

NAG Toolbox

nag_pde_1d_parab_dae_fd (d03ph)

1 Purpose

`nag_pde_1d_parab_dae_fd` (d03ph) integrates a system of linear or nonlinear parabolic partial differential equations (PDEs) in one space variable, with scope for coupled ordinary differential equations (ODEs). The spatial discretization is performed using finite differences, and the method of lines is employed to reduce the PDEs to a system of ODEs. The resulting system is solved using a backward differentiation formula method or a Theta method (switching between Newton's method and functional iteration).

2 Syntax

```
[ts, u, rsave, isave, ind, user, cwsav, lwsav, iwsav, rwsav, ifail] =
nag_pde_1d_parab_dae_fd(npde, m, ts, tout, pdedef, bndary, u, x, ncode, odedef,
xi, rtol, atol, itol, norm_p, laopt, algopt, rsave, isave, itask, itrace, ind,
cwsav, lwsav, iwsav, rwsav, 'npts', npts, 'nxi', nxi, 'neqn', neqn, 'lisave',
lisave, 'user', user)

[ts, u, rsave, isave, ind, user, cwsav, lwsav, iwsav, rwsav, ifail] = d03ph
(npde, m, ts, tout, pdedef, bndary, u, x, ncode, odedef, xi, rtol, atol, itol,
norm_p, laopt, algopt, rsave, isave, itask, itrace, ind, cwsav, lwsav, iwsav,
rwsav, 'npts', npts, 'nxi', nxi, 'neqn', neqn, 'lisave', lisave, 'user', user)
```

Note: the interface to this routine has changed since earlier releases of the toolbox:

At Mark 22: *lrsave* was removed from the interface.

3 Description

`nag_pde_1d_parab_dae_fd` (d03ph) integrates the system of parabolic-elliptic equations and coupled ODEs

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

$$F_i(t, V, \dot{V}, \xi, U^*, U_x^*, R^*, U_t^*, U_{xt}^*) = 0, \quad i = 1, 2, \dots, \text{ncode}, \quad (2)$$

where (1) defines the PDE part and (2) generalizes the coupled ODE part of the problem.

In (1), $P_{i,j}$ and R_i depend on x, t, U, U_x and V ; Q_i depends on x, t, U, U_x, V and **linearly** on \dot{V} . The vector U is the set of PDE solution values

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

and the vector U_x is the partial derivative with respect to x . The vector V is the set of ODE solution values

$$V(t) = [V_1(t), \dots, V_{\text{ncode}}(t)]^T,$$

and \dot{V} denotes its derivative with respect to time.

In (2), 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 some of the PDE spatial mesh points. U^*, U_x^*, R^*, U_t^* and U_{xt}^* are the functions U, U_x, R, U_t and U_{xt} evaluated at these coupling points. Each F_i may only depend linearly on time derivatives. Hence the equation (2) may be written more precisely as

$$F = G - A\dot{V} - B \begin{pmatrix} U_t^* \\ U_{xt}^* \end{pmatrix}, \quad (3)$$

where $F = [F_1, \dots, F_{\mathbf{ncode}}]^T$, G is a vector of length \mathbf{ncode} , A is an \mathbf{ncode} by \mathbf{ncode} matrix, B is an \mathbf{ncode} by $(n_\xi \times \mathbf{npde})$ matrix and the entries in G , A and B may depend on t , ξ , U^* , U_x^* and V . In practice you only need to supply a vector of information to define the ODEs and not the matrices A and B . (See Section 5 for the specification of **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 $b = x_{\mathbf{npts}}$ are the leftmost and rightmost points of a user-defined mesh $x_1, x_2, \dots, x_{\mathbf{npts}}$. The coordinate system in space is defined by the values of m ; $m = 0$ for Cartesian coordinates, $m = 1$ for cylindrical polar coordinates and $m = 2$ for spherical polar coordinates.

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

The initial values of the functions $U(x, t)$ and $V(t)$ must be given at $t = t_0$.

The functions R_i which may be thought of as fluxes, are also used in the definition of the boundary conditions. The boundary conditions must have the form

$$\beta_i(x, t)R_i(x, t, U, U_x, V) = \gamma_i(x, t, U, U_x, V, \dot{V}), \quad i = 1, 2, \dots, \mathbf{npde}, \quad (4)$$

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

The boundary conditions must be specified in **bdnary**. The function γ_i may depend **linearly** on \dot{V} .

The problem is subject to the following restrictions:

- (i) In (1), $\dot{V}_j(t)$, for $j = 1, 2, \dots, \mathbf{ncode}$, may only appear **linearly** in the functions Q_i , for $i = 1, 2, \dots, \mathbf{npde}$, with a similar restriction for γ ;
- (ii) $P_{i,j}$ and the flux R_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 $P_{i,j}$, Q_i and R_i is done approximately at the mid-points of the mesh $\mathbf{x}(i)$, for $i = 1, 2, \dots, \mathbf{npts}$, by calling the **pdedef** for each mid-point 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 nonzero so that there is a time derivative present in the PDE problem;
- (vi) 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 9 below.

The algebraic-differential equation system which is defined by the functions F_i must be specified in **odedef**. You must also specify the coupling points ξ in the array **xi**.

The parabolic equations are approximated by a system of ODEs in time for the values of U_i at mesh points. For simple problems in Cartesian coordinates, this system is obtained by replacing the space derivatives by the usual central, three-point finite difference formula. However, for polar and spherical problems, or problems with nonlinear coefficients, the space derivatives are replaced by a modified three-point formula which maintains second order accuracy. In total there are $\mathbf{npde} \times \mathbf{npts} + \mathbf{ncode}$ ODEs in the time direction. This system is then integrated forwards in time using a backward differentiation formula (BDF) or a Theta method.

4 References

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

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

Berzins M and Furzeland R M (1992) An adaptive theta method for the solution of stiff and nonstiff differential equations *Appl. Numer. Math.* **9** 1–19

Skeel R D and Berzins M (1990) A method for the spatial discretization of parabolic equations in one space variable *SIAM J. Sci. Statist. Comput.* **11(1)** 1–32

5 Parameters

5.1 Compulsory Input Parameters

1: **npde** – INTEGER

The number of PDEs to be solved.

Constraint: **npde** \geq 1.

2: **m** – INTEGER

The coordinate system used:

m = 0

Indicates Cartesian coordinates.

m = 1

Indicates cylindrical polar coordinates.

m = 2

Indicates spherical polar coordinates.

Constraint: **m** = 0, 1 or 2.

3: **ts** – REAL (KIND=nag_wp)

The initial value of the independent variable t .

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

4: **tout** – REAL (KIND=nag_wp)

The final value of t to which the integration is to be carried out.

5: **pdedef** – SUBROUTINE, supplied by the user.

pdedef must evaluate the functions $P_{i,j}$, Q_i and R_i which define the system of PDEs. The functions may depend on x , t , U , U_x and V . Q_i may depend linearly on \dot{V} . **pdedef** is called approximately midway between each pair of mesh points in turn by nag_pde_1d_parab_dae_fd (d03ph).

```
[p, q, r, ires, user] = pdedef(npde, t, x, u, ux, ncode, v, vdot, ires,
user)
```

Input Parameters

1: **npde** – INTEGER

The number of PDEs in the system.

2: **t** – REAL (KIND=nag_wp)

The current value of the independent variable t .

3: **x** – REAL (KIND=nag_wp)

The current value of the space variable x .

- 4: **u(npde)** – REAL (KIND=nag_wp) array
u(i) contains the value of the component $U_i(x,t)$, for $i = 1, 2, \dots, \mathbf{npde}$.
- 5: **ux(npde)** – REAL (KIND=nag_wp) array
ux(i) contains the value of the component $\frac{\partial U_i(x,t)}{\partial x}$, for $i = 1, 2, \dots, \mathbf{npde}$.
- 6: **ncode** – INTEGER
The number of coupled ODEs in the system.
- 7: **v(ncode)** – REAL (KIND=nag_wp) array
If **ncode** > 0, **v(i)** contains the value of the component $V_i(t)$, for $i = 1, 2, \dots, \mathbf{ncode}$.
- 8: **vdot(ncode)** – REAL (KIND=nag_wp) array
If **ncode** > 0, **vdot(i)** contains the value of component $\dot{V}_i(t)$, for $i = 1, 2, \dots, \mathbf{ncode}$.
Note: $\dot{V}_i(t)$, for $i = 1, 2, \dots, \mathbf{ncode}$, may only appear linearly in Q_j , for $j = 1, 2, \dots, \mathbf{npde}$.
- 9: **ires** – INTEGER
Set to -1 or 1.
- 10: **user** – INTEGER array
pdedef is called from `nag_pde_1d_parab_dae_fd` (d03ph) with the object supplied to `nag_pde_1d_parab_dae_fd` (d03ph).

Output Parameters

- 1: **p(npde, npde)** – REAL (KIND=nag_wp) array
p(i, j) must be set to the value of $P_{i,j}(x, t, U, U_x, V)$, for $i = 1, 2, \dots, \mathbf{npde}$ and $j = 1, 2, \dots, \mathbf{npde}$.
- 2: **q(npde)** – REAL (KIND=nag_wp) array
q(i) must be set to the value of $Q_i(x, t, U, U_x, V, \dot{V})$, for $i = 1, 2, \dots, \mathbf{npde}$.
- 3: **r(npde)** – REAL (KIND=nag_wp) array
r(i) must be set to the value of $R_i(x, t, U, U_x, V)$, for $i = 1, 2, \dots, \mathbf{npde}$.
- 4: **ires** – INTEGER
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 (sub)routine with the error indicator set to **ifail** = 6.
- 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_1d_parab_dae_fd` (d03ph) returns to the calling function with the error indicator set to **ifail** = 4.

5: **user** – INTEGER array

6: **bdnary** – SUBROUTINE, supplied by the user.

bdnary must evaluate the functions β_i and γ_i which describe the boundary conditions, as given in (4).

```
[beta, gamma, ires, user] = bdnary(npde, t, u, ux, ncode, v, vdot, ibnd,
ires, user)
```

Input Parameters

1: **npde** – INTEGER

The number of PDEs in the system.

2: **t** – REAL (KIND=nag_wp)

The current value of the independent variable t .

3: **u(npde)** – REAL (KIND=nag_wp) array

u(i) contains the value of the component $U_i(x, t)$ at the boundary specified by **ibnd**, for $i = 1, 2, \dots, \mathbf{npde}$.

4: **ux(npde)** – REAL (KIND=nag_wp) array

ux(i) contains the value of the component $\frac{\partial U_i(x, t)}{\partial x}$ at the boundary specified by **ibnd**, for $i = 1, 2, \dots, \mathbf{npde}$.

5: **ncode** – INTEGER

The number of coupled ODEs in the system.

6: **v(ncode)** – REAL (KIND=nag_wp) array

If **ncode** > 0 , **v**(i) contains the value of the component $V_i(t)$, for $i = 1, 2, \dots, \mathbf{ncode}$.

7: **vdot(ncode)** – REAL (KIND=nag_wp) array

If **ncode** > 0 , **vdot**(i) contains the value of component $\dot{V}_i(t)$, for $i = 1, 2, \dots, \mathbf{ncode}$.

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

8: **ibnd** – INTEGER

Specifies which boundary conditions are to be evaluated.

ibnd = 0

bdnary must set up the coefficients of the left-hand boundary, $x = a$.

ibnd $\neq 0$

bdnary must set up the coefficients of the right-hand boundary, $x = b$.

9: **ires** – INTEGER

Set to -1 or 1 .

10: **user** – INTEGER array

bdnary is called from nag_pde_1d_parab_dae_fd (d03ph) with the object supplied to nag_pde_1d_parab_dae_fd (d03ph).

Output Parameters

- 1: **beta(npde)** – REAL (KIND=nag_wp) array
beta(i) must be set to the value of $\beta_i(x, t)$ at the boundary specified by **ibnd**, for $i = 1, 2, \dots, \text{npde}$.
- 2: **gamma(npde)** – REAL (KIND=nag_wp) array
gamma(i) must be set to the value of $\gamma_i(x, t, U, U_x, V, \dot{V})$ at the boundary specified by **ibnd**, for $i = 1, 2, \dots, \text{npde}$.
- 3: **ires** – INTEGER
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 (sub)routine with the error indicator set to **ifail** = 6.
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_1d_parab_dae_fd` (d03ph) returns to the calling function with the error indicator set to **ifail** = 4.
- 4: **user** – INTEGER array

- 7: **u(neqn)** – REAL (KIND=nag_wp) array
The initial values of the dependent variables defined as follows:
u(npde × (j - 1) + i) contain $U_i(x_j, t_0)$, for $i = 1, 2, \dots, \text{npde}$ and $j = 1, 2, \dots, \text{npts}$, and
u(npts × npde + i) contain $V_i(t_0)$, for $i = 1, 2, \dots, \text{ncode}$.
- 8: **x(npts)** – REAL (KIND=nag_wp) array
The mesh points in the space direction. **x(1)** must specify the left-hand boundary, a , and **x(npts)** must specify the right-hand boundary, b .
Constraint: $\mathbf{x}(1) < \mathbf{x}(2) < \dots < \mathbf{x}(\text{npts})$.
- 9: **ncode** – INTEGER
The number of coupled ODE components.
Constraint: **ncode** ≥ 0.
- 10: **odedef** – SUBROUTINE, supplied by the NAG Library or the user.
odedef must evaluate the functions F , which define the system of ODEs, as given in (3).
If you wish to compute the solution of a system of PDEs only (**ncode** = 0), **odedef** must be the string `nag_pde_1d_parab_remesh_fd_dummy_odedef` (d53pck).

```
[f, ires, user] = odedef(npde, t, ncode, v, vdot, nxi, xi, ucp, ucpx, rcp,
ucpt, ucptx, ires, user)
```

Input Parameters

- 1: **npde** – INTEGER
The number of PDEs in the system.
- 2: **t** – REAL (KIND=nag_wp)
The current value of the independent variable t .
- 3: **ncode** – INTEGER
The number of coupled ODEs in the system.
- 4: **v(ncode)** – REAL (KIND=nag_wp) array
If **ncode** > 0, **v**(i) contains the value of the component $V_i(t)$, for $i = 1, 2, \dots, \mathbf{ncode}$.
- 5: **vdot(ncode)** – REAL (KIND=nag_wp) array
If **ncode** > 0, **vdot**(i) contains the value of component $\dot{V}_i(t)$, for $i = 1, 2, \dots, \mathbf{ncode}$.
- 6: **nxi** – INTEGER
The number of ODE/PDE coupling points.
- 7: **xi(nxi)** – REAL (KIND=nag_wp) array
If **nxi** > 0, **xi**(i) contains the ODE/PDE coupling points, ξ_i , for $i = 1, 2, \dots, \mathbf{nxi}$.
- 8: **ucp(npde, :)** – REAL (KIND=nag_wp) array
The second dimension of the array **ucp** must be at least $\max(1, \mathbf{nxi})$.
If **nxi** > 0, **ucp**(i, j) contains the value of $U_i(x, t)$ at the coupling point $x = \xi_j$, for $i = 1, 2, \dots, \mathbf{npde}$ and $j = 1, 2, \dots, \mathbf{nxi}$.
- 9: **ucpx(npde, :)** – REAL (KIND=nag_wp) array
The second dimension of the array **ucpx** must be at least $\max(1, \mathbf{nxi})$.
If **nxi** > 0, **ucpx**(i, j) contains the value of $\frac{\partial U_i(x, t)}{\partial x}$ at the coupling point $x = \xi_j$, for $i = 1, 2, \dots, \mathbf{npde}$ and $j = 1, 2, \dots, \mathbf{nxi}$.
- 10: **rcp(npde, :)** – REAL (KIND=nag_wp) array
The second dimension of the array **rcp** must be at least $\max(1, \mathbf{nxi})$.
rcp(i, j) contains the value of the flux R_i at the coupling point $x = \xi_j$, for $i = 1, 2, \dots, \mathbf{npde}$ and $j = 1, 2, \dots, \mathbf{nxi}$.
- 11: **ucpt(npde, :)** – REAL (KIND=nag_wp) array
The second dimension of the array **ucpt** must be at least $\max(1, \mathbf{nxi})$.
If **nxi** > 0, **ucpt**(i, j) contains the value of $\frac{\partial U_i}{\partial t}$ at the coupling point $x = \xi_j$, for $i = 1, 2, \dots, \mathbf{npde}$ and $j = 1, 2, \dots, \mathbf{nxi}$.

- 12: **ucptx**(**npde**,:) – REAL (KIND=**nag_wp**) array
 The second dimension of the array **ucptx** must be at least $\max(1, \mathbf{nxi})$.
ucptx(i, j) contains the value of $\frac{\partial^2 U_i}{\partial x \partial t}$ at the coupling point $x = \xi_j$, for $i = 1, 2, \dots, \mathbf{npde}$ and $j = 1, 2, \dots, \mathbf{nxi}$.
- 13: **ires** – INTEGER
 The form of F that must be returned in the array **f**.
ires = 1
 Equation (5) must be used.
ires = -1
 Equation (6) must be used.
- 14: **user** – INTEGER array
odedef is called from `nag_pde_1d_parab_dae_fd` (d03ph) with the object supplied to `nag_pde_1d_parab_dae_fd` (d03ph).

Output Parameters

- 1: **f**(**ncode**) – REAL (KIND=**nag_wp**) array
f(i) must contain the i th component of F , for $i = 1, 2, \dots, \mathbf{ncode}$, where F is defined as

$$F = G - A\dot{V} - B \begin{pmatrix} U_t^* \\ U_{xt}^* \end{pmatrix}, \quad (5)$$

or

$$F = -A\dot{V} - B \begin{pmatrix} U_t^* \\ U_{xt}^* \end{pmatrix}. \quad (6)$$

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

- 2: **ires** – INTEGER
 Should usually remain unchanged. However, you 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 (sub)routine with the error indicator set to **ifail** = 6.
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_1d_parab_dae_fd` (d03ph) returns to the calling function with the error indicator set to **ifail** = 4.

- 3: **user** – INTEGER array

- 11: **xi**(**nxi**) – REAL (KIND=**nag_wp**) array
 If **nxi** > 0, **xi**(i), for $i = 1, 2, \dots, \mathbf{nxi}$, must be set to the ODE/PDE coupling points.
 Constraint: $\mathbf{x}(1) \leq \mathbf{xi}(1) < \mathbf{xi}(2) < \dots < \mathbf{xi}(\mathbf{nxi}) \leq \mathbf{x}(\mathbf{npts})$.

12: **rtol**(:) – REAL (KIND=nag_wp) array

The dimension of the array **rtol** must be at least 1 if **itol** = 1 or 2 and at least **neqn** if **itol** = 3 or 4

The relative local error tolerance.

Constraint: $\mathbf{rtol}(i) \geq 0.0$ for all relevant i .

13: **atol**(:) – REAL (KIND=nag_wp) array

The dimension of the array **atol** must be at least 1 if **itol** = 1 or 3 and at least **neqn** if **itol** = 2 or 4

The absolute local error tolerance.

Constraint: $\mathbf{atol}(i) \geq 0.0$ for all relevant i .

Note: corresponding elements of **rtol** and **atol** cannot both be 0.0.

14: **itol** – INTEGER

A value to indicate the form of the local error test. **itol** indicates to nag_pde_1d_parab_dae_fd (d03ph) whether to interpret either or both of **rtol** or **atol** as a vector or scalar. The error test to be satisfied is $\|e_i/w_i\| < 1.0$, where w_i is defined as follows:

itol	rtol	atol	w_i
1	scalar	scalar	$\mathbf{rtol}(1) \times U_i + \mathbf{atol}(1)$
2	scalar	vector	$\mathbf{rtol}(1) \times U_i + \mathbf{atol}(i)$
3	vector	scalar	$\mathbf{rtol}(i) \times U_i + \mathbf{atol}(1)$
4	vector	vector	$\mathbf{rtol}(i) \times U_i + \mathbf{atol}(i)$

In the above, e_i denotes the estimated local error for the i th component of the coupled PDE/ODE system in time, $\mathbf{u}(i)$, for $i = 1, 2, \dots, \mathbf{neqn}$.

The choice of norm used is defined by the argument **norm_p**.

Constraint: $1 \leq \mathbf{itol} \leq 4$.

15: **norm_p** – CHARACTER(1)

The type of norm to be used.

norm_p = 'M'

Maximum norm.

norm_p = 'A'

Averaged L_2 norm.

If \mathbf{u}_{norm} denotes the norm of the vector \mathbf{u} of length **neqn**, then for the averaged L_2 norm

$$\mathbf{u}_{\text{norm}} = \sqrt{\frac{1}{\mathbf{neqn}} \sum_{i=1}^{\mathbf{neqn}} (\mathbf{u}(i)/w_i)^2},$$

while for the maximum norm

$$\mathbf{u}_{\text{norm}} = \max_i |\mathbf{u}(i)/w_i|.$$

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

Constraint: **norm_p** = 'M' or 'A'.

16: **laopt** – CHARACTER(1)

The type of matrix algebra required.

laopt = 'F'

Full matrix methods to be used.

laopt = 'B'

Banded matrix methods to be used.

laopt = 'S'

Sparse matrix methods to be used.

Constraint: **laopt** = 'F', 'B' or 'S'.

Note: you are recommended to use the banded option when no coupled ODEs are present (i.e., **ncode** = 0).

17: **algopt(30)** – REAL (KIND=nag_wp) array

May be set to control various options available in the integrator. If you wish to employ all the default options, then **algopt(1)** 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(1)

Selects the ODE integration method to be used. If **algopt(1)** = 1.0, a BDF method is used and if **algopt(1)** = 2.0, a Theta method is used. The default value is **algopt(1)** = 1.0.

If **algopt(1)** = 2.0, then **algopt(i)**, for $i = 2, 3, 4$ are not used.

algopt(2)

Specifies the maximum order of the BDF integration formula to be used. **algopt(2)** may be 1.0, 2.0, 3.0, 4.0 or 5.0. The default value is **algopt(2)** = 5.0.

algopt(3)

Specifies what method is to be used to solve the system of nonlinear equations arising on each step of the BDF method. If **algopt(3)** = 1.0 a modified Newton iteration is used and if **algopt(3)** = 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(3)** = 1.0.

algopt(4)

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 $j = 1, 2, \dots, \mathbf{npde}$, for some i or when there is no $\dot{V}_i(t)$ dependence in the coupled ODE system. If **algopt(4)** = 1.0, then the Petzold test is used. If **algopt(4)** = 2.0, then the Petzold test is not used. The default value is **algopt(4)** = 1.0.

If **algopt(1)** = 1.0, then **algopt(i)**, for $i = 5, 6, 7$, are not used.

algopt(5)

Specifies the value of Theta to be used in the Theta integration method. $0.51 \leq \mathbf{algopt(5)} \leq 0.99$. The default value is **algopt(5)** = 0.55.

algopt(6)

Specifies what method is to be used to solve the system of nonlinear equations arising on each step of the Theta method. If **algopt(6)** = 1.0, a modified Newton iteration is used and if **algopt(6)** = 2.0, a functional iteration method is used. The default value is **algopt(6)** = 1.0.

algopt(7)

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(7)** = 1.0, then switching is allowed and if **algopt(7)** = 2.0, then switching is not allowed. The default value is **algopt(7)** = 1.0.

algotp(11)

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 argument **itask**. If **algotp(1)** \neq 0.0, a value of 0.0 for **algotp(11)**, say, should be specified even if **itask** subsequently specifies that t_{crit} will not be used.

algotp(12)

Specifies the minimum absolute step size to be allowed in the time integration. If this option is not required, **algotp(12)** should be set to 0.0.

algotp(13)

Specifies the maximum absolute step size to be allowed in the time integration. If this option is not required, **algotp(13)** should be set to 0.0.

algotp(14)

Specifies the initial step size to be attempted by the integrator. If **algotp(14)** = 0.0, then the initial step size is calculated internally.

algotp(15)

Specifies the maximum number of steps to be attempted by the integrator in any one call. If **algotp(15)** = 0.0, then no limit is imposed.

algotp(23)

Specifies what method is to be used to solve the nonlinear equations at the initial point to initialize the values of U , U_t , V and \dot{V} . If **algotp(23)** = 1.0, a modified Newton iteration is used and if **algotp(23)** = 2.0, functional iteration is used. The default value is **algotp(23)** = 1.0.

algotp(29) and **algotp(30)** are used only for the sparse matrix algebra option, **laopt** = 'S'.

algotp(29)

Governs the choice of pivots during the decomposition of the first Jacobian matrix. It should lie in the range $0.0 < \text{algotp}(29) < 1.0$, with smaller values biasing the algorithm towards maintaining sparsity at the expense of numerical stability. If **algotp(29)** lies outside this range then the default value is used. If the functions regard the Jacobian matrix as numerically singular then increasing **algotp(29)** towards 1.0 may help, but at the cost of increased fill-in. The default value is **algotp(29)** = 0.1.

algotp(30)

Is used as a relative pivot threshold during subsequent Jacobian decompositions (see **algotp(29)**) below which an internal error is invoked. If **algotp(30)** is greater than 1.0 no check is made on the pivot size, and this may be a necessary option if the Jacobian is found to be numerically singular (see **algotp(29)**). The default value is **algotp(30)** = 0.0001.

18: **rsave**(*lrsave*) – REAL (KIND=nag_wp) array

lrsave, the dimension of the array, must satisfy the constraint

If **laopt** = 'F', $lrsave \geq \text{neqn} \times \text{neqn} + \text{neqn} + \text{nwkres} + \text{lenode}$.

If **laopt** = 'B', $lrsave \geq (3 \times \text{mlu} + 1) \times \text{neqn} + \text{nwkres} + \text{lenode}$.

If **laopt** = 'S', $lrsave \geq 4 \times \text{neqn} + 11 \times \text{neqn}/2 + 1 + \text{nwkres} + \text{lenode}$.

Note: when **laopt** = 'S', 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 **ifail** = 15..

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.

19: **isave**(**lisave**) – INTEGER 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(1)

Contains the number of steps taken in time.

isave(2)

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(3)

Contains the number of Jacobian evaluations performed by the time integrator.

isave(4)

Contains the order of the last backward differentiation formula method used.

isave(5)

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.

20: **itask** – INTEGER

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 $t = \mathbf{tout}$.

itask = 4

Normal computation of output values **u** at $t = \mathbf{tout}$ but without overshooting $t = t_{\text{crit}}$ where t_{crit} is described under the argument **algot**.

itask = 5

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

Constraint: **itask** = 1, 2, 3, 4 or 5.

21: **itrace** – INTEGER

The level of trace information required from `nag_pde_1d_parab_dae_fd` (d03ph) 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 on the current error message unit (see `nag_file_set_unit_error` (x04aa)).

itrace > 0

Output from the underlying ODE solver is printed on the current advisory message unit (see `nag_file_set_unit_advisory` (x04ab)). 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. You are advised to set **itrace** = 0, unless you are experienced with Sub-chapter D02M–N.

22: **ind** – INTEGER

Indicates whether this is a continuation call or a new integration.

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 **ifail** should be reset between calls to `nag_pde_1d_parab_dae_fd` (d03ph).

Constraint: **ind** = 0 or 1.

23: **cwsav**(10) – CHARACTER(80) array

24: **lwsav**(100) – LOGICAL array

25: **iwsav**(505) – INTEGER array

26: **rwsav**(1100) – REAL (KIND=nag_wp) array

5.2 Optional Input Parameters

1: **npts** – INTEGER

Default: the dimension of the array **x**.

The number of mesh points in the interval $[a, b]$.

Constraint: **npts** \geq 3.

2: **nxi** – INTEGER

Default: the dimension of the array **xi**.

The number of ODE/PDE coupling points.

Constraints:

if **ncode** = 0, **nxi** = 0;

if **ncode** > 0, **nxi** \geq 0.

3: **neqn** – INTEGER

Default: the dimension of the array **u**.

The number of ODEs in the time direction.

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

4: **lisave** – INTEGER

Default: the dimension of the array **isave**.

The dimension of the array **isave**. its size depends on the type of matrix algebra selected:

if **laopt** = 'F', **lisave** \geq 24;

if **laopt** = 'B', **lisave** \geq **neqn** + 24;

if **laopt** = 'S', **lisave** \geq 25 \times **neqn** + 24.

Note: when using the sparse option, 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 **ifail** = 15.

5: **user** – INTEGER array

user is not used by `nag_pde_1d_parab_dae_fd` (d03ph), but is passed to **pdedef**, **boundary** and **odedef**. Note that for large objects it may be more efficient to use a global variable which is accessible from the m-files than to use **user**.

5.3 Output Parameters

1: **ts** – REAL (KIND=nag_wp)

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

2: **u(neqn)** – REAL (KIND=nag_wp) array

The computed solution $U_i(x_j, t)$, for $i = 1, 2, \dots, \mathbf{npde}$ and $j = 1, 2, \dots, \mathbf{npts}$, and $V_k(t)$, for $k = 1, 2, \dots, \mathbf{ncode}$, evaluated at $t = \mathbf{ts}$.

3: **rsave(lrsave)** – REAL (KIND=nag_wp) array

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

4: **isave(lisave)** – INTEGER array

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(1)

Contains the number of steps taken in time.

isave(2)

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(3)

Contains the number of Jacobian evaluations performed by the time integrator.

isave(4)

Contains the order of the last backward differentiation formula method used.

isave(5)

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.

5: **ind** – INTEGER

ind = 1.

6: **user** – INTEGER array

7: **cwsav(10)** – CHARACTER(80) array

8: **lwsav(100)** – LOGICAL array

9: **iwsav(505)** – INTEGER array

10: **rwsav(1100)** – REAL (KIND=nag_wp) array

11: **ifail** – INTEGER

ifail = 0 unless the function detects an error (see Section 5).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail = 1

On entry, **tout** – **ts** is too small,
 or **itask** \neq 1, 2, 3, 4 or 5,
 or **m** \neq 0, 1 or 2,
 or at least one of the coupling points defined in array **xi** is outside the interval $[\mathbf{x}(1), \mathbf{x}(\mathbf{npts})]$,
 or **m** > 0 and $\mathbf{x}(1) < 0.0$,
 or **npts** < 3,
 or **npde** < 1,
 or **norm_p** \neq 'A' or 'M',
 or **laopt** \neq 'F', 'B' or 'S',
 or **itol** \neq 1, 2, 3 or 4,
 or **ind** \neq 0 or 1,
 or mesh points $\mathbf{x}(i)$ are badly ordered,
 or *lrsave* is too small,
 or **lisave** is too small,
 or **ncode** and **nxi** are incorrectly defined,
 or **neqn** \neq **npde** \times **npts** + **ncode**,
 or either an element of **rtol** or **atol** < 0.0,
 or all the elements of **rtol** and **atol** are zero.

ifail = 2 (*warning*)

The underlying ODE solver cannot make any further progress, with the values of **atol** and **rtol**, across the integration range from the current point $t = \mathbf{ts}$. The components of **u** contain the computed values at the current point $t = \mathbf{ts}$.

ifail = 3 (*warning*)

In the underlying ODE solver, there were repeated error test failures on an attempted step, before completing the requested task, but the integration was successful as far as $t = \mathbf{ts}$. The problem may have a singularity, or the error requirement may be inappropriate.

ifail = 4

In setting up the ODE system, the internal initialization function was unable to initialize the derivative of the ODE system. This could be due to the fact that **ires** was repeatedly set to 3 in at least **pdedef**, **boundary** or **odedef**, when the residual in the underlying ODE solver was being evaluated.

ifail = 5

In solving the ODE system, a singular Jacobian has been encountered. You should check your problem formulation.

ifail = 6 (*warning*)

When evaluating the residual in solving the ODE system, **ires** was set to 2 in at least **pdedef**, **boundary** or **odedef**. Integration was successful as far as $t = \mathbf{ts}$.

ifail = 7

The values of **atol** and **rtol** are so small that the function is unable to start the integration in time.

ifail = 8

In one of **pdedef**, **bndary** or **odedef**, **ires** was set to an invalid value.

ifail = 9 (`nag_ode_ivp_stiff_imp_revcom (d02nn)`)

A serious error has occurred in an internal call to the specified function. Check the problem specification and all arguments and array dimensions. Setting **itrace** = 1 may provide more information. If the problem persists, contact NAG.

ifail = 10 (*warning*)

The required task has been completed, but it is estimated that a small change in **atol** and **rtol** is unlikely to produce any change in the computed solution. (Only applies when you are not operating in one step mode, that is when **itask** \neq 2 or 5.)

ifail = 11

An error occurred during Jacobian formulation of the ODE system (a more detailed error description may be directed to the current error message unit). If using the sparse matrix algebra option, the values of **algopt**(29) and **algopt**(30) may be inappropriate.

ifail = 12

In solving the ODE system, the maximum number of steps specified in **algopt**(15) have been taken.

ifail = 13 (*warning*)

Some error weights w_i became zero during the time integration (see the description of **itol**). Pure relative error control (**atol**(i) = 0.0) was requested on a variable (the i th) which has become zero. The integration was successful as far as $t = \mathbf{ts}$.

ifail = 14

The flux function R_i was detected as depending on time derivatives, which is not permissible.

ifail = 15

When using the sparse option, the value of **lisave** or *lrsave* was not sufficient (more detailed information may be directed to the current error message unit).

ifail = -99

An unexpected error has been triggered by this routine. Please contact NAG.

ifail = -399

Your licence key may have expired or may not have been installed correctly.

ifail = -999

Dynamic memory allocation failed.

7 Accuracy

`nag_pde_1d_parab_dae_fd (d03ph)` 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 accuracy arguments **atol** and **rtol**.

8 Further Comments

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. It may be advisable in such cases to reduce the whole system to first-order and to use the Keller box scheme function `nag_pde_1d_parab_dae_keller` (d03pk).

The time taken depends on the complexity of the parabolic system and on the accuracy requested. For a given system and a fixed accuracy it is approximately proportional to **neqn**.

9 Example

This example provides a simple coupled system of one PDE and one ODE.

$$(V_1)^2 \frac{\partial U_1}{\partial t} - x V_1 \dot{V}_1 \frac{\partial U_1}{\partial x} = \frac{\partial^2 U_1}{\partial x^2}$$

$$\dot{V}_1 = V_1 U_1 + \frac{\partial U_1}{\partial x} + 1 + t,$$

for $t \in [10^{-4}, 0.1 \times 2^i]$; $i = 1, 2, \dots, 5$; $x \in [0, 1]$.

The left boundary condition at $x = 0$ is

$$\frac{\partial U_1}{\partial x} = -V_1 \exp t.$$

The right boundary condition at $x = 1$ is

$$\frac{\partial U_1}{\partial x} = -V_1 \dot{V}_1.$$

The initial conditions at $t = 10^{-4}$ are defined by the exact solution:

$$V_1 = t, \quad \text{and} \quad U_1(x, t) = \exp\{t(1-x)\} - 1.0, \quad x \in [0, 1],$$

and the coupling point is at $\xi_1 = 1.0$.

9.1 Program Text

```
function d03ph_example

fprintf('d03ph example results\n\n');

npde   = nag_int(1);
m      = nag_int(0);
ts     = 0.0001;
tout   = 0.2;
x      = [0:0.05:1];
u      = [exp(ts*(1-x))-1,ts];
ncode  = nag_int(1);
xi     = [1];
rtol   = [0.0001];
atol   = [0.0001];
itol   = nag_int(1);
normt  = 'A';
laopt  = 'F';
algopt = zeros(30,1);
rsave  = zeros(4000, 1);
isave  = zeros(100, 1, nag_int_name);
itask  = nag_int(1);
itrace = nag_int(0);
ind    = nag_int(0);
cwsav  = {''; '''; '''; '''; '''; '''; '''; '''; '''; '''; '''};
lwsav  = false(100, 1);
iwsav  = zeros(505, 1, nag_int_name);
rwsav  = zeros(1100, 1);
```

```

% Loop over t values
nt = 20;
t = zeros(nt,1);
alpha = (32)^(1/19);
for j = 1:nt
    t(j) = 0.1*alpha^(j-1);
end

for t_i = 1:nt
    tout = t(t_i);
    [ts, u, rsave, isave, ind, user, cwsav, lwsav, iwsav, rwsav, ifail] = ...
    d03ph( ...
        npde, m, ts, tout, @pdedef, @bndary, u, x, ncode, ...
        @odedef, xi, rtol, atol, itol, normt, laopt, algopt, ...
        rsave, isave, itask, itrace, ind, cwsav, lwsav, iwsav, rwsav);

    if mod(t_i+4,6)==0
        fprintf('\n\nThe solution at t = %7.4f is:\n',ts);
        for j = 0:2
            fprintf('%10s%12s', 'x', 'u(x,t)');
        end
        fprintf('\n');
        for i = 1:7
            for j = 0:2
                fprintf('%12.2f%10.4f',x(i+j*7),u(i+j*7));
            end
            fprintf('\n');
        end
        end
        v(:,t_i) = u(1:(end-1));
    end

    fig1 = figure;
    mesh(t,x,v);
    xlabel('t');
    ylabel('x');
    zlabel('u(x,t)');
    title('Coupled Parabolic PDE/ODE using Finite-differences and BDF');

function [p, q, r, ires, user] = pdedef(npde, t, x, u, ux, ncode, v, vdot, ...
    ires, user)

    p = zeros(npde, npde);
    q = zeros(npde, 1);
    r = zeros(npde, 1);

    p(1,1) = v(1)*v(1);
    r(1) = ux(1);
    q(1) = -x*ux(1)*v(1)*vdot(1);

function [beta, gamma, ires, user] = bndary(npde, t, u, ux, ncode, ...
    v, vdot, ibnd, ires, user)

    beta = zeros(npde, 1);
    gamma = zeros(npde, 1);
    beta(1) = 1.0d0;
    if (ibnd == 0)
        gamma(1) = -v(1)*exp(t);
    else
        gamma(1) = -v(1)*vdot(1);
    end

function [f, ires, user] = odedef(npde, t, ncode, v, vdot, nxi, xi, ucp, ...
    ucp, rcp, ucpt, ucptx, ires, user)

    f = zeros(ncode,1);
    if (ires == 1)
        f(1) = vdot(1) - v(1)*ucp(1,1) - ucp(1,1) - 1 - t;
    elseif (ires == -1)
        f(1) = vdot(1);
    end
end

```

9.2 Program Results

d03ph example results

The solution at $t = 0.1200$ is:

x	u(x,t)	x	u(x,t)	x	u(x,t)
0.00	0.1279	0.35	0.0816	0.70	0.0371
0.05	0.1212	0.40	0.0751	0.75	0.0309
0.10	0.1145	0.45	0.0687	0.80	0.0248
0.15	0.1078	0.50	0.0623	0.85	0.0186
0.20	0.1012	0.55	0.0559	0.90	0.0126
0.25	0.0946	0.60	0.0496	0.95	0.0065
0.30	0.0881	0.65	0.0434	1.00	0.0005

The solution at $t = 0.3585$ is:

x	u(x,t)	x	u(x,t)	x	u(x,t)
0.00	0.4327	0.35	0.2640	0.70	0.1154
0.05	0.4073	0.40	0.2416	0.75	0.0956
0.10	0.3823	0.45	0.2196	0.80	0.0762
0.15	0.3578	0.50	0.1980	0.85	0.0572
0.20	0.3337	0.55	0.1768	0.90	0.0385
0.25	0.3101	0.60	0.1560	0.95	0.0201
0.30	0.2869	0.65	0.1355	1.00	0.0020

The solution at $t = 1.0711$ is:

x	u(x,t)	x	u(x,t)	x	u(x,t)
0.00	1.9236	0.35	1.0146	0.70	0.3902
0.05	1.7720	0.40	0.9104	0.75	0.3187
0.10	1.6283	0.45	0.8116	0.80	0.2509
0.15	1.4920	0.50	0.7180	0.85	0.1868
0.20	1.3629	0.55	0.6294	0.90	0.1260
0.25	1.2405	0.60	0.5453	0.95	0.0683
0.30	1.1245	0.65	0.4657	1.00	0.0138

The solution at $t = 3.2000$ is:

x	u(x,t)	x	u(x,t)	x	u(x,t)
0.00	23.4723	0.35	7.0665	0.70	1.6807
0.05	19.8823	0.40	5.8860	0.75	1.2948
0.10	16.8191	0.45	4.8793	0.80	0.9662
0.15	14.2055	0.50	4.0210	0.85	0.6865
0.20	11.9756	0.55	3.2891	0.90	0.4485
0.25	10.0733	0.60	2.6653	0.95	0.2460
0.30	8.4506	0.65	2.1337	1.00	0.0740

Coupled Parabolic PDE/ODE using Finite-differences and BDF

