

NAG Library Routine Document

D03PHF/D03PHA

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details.

1 Purpose

D03PHF/D03PHA 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).

D03PHA is a version of D03PHF that has additional parameters in order to make it safe for use in multithreaded applications (see Section 5).

2 Specification

2.1 Specification for D03PHF

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SUBROUTINE D03PHF(NPDE, M, TS, TOUT, PDEDEF, BNDARY, U, NPTS, X, NCODE,
1      ODEDEF, NXI, XI, NEQN, RTOL, ATOL, ITOL, NORM, LAOPT,
2      ALGOPT, RSAVE, LRSAVE, ISAVE, LISAVE, ITASK, ITRACE,
3      IND, IFAIL)

  INTEGER      NPDE, M, NPTS, NCODE, NXI, NEQN, ITOL, LRSAVE,
1      ISAVE(LISAVE), LISAVE, ITASK, ITRACE, IND, IFAIL
  double precision TS, TOUT, U(NEQN), X(NPTS), XI(NXI), RTOL(*), ATOL(*),
1      ALGOPT(30), RSAVE(LRSAVE)
  CHARACTER*1  NORM, LAOPT
  EXTERNAL     PDEDEF, BNDARY, ODEDEF

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2.2 Specification for D03PHA

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SUBROUTINE D03PHA(NPDE, M, TS, TOUT, PDEDEF, BNDARY, U, NPTS, X, NCODE,
1      ODEDEF, NXI, XI, NEQN, RTOL, ATOL, ITOL, NORM, LAOPT,
2      ALGOPT, RSAVE, LRSAVE, ISAVE, LISAVE, ITASK, ITRACE,
3      IND, IUSER, RUSER, CWSAV, LWSAV, IWSAV, RWSAV, IFAIL)

  INTEGER      NPDE, M, NPTS, NCODE, NXI, NEQN, ITOL, LRSAVE,
1      ISAVE(LISAVE), LISAVE, ITASK, ITRACE, IND, IUSER(*),
2      IWSAV(505), IFAIL
  double precision TS, TOUT, U(NEQN), X(NPTS), XI(NXI), RTOL(*), ATOL(*),
1      ALGOPT(30), RSAVE(LRSAVE), RUSER(*), RWSAV(1100)
  LOGICAL      LWSAV(100)
  CHARACTER*1  NORM, LAOPT
  CHARACTER*80 CWSAV(10)
  EXTERNAL     PDEDEF, BNDARY, ODEDEF

```

3 Description

D03PHF/D03PHA integrates the system of parabolic-elliptic equations and coupled ODEs

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

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

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 $F = [F_1, \dots, F_{\text{NCODE}}]^T$, G is a vector of length NCODE, A is an NCODE by NCODE matrix, B is an NCODE by $(n_\xi \times \text{NPDE})$ 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 $b = x_{\text{NPTS}}$ are the leftmost and rightmost points of a user-defined mesh $x_1, x_2, \dots, x_{\text{NPTS}}$. The co-ordinate system in space is defined by the values of m ; $m = 0$ for Cartesian co-ordinates, $m = 1$ for cylindrical polar co-ordinates and $m = 2$ for spherical polar co-ordinates.

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

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

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

The boundary conditions must be specified in BNDARY. 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 $j = 1, 2, \dots, \text{NCODE}$, may only appear **linearly** in the functions Q_i , for $i = 1, 2, \dots, \text{NPDE}$, 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 $X(i)$, for $i = 1, 2, \dots, \text{NPTS}$, 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 $x_1, x_2, \dots, x_{\text{NPTS}}$;
- (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 8 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 co-ordinates, 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 $\text{NPDE} \times \text{NPTS} + \text{NCODE}$ 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 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

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

- 1: NPDE – INTEGER *Input*
On entry: the number of PDEs to be solved.
Constraint: $\text{NPDE} \geq 1$.
- 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: M = 0, 1 or 2.
- 3: TS – **double precision** *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 precision** *Input*
On entry: the final value of t to which the integration is to be carried out.
- 5: PDEDEF – SUBROUTINE, supplied by the user. *External Procedure*
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 D03PHF/D03PHA.

The specification of PDEDEF for D03PHF is:

```

SUBROUTINE PDEDEF(NPDE, T, X, U, UX, NCODE, V, VDOT, P, Q, R, IRES)
  INTEGER          NPDE, NCODE, IRES
  double precision T, X, U(NPDE), UX(NPDE), V(NCODE), VDOT(NCODE),
1                  P(NPDE,NPDE), Q(NPDE), R(NPDE)

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The specification of PDEDEF for D03PHA is:

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SUBROUTINE PDEDEF(NPDE, T, X, U, UX, NCODE, V, VDOT, P, Q, R, IRES,
1                  IUSER, RUSER)
  INTEGER          NPDE, NCODE, IRES, IUSER(*)
  double precision T, X, U(NPDE), UX(NPDE), V(NCODE), VDOT(NCODE),
1                  P(NPDE,NPDE), Q(NPDE), R(NPDE), RUSER(*)

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|-----|---|---------------|
| 1: | NPDE – INTEGER | <i>Input</i> |
| | <i>On entry:</i> the number of PDEs in the system. | |
| 2: | T – double precision | <i>Input</i> |
| | <i>On entry:</i> the current value of the independent variable t . | |
| 3: | X – double precision | <i>Input</i> |
| | <i>On entry:</i> the current value of the space variable x . | |
| 4: | U(NPDE) – double precision array | <i>Input</i> |
| | <i>On entry:</i> U(i) contains the value of the component $U_i(x, t)$, for $i = 1, 2, \dots, \text{NPDE}$. | |
| 5: | UX(NPDE) – double precision array | <i>Input</i> |
| | <i>On entry:</i> UX(i) contains the value of the component $\frac{\partial U_i(x, t)}{\partial x}$, for $i = 1, 2, \dots, \text{NPDE}$. | |
| 6: | NCODE – INTEGER | <i>Input</i> |
| | <i>On entry:</i> the number of coupled ODEs in the system. | |
| 7: | V(NCODE) – double precision array | <i>Input</i> |
| | <i>On entry:</i> if NCODE > 0, V(i) contains the value of component $V_i(t)$, for $i = 1, 2, \dots, \text{NCODE}$. | |
| 8: | VDOT(NCODE) – double precision array | <i>Input</i> |
| | <i>On entry:</i> if NCODE > 0, VDOT(i) contains the value of component $\dot{V}_i(t)$, for $i = 1, 2, \dots, \text{NCODE}$. | |
| | Note: $\dot{V}_i(t)$, for $i = 1, 2, \dots, \text{NCODE}$, may only appear linearly in Q_j , for $j = 1, 2, \dots, \text{NPDE}$. | |
| 9: | P(NPDE,NPDE) – double precision array | <i>Output</i> |
| | <i>On exit:</i> P(i, j) must be set to the value of $P_{i,j}(x, t, U, U_x, V)$, for $i, j = 1, 2, \dots, \text{NPDE}$. | |
| 10: | Q(NPDE) – double precision array | <i>Output</i> |
| | <i>On exit:</i> Q(i) must be set to the value of $Q_i(x, t, U, U_x, V, \dot{V})$, for $i = 1, 2, \dots, \text{NPDE}$. | |
| 11: | R(NPDE) – double precision array | <i>Output</i> |
| | <i>On exit:</i> R(i) must be set to the value of $R_i(x, t, U, U_x, V)$, for $i = 1, 2, \dots, \text{NPDE}$. | |

12:	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 routine to take certain actions as described below:	
	IRES = 2	
	Indicates to the integrator that control should be passed back immediately to the calling subroutine 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 D03PHF/D03PHA returns to the calling subroutine with the error indicator set to IFAIL = 4.	
	Note: the following are additional parameters for specific use with D03PHA. Users of D03PHF therefore need not read the remainder of this description.	
13:	IUSER(*) – INTEGER array	<i>User Workspace</i>
14:	RUSER(*) – double precision array	<i>User Workspace</i>
	PDEDEF is called from D03PHA with the parameters IUSER and RUSER as supplied to D03PHA. You are free to use the arrays IUSER and RUSER to supply information to PDEDEF.	

PDEDEF must be declared as EXTERNAL in the (sub)program from which D03PHF/D03PHA is called. Parameters denoted as *Input* must **not** be changed by this procedure.

- 6: BNDARY – SUBROUTINE, supplied by the user. *External Procedure*
- BNDARY must evaluate the functions β_i and γ_i which describe the boundary conditions, as given in (4).

The specification of BNDARY for D03PHF is:

```

SUBROUTINE BNDARY(NPDE, T, U, UX, NCODE, V, VDOT, IBND, BETA, GAMMA,
1 IRES)
INTEGER NPDE, NCODE, IBND, IRES
double precision T, U(NPDE), UX(NPDE), V(NCODE), VDOT(NCODE),
1 BETA(NPDE), GAMMA(NPDE)

```

The specification of BNDARY for D03PHA is:

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SUBROUTINE BNDARY(NPDE, T, U, UX, NCODE, V, VDOT, IBND, BETA, GAMMA,
1 IRES, IUSER, RUSER)
INTEGER NPDE, NCODE, IBND, IRES, IUSER(*)
double precision T, U(NPDE), UX(NPDE), V(NCODE), VDOT(NCODE),
1 BETA(NPDE), GAMMA(NPDE), RUSER(*)

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- | | | |
|----|---|--------------|
| 1: | NPDE – INTEGER | <i>Input</i> |
| | <i>On entry:</i> the number of PDEs in the system. | |
| 2: | T – double precision | <i>Input</i> |
| | <i>On entry:</i> the current value of the independent variable t . | |
| 3: | U(NPDE) – double precision array | <i>Input</i> |
| | <i>On entry:</i> U(i) 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) – <i>double precision</i> array	Input
	<i>On entry:</i> UX(<i>i</i>) contains the value of the component $\frac{\partial U_i(x,t)}{\partial x}$ at the boundary specified by IBND, for $i = 1, 2, \dots, \text{NPDE}$.	
5:	NCODE – INTEGER	Input
	<i>On entry:</i> the number of coupled ODEs in the system.	
6:	V(NCODE) – <i>double precision</i> array	Input
	<i>On entry:</i> if NCODE > 0, V(<i>i</i>) contains the value of component $V_i(t)$, for $i = 1, 2, \dots, \text{NCODE}$.	
7:	VDOT(NCODE) – <i>double precision</i> array	Input
	<i>On entry:</i> if NCODE > 0, VDOT(<i>i</i>) contains the value of component $\dot{V}_i(t)$, for $i = 1, 2, \dots, \text{NCODE}$.	
	Note: $\dot{V}_i(t)$, for $i = 1, 2, \dots, \text{NCODE}$, may only appear linearly in Q_j , for $j = 1, 2, \dots, \text{NPDE}$.	
8:	IBND – INTEGER	Input
	<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 $\neq$ 0 BNDARY must set up the coefficients of the right-hand boundary, $x = b$.	
9:	BETA(NPDE) – <i>double precision</i> array	Output
	<i>On exit:</i> BETA(<i>i</i>) must be set to the value of $\beta_i(x,t)$ at the boundary specified by IBND, for $i = 1, 2, \dots, \text{NPDE}$.	
10:	GAMMA(NPDE) – <i>double precision</i> array	Output
	<i>On exit:</i> GAMMA(<i>i</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 $i = 1, 2, \dots, \text{NPDE}$.	
11:	IRES – INTEGER	Input/Output
	<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 routine to take certain actions as described below:	
	IRES = 2 Indicates to the integrator that control should be passed back immediately to the calling subroutine 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 D03PHF/D03PHA returns to the calling subroutine with the error indicator set to IFAIL = 4.	
	Note: the following are additional parameters for specific use with D03PHA. Users of D03PHF therefore need not read the remainder of this description.	

12:	IUSER(*) – INTEGER array	User Workspace
13:	RUSER(*) – double precision array	User Workspace
BNDARY is called from D03PHA with the parameters IUSER and RUSER as supplied to D03PHA. You are free to use the arrays IUSER and RUSER to supply information to BNDARY.		

BNDARY must be declared as EXTERNAL in the (sub)program from which D03PHF/D03PHA is called. Parameters denoted as *Input* must **not** be changed by this procedure.

- 7: U(NEQN) – **double precision** array *Input/Output*

On entry: the initial values of the dependent variables defined as follows:

U(NPDE $\times$ (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 $\times$ NPDE + i) contain $V_i(t_0)$, for $i = 1, 2, \dots, \text{NCODE}$.

On exit: the computed solution $U_i(x_j, t)$, for $i = 1, 2, \dots, \text{NPDE}$ and $j = 1, 2, \dots, \text{NPTS}$, and $V_k(t)$, for $k = 1, 2, \dots, \text{NCODE}$, evaluated at $t = \text{TS}$.

- 8: NPTS – INTEGER *Input*

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

Constraint: NPTS ≥ 3 .

- 9: X(NPTS) – **double precision** array *Input*

On entry: 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: X(1) < X(2) < $\dots$ < X(NPTS).

- 10: NCODE – INTEGER *Input*

On entry: the number of coupled ODE components.

Constraint: NCODE ≥ 0 .

- 11: ODEDEF – SUBROUTINE, supplied by the NAG Library or the user. *External Procedure*

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 dummy routine D03PCK/D53PCK for D03PHF (or D53PCK for D03PHA). D03PCK/D53PCK and D53PCK are included in the NAG Library.

The specification of ODEDEF for D03PHF is:

```

SUBROUTINE ODEDEF(NPDE, T, NCODE, V, VDOT, NXI, XI, UCP, UCPX, RCP,
1 UCPT, UCPTX, F, IRES)
    INTEGER NPDE, NCODE, NXI, IRES
    double precision T, V(NCODE), VDOT(NCODE), XI(NXI), UCP(NPDE,*),
1 UCPX(NPDE,*), RCP(NPDE,*), UCPT(NPDE,*),
2 UCPTX(NPDE,*), F(NCODE)
```

The specification of ODEDEF for D03PHA is:

```

SUBROUTINE ODEDEF(NPDE, T, NCODE, V, VDOT, NXI, XI, UCP, UCPX, RCP,
1 UCPT, UCPTX, F, IRES, IUSER, RUSER)
    INTEGER NPDE, NCODE, NXI, IRES, IUSER(*)
    double precision T, V(NCODE), VDOT(NCODE), XI(NXI), UCP(NPDE,*),
1 UCPX(NPDE,*), RCP(NPDE,*), UCPT(NPDE,*),
2 UCPTX(NPDE,*), F(NCODE), RUSER(*)
```

1:	NPDE – INTEGER	Input
	<i>On entry:</i> the number of PDEs in the system.	
2:	T – double precision	Input
	<i>On entry:</i> the current value of the independent variable t .	
3:	NCODE – INTEGER	Input
	<i>On entry:</i> the number of coupled ODEs in the system.	
4:	V(NCODE) – double precision array	Input
	<i>On entry:</i> if NCODE > 0, V(i) contains the value of component $V_i(t)$, for $i = 1, 2, \dots, \text{NCODE}$.	
5:	VDOT(NCODE) – double precision array	Input
	<i>On entry:</i> if NCODE > 0, VDOT(i) contains the value of component $\dot{V}_i(t)$, for $i = 1, 2, \dots, \text{NCODE}$.	
6:	NXI – INTEGER	Input
	<i>On entry:</i> the number of ODE/PDE coupling points.	
7:	XI(NXI) – double precision array	Input
	<i>On entry:</i> if NXI > 0, XI(i) contains the ODE/PDE coupling points, ξ_i , for $i = 1, 2, \dots, \text{NXI}$.	
8:	UCP(NPDE,*) – double precision array	Input
	Note: the second dimension of the array UCP is max(1, NXI).	
	<i>On entry:</i> if NXI > 0, UCP(i, j) contains the value of $U_i(x, t)$ at the coupling point $x = \xi_j$, for $i = 1, 2, \dots, \text{NPDE}$ and $j = 1, 2, \dots, \text{NXI}$.	
9:	UCPX(NPDE,*) – double precision array	Input
	Note: the second dimension of the array UCPX is max(1, NXI).	
	<i>On entry:</i> 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 $i = 1, 2, \dots, \text{NPDE}$ and $j = 1, 2, \dots, \text{NXI}$.	
10:	RCP(NPDE,*) – double precision array	Input
	Note: the second dimension of the array RCP is max(1, NXI).	
	<i>On entry:</i> RCP(i, j) contains the value of the flux R_i at the coupling point $x = \xi_j$, for $i = 1, 2, \dots, \text{NPDE}$ and $j = 1, 2, \dots, \text{NXI}$.	
11:	UCPT(NPDE,*) – double precision array	Input
	Note: the second dimension of the array UCPT is max(1, NXI).	
	<i>On entry:</i> if NXI > 0, UCPT(i, j) contains the value of $\frac{\partial U_i}{\partial t}$ at the coupling point $x = \xi_j$, for $i = 1, 2, \dots, \text{NPDE}$ and $j = 1, 2, \dots, \text{NXI}$.	

12:	UCPTX(NPDE,*) – double precision array	<i>Input</i>
	Note: the second dimension of the array UCPTX is max(1,NXI).	
	<i>On entry:</i> UCPTX(<i>i</i> , <i>j</i>) contains the value of $\frac{\partial^2 U_i}{\partial x \partial t}$ at the coupling point $x = \xi_j$, for $i = 1, 2, \dots, \text{NPDE}$ and $j = 1, 2, \dots, \text{NXI}$.	
13:	F(NCODE) – double precision array	<i>Output</i>
	<i>On exit:</i> F(<i>i</i>) must contain the <i>i</i> th component of <i>F</i> , for $i = 1, 2, \dots, \text{NCODE}$, where <i>F</i> 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 <i>F</i> is determined by the input value of IRES.	
14:	IRES – INTEGER	<i>Input/Output</i>
	<i>On entry:</i> the form of <i>F</i> that must be returned in the array F.	
	IRES = 1 Equation (5) must be used.	
	IRES = -1 Equation (6) must be used.	
	<i>On exit:</i> should usually remain unchanged. However, you may reset IRES to force the integration routine to take certain actions as described below:	
	IRES = 2 Indicates to the integrator that control should be passed back immediately to the calling subroutine 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 D03PHF/D03PHA returns to the calling subroutine with the error indicator set to IFAIL = 4.	
	Note: the following are additional parameters for specific use with D03PHA. Users of D03PHF therefore need not read the remainder of this description.	
15:	IUSER(*) – INTEGER array	<i>User Workspace</i>
16:	RUSER(*) – double precision array	<i>User Workspace</i>
	ODEDEF is called from D03PHA with the parameters IUSER and RUSER as supplied to D03PHA. You are free to use the arrays IUSER and RUSER to supply information to ODEDEF.	

ODEDEF must be declared as EXTERNAL in the (sub)program from which D03PHF/D03PHA is called. Parameters denoted as *Input* must **not** be changed by this procedure.

- | | | |
|-----|---|--------------|
| 12: | NXI – INTEGER | <i>Input</i> |
| | <i>On entry:</i> the number of ODE/PDE coupling points. | |

Constraints:

if NCODE = 0, NXI = 0;
 if NCODE > 0, NXI ≥ 0.

13: XI(NXI) – **double precision** array *Input*

On entry: if NXI > 0, XI(*i*), for $i = 1, 2, \dots, \text{NXI}$, must be set to the ODE/PDE coupling points.

Constraint: $X(1) \leq \text{XI}(1) < \text{XI}(2) < \dots < \text{XI}(\text{NXI}) \leq X(\text{NPTS})$.

14: NEQN – INTEGER *Input*

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

Constraint: $\text{NEQN} = \text{NPDE} \times \text{NPTS} + \text{NCODE}$.

15: RTOL(*) – **double precision** array *Input*

Note: 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.

On entry: the relative local error tolerance.

Constraint: $\text{RTOL}(i) \geq 0$ for all relevant *i*.

16: ATOL(*) – **double precision** array *Input*

Note: 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.

On entry: the absolute local error tolerance.

Constraint: $\text{ATOL}(i) \geq 0$ for all relevant *i*.

Note: corresponding elements of RTOL and ATOL cannot both be 0.0.

17: ITOL – INTEGER *Input*

On entry: a value to indicate the form of the local error test. ITOL indicates to D03PHF/D03PHA 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	$\text{RTOL}(1) \times U_i + \text{ATOL}(1)$
2	scalar	vector	$\text{RTOL}(1) \times U_i + \text{ATOL}(i)$
3	vector	scalar	$\text{RTOL}(i) \times U_i + \text{ATOL}(1)$
4	vector	vector	$\text{RTOL}(i) \times U_i + \text{ATOL}(i)$

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

The choice of norm used is defined by the parameter NORM.

Constraint: $1 \leq \text{ITOL} \leq 4$.

18: NORM – CHARACTER*1 *Input*

On entry: the type of norm to be used.

NORM = 'M'

Maximum norm.

NORM = 'A'

Averaged L_2 norm.

If U_{norm} denotes the norm of the vector U of length NEQN, then for the averaged L_2 norm

$$U_{\text{norm}} = \sqrt{\frac{1}{\text{NEQN}} \sum_{i=1}^{\text{NEQN}} (U(i)/w_i)^2},$$

while for the maximum norm

$$U_{\text{norm}} = \max_i |U(i)/w_i|.$$

See the description of ITOL for the formulation of the weight vector w .

Constraint: NORM = 'M' or 'A'.

19: LAOPT – CHARACTER*1

Input

On entry: 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).

20: ALGOPT(30) – *double precision* array

Input

On entry: 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 $j = 1, 2, \dots, \text{NPDE}$ 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 $\text{ALGOPT}(1) = 1.0$, then $\text{ALGOPT}(i)$, for $i = 5, 6, 7$ are not used.

ALGOPT(5)

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

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 $\text{ALGOPT}(6) = 1.0$, a modified Newton iteration is used and if $\text{ALGOPT}(6) = 2.0$, a functional iteration method is used. The default value is $\text{ALGOPT}(6) = 1.0$.

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 $\text{ALGOPT}(7) = 1.0$, then switching is allowed and if $\text{ALGOPT}(7) = 2.0$, then switching is not allowed. The default value is $\text{ALGOPT}(7) = 1.0$.

ALGOPT(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 parameter ITASK. If $\text{ALGOPT}(1) \neq 0.0$, a value of 0.0 for $\text{ALGOPT}(11)$, say, should be specified even if ITASK subsequently specifies that t_{crit} will not be used.

ALGOPT(12)

Specifies the minimum absolute step size to be allowed in the time integration. If this option is not required, $\text{ALGOPT}(12)$ should be set to 0.0.

ALGOPT(13)

Specifies the maximum absolute step size to be allowed in the time integration. If this option is not required, $\text{ALGOPT}(13)$ should be set to 0.0.

ALGOPT(14)

Specifies the initial step size to be attempted by the integrator. If $\text{ALGOPT}(14) = 0.0$, then the initial step size is calculated internally.

ALGOPT(15)

Specifies the maximum number of steps to be attempted by the integrator in any one call. If $\text{ALGOPT}(15) = 0.0$, then no limit is imposed.

ALGOPT(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 $\text{ALGOPT}(23) = 1.0$, a modified Newton iteration is used and if $\text{ALGOPT}(23) = 2.0$, functional iteration is used. The default value is $\text{ALGOPT}(23) = 1.0$.

$\text{ALGOPT}(29)$ and $\text{ALGOPT}(30)$ are used only for the sparse matrix algebra option, $\text{LAOPT} = 'S'$.

ALGOPT(29)

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

ALGOPT(30)

Is used as a relative pivot threshold during subsequent Jacobian decompositions (see $\text{ALGOPT}(29)$) below which an internal error is invoked. If $\text{ALGOPT}(30)$ 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 $\text{ALGOPT}(29)$). The default value is $\text{ALGOPT}(30) = 0.0001$.

- 21: RSAVE(LRSAVE) – **double precision** array *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 routine because it contains required information about the iteration.

- 22: LRSAVE – INTEGER *Input*

On entry: the dimension of the array RSAVE as declared in the (sub)program from which D03PHF/D03PHA is called.

If LAOPT = 'F', $LRSAVE \geq NEQN \times NEQN + NEQN + nwkres + lenode$.

If LAOPT = 'B', $LRSAVE \geq (3 \times mlu + 1) \times NEQN + nwkres + lenode$.

If LAOPT = 'S', $LRSAVE \geq 4 \times NEQN + 11 \times NEQN/2 + 1 + nwkres + lenode$.

Where

mlu is the lower or upper half bandwidths such that

$mlu = 3 \times NPDE - 1$, for PDE problems only (no coupled ODEs); or

$mlu = NEQN - 1$, for coupled PDE/ODE problems.

$$nwkres = \begin{cases} NPDE \times (2 \times NPTS + 6 \times NXI + 3 \times NPDE + 26) + NXI + NCODE + 7 \times NPTS + 2, & \text{when } NCODE > 0 \text{ and } NXI > 0; \\ NPDE \times (2 \times NPTS + 3 \times NPDE + 32) + NCODE + 7 \times NPTS + 3, & \text{when } NCODE > 0 \text{ and } NXI = 0; \\ NPDE \times (2 \times NPTS + 3 \times NPDE + 32) + 7 \times NPTS + 4, & \text{when } NCODE = 0. \end{cases}$$

$$lenode = \begin{cases} (6 + \text{int}(\text{ALGOPT}(2))) \times NEQN + 50, & \text{when the BDF method is used;} \\ 9 \times NEQN + 50, & \text{when the Theta method is used.} \end{cases}$$

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 routine returns with IFAIL = 15.

- 23: ISAVE(LISAVE) – INTEGER array *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 routine 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.

24: LISAVE – INTEGER *Input*

On entry: the dimension of the array ISAVE as declared in the (sub)program from which D03PHF/D03PHA is called. Its size depends on the type of matrix algebra selected:

- if LAOPT = 'F', LISAVE ≥ 24 ;
- if LAOPT = 'B', LISAVE $\geq \text{NEQN} + 24$;
- if LAOPT = 'S', LISAVE $\geq 25 \times \text{NEQN} + 24$.

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 routine returns with IFAIL = 15.

25: ITASK – INTEGER *Input*

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

ITASK = 1

Normal computation of output values U at $t = \text{TOUT}$.

ITASK = 2

One step and return.

ITASK = 3

Stop at first internal integration point at or beyond $t = \text{TOUT}$.

ITASK = 4

Normal computation of output values U at $t = \text{TOUT}$ but without overshooting $t = t_{\text{crit}}$ where t_{crit} is described under the parameter ALGOPT.

ITASK = 5

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

Constraint: ITASK = 1, 2, 3, 4 or 5.

26: ITRACE – INTEGER *Input*

On entry: the level of trace information required from D03PHF/D03PHA 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 X04AAF).

ITRACE > 0

Output from the underlying ODE solver is printed on the current advisory message unit (see X04ABF). 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.

27: IND – INTEGER *Input/Output*

On entry: 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 routine. In this case, only the parameters TOUT and IFAIL should be reset between calls to D03PHF/D03PHA.

Constraint: IND = 0 or 1.

On exit: IND = 1.

28: IFAIL – INTEGER

Input/Output

Note: for D03PHA, IFAIL does not occur in this position in the parameter list. See the additional parameters described below.

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this parameter, the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

Note: the following are additional parameters for specific use with D03PHA. Users of D03PHF therefore need not read the remainder of this description.

28: IUSER(*) – INTEGER array

User Workspace

Note: the dimension of the array IUSER must be at least 1.

IUSER is not used by D03PHA, but is passed directly to PDEDEF, BNDARY and ODEDEF and may be used to pass information to these routines.

29: RUSER(*) – **double precision** array

User Workspace

Note: the dimension of the array RUSER must be at least 1.

RUSER is not used by D03PHA, but is passed directly to PDEDEF, BNDARY and ODEDEF and may be used to pass information to these routines.

31: CWSAV(10) – CHARACTER*80 array

Communication Array

32: LWSAV(100) – LOGICAL array

Communication Array

33: IWSAV(505) – INTEGER array

Communication Array

34: RWSAV(1100) – **double precision** array

Communication Array

34: IFAIL – INTEGER

Input/Output

Note: see the parameter description for IFAIL above.

6 Error Indicators and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

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 $[X(1), X(NPTS)]$,
- or $M > 0$ and $X(1) < 0.0$,
- or $NPTS < 3$,
- or $NPDE < 1$,
- or $NORM \neq 'A'$ 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 $X(i)$ 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

The underlying ODE solver cannot make any further progress, with the values of $ATOL$ and $RTOL$, across the integration range from the current point $t = TS$. The components of U contain the computed values at the current point $t = TS$.

IFAIL = 3

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 $t = TS$. The problem may have a singularity, or the error requirement may be inappropriate.

IFAIL = 4

In setting up the ODE system, the internal initialization routine 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 $PDEDEF$, $BNDARY$ 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

When evaluating the residual in solving the ODE system, $IRES$ was set to 2 in at least $PDEDEF$, $BNDARY$ or $ODEDEF$. Integration was successful as far as $t = TS$.

IFAIL = 7

The values of $ATOL$ and $RTOL$ are so small that the routine 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 (D02NNF)

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

IFAIL = 10

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

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 $t = TS$.

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).

7 Accuracy

D03PHF/D03PHA 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 parameters ATOL and RTOL.

8 Further Comments

The parameter 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 routine D03PKF.

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:

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

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

9.1 Program Text

Note: the following program illustrates the use of D03PHF. An equivalent program illustrating the use of D03PHA is available with the supplied Library and is also available from the NAG web site.

```
*      D03PHF Example Program Text
*      Mark 16 Revised. NAG Copyright 1993.
*      .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          NPDE, NPTS, NCODE, M, NXI, NEQN, LISAVE, NWKRES,
+      LENODE, LRSAVE
      PARAMETER        (NPDE=1, NPTS=21, NCODE=1, M=0, NXI=1,
+      NEQN=NPDE*NPTS+NCODE, LISAVE=24,
+      NWKRES=NPDE*(NPTS+6*NXI+3*NPDE+15)
+      +NCODE+NXI+7*NPTS+2, LENODE=11*NEQN+50,
+      LRSAVE=NEQN*NEQN+NEQN+NWKRES+LENODE)
*      .. Scalars in Common ..
      DOUBLE PRECISION TS
*      .. Local Scalars ..
      DOUBLE PRECISION TOUT
      INTEGER          I, IFAIL, IND, IT, ITASK, ITOL, ITRACE
      LOGICAL          THETA
      CHARACTER        LAOPT, NORM
*      .. Local Arrays ..
      DOUBLE PRECISION ALGOPT(30), ATOL(1), EXY(NPTS), RSAVE(LRSAVE),
+      RTOL(1), U(NEQN), X(NPTS), XI(1)
      INTEGER          ISAVE(LISAVE)
*      .. External Subroutines ..
      EXTERNAL          BNDARY, D03PHF, EXACT, ODEDEF, PDEDEF, UVINIT
*      .. Common blocks ..
      COMMON            /TAXIS/TS
*      .. Executable Statements ..
      WRITE (NOUT,*) 'D03PHF Example Program Results'
      ITRACE = 0
      ITOL = 1
      ATOL(1) = 1.0D-4
      RTOL(1) = ATOL(1)

*
*      Set break-points
*
      DO 20 I = 1, NPTS
          X(I) = (I-1.0D0)/(NPTS-1.0D0)
20  CONTINUE

*
      XI(1) = 1.0D0
      NORM = 'A'
      LAOPT = 'F'
      IND = 0
      ITASK = 1

*
*      Set THETA to .TRUE. if the Theta integrator is required
*
      THETA = .FALSE.
```

```

      DO 40 I = 1, 30
        ALGOPT(I) = 0.0D0
40    CONTINUE
      IF (THETA) THEN
        ALGOPT(1) = 2.0D0
      ELSE
        ALGOPT(1) = 0.0D0
      END IF

*
*   Loop over output value of t
*
      TS = 1.0D-4
      TOUT = 0.0D0
      CALL UVINIT(NPDE,NPTS,X,U,NCODE,NEQN)
      DO 60 IT = 1, 5
        TOUT = 0.1D0*(2**IT)
        IFAIL = 1

*
        CALL D03PHF(NPDE,M,TS,TOUT,PDEDEF,BNDARY,U,NPTS,X,NCODE,ODEDEF,
+          NXI,XI,NEQN,RTOL,ATOL,ITOL,NORM,LAOPT,ALGOPT,RSAVE,
+          LRSAVE,ISAVE,LISAVE,ITASK,ITRACE,IND,IFAIL)

*
        IF (IFAIL.NE.0) THEN
          WRITE (NOUT,99993) IFAIL
          GO TO 80
        ELSE IF (IT.EQ.1) THEN
          WRITE (NOUT,99997) ATOL, NPTS
          WRITE (NOUT,99999) X(1), X(5), X(9), X(13), X(21)
        END IF

*
*   Check against the exact solution
*
        CALL EXACT(TOUT,NPTS,X,EXY)
        WRITE (NOUT,99998) TS
        WRITE (NOUT,99995) U(1), U(5), U(9), U(13), U(21), U(22)
        WRITE (NOUT,99994) EXY(1), EXY(5), EXY(9), EXY(13), EXY(21), TS
60    CONTINUE
        WRITE (NOUT,99996) ISAVE(1), ISAVE(2), ISAVE(3), ISAVE(5)

*
      80 CONTINUE

*
99999 FORMAT (' X ',5F9.3,/)
99998 FORMAT (' T = ',F6.3)
99997 FORMAT (/' Simple coupled PDE using BDF ',/' Accuracy require',
+   'ment =',E10.3,' Number of points = ',I4,/)
99996 FORMAT (' Number of integration steps in time = ',I6,/' Number o',
+   'f function evaluations = ',I6,/' Number of Jacobian eval',
+   'uations = ',I6,/' Number of iterations = ',I6)
99995 FORMAT (1X,'App. sol. ',F7.3,4F9.3,' ODE sol. =',F8.3)
99994 FORMAT (1X,'Exact sol. ',F7.3,4F9.3,' ODE sol. =',F8.3,/)
99993 FORMAT (1X,/1X,' ** D03PHF returned with IFAIL = ',I5)
      END

*
      SUBROUTINE UVINIT(NPDE,NPTS,X,U,NCODE,NEQN)
*   Routine for PDE initial values
*   .. Scalar Arguments ..
      INTEGER          NCODE, NEQN, NPDE, NPTS
*   .. Array Arguments ..
      DOUBLE PRECISION U(NEQN), X(NPTS)
*   .. Scalars in Common ..
      DOUBLE PRECISION TS
*   .. Local Scalars ..
      INTEGER          I
*   .. Intrinsic Functions ..
      INTRINSIC        EXP
*   .. Common blocks ..
      COMMON            /TAXIS/TS
*   .. Executable Statements ..
      DO 20 I = 1, NPTS
        U(I) = EXP(TS*(1.0D0-X(I))) - 1.0D0
20    CONTINUE

```

```

      U(NEQN) = TS
      RETURN
      END

*
      SUBROUTINE ODEDEF(NPDE,T,NCODE,V,VDOT,NXI,XI,UCP,UCPX,RCP,UCPT,
+          UCPTX,F,IRES)
*
      .. Scalar Arguments ..
      DOUBLE PRECISION T
      INTEGER          IRES, NCODE, NPDE, NXI
*
      .. Array Arguments ..
      DOUBLE PRECISION F(NCODE), RCP(NPDE,*), UCP(NPDE,*), UCPT(NPDE,*),
+          UCPTX(NPDE,*), UCPX(NPDE,*), V(NCODE),
+          VDOT(NCODE), XI(NXI)
*
      .. Executable Statements ..
      IF (IRES.EQ.1) THEN
          F(1) = VDOT(1) - V(1)*UCP(1,1) - UCPX(1,1) - 1.0D0 - T
      ELSE IF (IRES.EQ.-1) THEN
          F(1) = VDOT(1)
      END IF
      RETURN
      END

*
      SUBROUTINE PDEDEF(NPDE,T,X,U,UX,NCODE,V,VDOT,P,Q,R,IRES)
*
      .. Scalar Arguments ..
      DOUBLE PRECISION T, X
      INTEGER          IRES, NCODE, NPDE
*
      .. Array Arguments ..
      DOUBLE PRECISION P(NPDE,NPDE), Q(NPDE), R(NPDE), U(NPDE),
+          UX(NPDE), V(NCODE), VDOT(NCODE)
*
      .. Executable Statements ..
      P(1,1) = V(1)*V(1)
      R(1) = UX(1)
      Q(1) = -X*UX(1)*V(1)*VDOT(1)
      RETURN
      END

*
      SUBROUTINE BNDARY(NPDE,T,U,UX,NCODE,V,VDOT,IBND,BETA,GAMMA,IRES)
*
      .. Scalar Arguments ..
      DOUBLE PRECISION T
      INTEGER          IBND, IRES, NCODE, NPDE
*
      .. Array Arguments ..
      DOUBLE PRECISION BETA(NPDE), GAMMA(NPDE), U(NPDE), UX(NPDE),
+          V(NCODE), VDOT(NCODE)
*
      .. Intrinsic Functions ..
      INTRINSIC      EXP
*
      .. Executable Statements ..
      BETA(1) = 1.0D0
      IF (IBND.EQ.0) THEN
          GAMMA(1) = -V(1)*EXP(T)
      ELSE
          GAMMA(1) = -V(1)*VDOT(1)
      END IF
      RETURN
      END

*
      SUBROUTINE EXACT(TIME,NPTS,X,U)
*
      Exact solution (for comparison purpose)
*
      .. Scalar Arguments ..
      DOUBLE PRECISION TIME
      INTEGER          NPTS
*
      .. Array Arguments ..
      DOUBLE PRECISION U(NPTS), X(NPTS)
*
      .. Local Scalars ..
      INTEGER          I
*
      .. Intrinsic Functions ..
      INTRINSIC      EXP
*
      .. Executable Statements ..

```

```

      DO 20 I = 1, NPTS
        U(I) = EXP(TIME*(1.0D0-X(I))) - 1.0D0
20  CONTINUE
      RETURN
      END

```

9.2 Program Data

None.

9.3 Program Results

D03PHF Example Program Results

```

Simple coupled PDE using BDF
Accuracy requirement = 0.100E-03 Number of points = 21

```

X	0.000	0.200	0.400	0.600	1.000		
T = 0.200							
App. sol.	0.222	0.174	0.128	0.084	0.001	ODE sol. =	0.200
Exact sol.	0.221	0.174	0.127	0.083	0.000	ODE sol. =	0.200
T = 0.400							
App. sol.	0.493	0.379	0.273	0.176	0.002	ODE sol. =	0.400
Exact sol.	0.492	0.377	0.271	0.174	0.000	ODE sol. =	0.400
T = 0.800							
App. sol.	1.229	0.901	0.622	0.384	0.008	ODE sol. =	0.798
Exact sol.	1.226	0.896	0.616	0.377	0.000	ODE sol. =	0.800
T = 1.600							
App. sol.	3.959	2.610	1.629	0.917	0.027	ODE sol. =	1.594
Exact sol.	3.953	2.597	1.612	0.896	0.000	ODE sol. =	1.600
T = 3.200							
App. sol.	23.468	11.973	5.885	2.665	0.074	ODE sol. =	3.184
Exact sol.	23.533	11.936	5.821	2.597	0.000	ODE sol. =	3.200
Number of integration steps in time = 36							
Number of function evaluations = 498							
Number of Jacobian evaluations = 17							
Number of iterations = 117							

Example Program
Parabolic PDE Coupled with ODE using Finite-differences and BDF

