -2.4850 -1.9957 -0.7623 0.7623 1.9957 2.4850

0.0010 u(1) 1.0000 0.8085 0.3088 -0.3088 -0.8085 -1.0000
      u(2) -2.5583 -1.9913 -0.7606 0.7606 1.9913 2.5583

0.0100 u(1) 1.0000 0.8051 0.3068 -0.3068 -0.8051 -1.0000
      u(2) -2.6962 -1.9481 -0.7439 0.7439 1.9481 2.6962

0.1000 u(1) 1.0000 0.7951 0.2985 -0.2985 -0.7951 -1.0000
      u(2) -2.9022 -1.8339 -0.6338 0.6338 1.8339 2.9022

1.0000 u(1) 1.0000 0.7939 0.2972 -0.2972 -0.7939 -1.0000
      u(2) -2.9233 -1.8247 -0.6120 0.6120 1.8247 2.9233
```

```
Number of integration steps in time 50
Number of residual evaluations of resulting ODE system 407
Number of Jacobian evaluations 18
Number of iterations of nonlinear solver 122
```
