

## NAG Library Function Document

### nag\_ode\_ivp\_bdf\_gen (d02ejc)

#### 1 Purpose

nag\_ode\_ivp\_bdf\_gen (d02ejc) integrates a stiff system of first-order ordinary differential equations over an interval with suitable initial conditions, using a variable-order, variable-step method implementing the Backward Differentiation Formulae (BDF), until a user-specified function, if supplied, of the solution is zero, and returns the solution at specified points, if desired.

#### 2 Specification

```
#include <nag.h>
#include <nagd02.h>

void nag_ode_ivp_bdf_gen (Integer neq,
    void (*fcn)(Integer neq, double x, const double y[], double f[],
        Nag_User *comm),
    void (*pederv)(Integer neq, double x, const double y[], double pw[],
        Nag_User *comm),
    double *x, double y[], double xend, double tol, Nag_ErrorControl err_c,
    void (*output)(Integer neq, double *xsol, const double y[],
        Nag_User *comm),
    double (*g)(Integer neq, double x, const double y[], Nag_User *comm),
    Nag_User *comm, NagError *fail)
```

#### 3 Description

nag\_ode\_ivp\_bdf\_gen (d02ejc) advances the solution of a system of ordinary differential equations

$$y'_i = f_i(x, y_1, y_2, \dots, y_{\mathbf{neq}}), \quad i = 1, 2, \dots, \mathbf{neq},$$

from  $x = \mathbf{x}$  to  $x = \mathbf{xend}$  using a variable-order, variable-step method implementing the BDF. The system is defined by **fcn**, which evaluates  $f_i$  in terms of  $x$  and  $y_1, y_2, \dots, y_{\mathbf{neq}}$  (see Section 5). The initial values of  $y_1, y_2, \dots, y_{\mathbf{neq}}$  must be given at  $x = \mathbf{x}$ .

The solution is returned via **output** at specified points, if desired: this solution is obtained by  $C^1$  interpolation on solution values produced by the method. As the integration proceeds a check can be made on the user-specified function  $g(x, y)$  to determine an interval where it changes sign. The position of this sign change is then determined accurately. It is assumed that  $g(x, y)$  is a continuous function of the variables, so that a solution of  $g(x, y) = 0.0$  can be determined by searching for a change in sign in  $g(x, y)$ . The accuracy of the integration, the interpolation and, indirectly, of the determination of the position where  $g(x, y) = 0.0$ , is controlled by the arguments **tol** and **err\_c**. The Jacobian of the system  $y' = f(x, y)$  may be supplied in function **pederv**, if it is available.

For a description of BDF and their practical implementation see Hall and Watt (1976).

#### 4 References

Hall G and Watt J M (ed.) (1976) *Modern Numerical Methods for Ordinary Differential Equations* Clarendon Press, Oxford

## 5 Arguments

1: **neq** – Integer *Input*

*On entry:* the number of differential equations.

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

2: **fcn** – function, supplied by the user *External Function*

**fcn** must evaluate the first derivatives  $y'_i$  (i.e., the functions  $f_i$ ) for given values of their arguments  $x, y_1, y_2, \dots, y_{\text{neq}}$ .

The specification of **fcn** is:

```
void fcn (Integer neq, double x, const double y[], double f[],
         Nag_User *comm)
```

1: **neq** – Integer *Input*

*On entry:* the number of differential equations.

2: **x** – double *Input*

*On entry:* the value of the independent variable  $x$ .

3: **y[neq]** – const double *Input*

*On entry:*  $y[i - 1]$  holds the value of the variable  $y_i$ , for  $i = 1, 2, \dots, \text{neq}$ .

4: **f[neq]** – double *Output*

*On exit:*  $f[i - 1]$  must contain the value of  $f_i$ , for  $i = 1, 2, \dots, \text{neq}$ .

5: **comm** – Nag\_User \*

Pointer to a structure of type Nag\_User with the following member:

**p** – Pointer

*On entry/exit:* the pointer **comm**→**p** should be cast to the required type, e.g.,  
`struct user *s = (struct user *)comm → p`, to obtain the original  
 object's address with appropriate type. (See the argument **comm** below.)

3: **pederv** – function, supplied by the user *External Function*

**pederv** must evaluate the Jacobian of the system (that is, the partial derivatives  $\frac{\partial f_i}{\partial y_j}$ ) for given values of the variables  $x, y_1, y_2, \dots, y_{\text{neq}}$ .

The specification of **pederv** is:

```
void pederv (Integer neq, double x, const double y[], double pw[],
            Nag_User *comm)
```

1: **neq** – Integer *Input*

*On entry:* the number of differential equations.

2: **x** – double *Input*

*On entry:* the value of the independent variable  $x$ .

3:	<b>y[neq]</b> – const double <i>On entry:</i> $y[i - 1]$ holds the value of the variable $y_i$ , for $i = 1, 2, \dots, \mathbf{neq}$ .	<i>Input</i>
4:	<b>pw[neq × neq]</b> – double <i>On exit:</i> <b>pw</b> $[(i - 1) \times \mathbf{neq} + j - 1]$ must contain the value of $\frac{\partial f_i}{\partial y_j}$ , for $i, j = 1, 2, \dots, \mathbf{neq}$ .	<i>Output</i>
5:	<b>comm</b> – Nag_User * Pointer to a structure of type Nag_User with the following member:  <b>p</b> – Pointer  <i>On entry/exit:</i> the pointer <b>comm</b> → <b>p</b> should be cast to the required type, e.g., struct user *s = (struct user *)comm → p, to obtain the original object's address with appropriate type. (See the argument <b>comm</b> below.)	

If you do not wish to supply the Jacobian, the actual argument **pederv** must be the NAG defined null function pointer **NULLFN**.

- 4: **x** – double \* *Input/Output*  
*On entry:* the value of the independent variable  $x$ .  
*Constraint:*  $\mathbf{x} \neq \mathbf{xend}$ .  
*On exit:* if  $g$  is supplied, **x** contains the point where  $g(x, y) = 0.0$ , unless  $g(x, y) \neq 0.0$  anywhere on the range **x** to **xend**, in which case, **x** will contain **xend**. If  $g$  is not supplied **x** contains **xend**, unless an error has occurred, when it contains the value of  $x$  at the error.
- 5: **y[neq]** – double *Input/Output*  
*On entry:*  $y[i - 1]$  holds the value of the variable  $y_i$ , for  $i = 1, 2, \dots, \mathbf{neq}$ .  
*On exit:* the computed values of the solution at the final point  $x = \mathbf{x}$ .
- 6: **xend** – double *Input*  
*On entry:* the final value of the independent variable.  
**xend** < **x**  
Integration proceeds in the negative direction.  
*Constraint:* **xend**  $\neq$  **x**.
- 7: **tol** – double *Input*  
*On entry:* a **positive** tolerance for controlling the error in the integration. Hence **tol** affects the determination of the position where  $g(x, y) = 0.0$ , if  $g$  is supplied.  
  
nag\_ode\_ivp\_bdf\_gen (d02ejc) has been designed so that, for most problems, a reduction in **tol** leads to an approximately proportional reduction in the error in the solution. However, the actual relation between **tol** and the accuracy achieved cannot be guaranteed. You are strongly recommended to call nag\_ode\_ivp\_bdf\_gen (d02ejc) with more than one value for **tol** and to compare the results obtained to estimate their accuracy. In the absence of any prior knowledge, you might compare the results obtained by calling nag\_ode\_ivp\_bdf\_gen (d02ejc) with **tol** =  $10^{-p}$  and **tol** =  $10^{-p-1}$  if  $p$  correct decimal digits are required in the solution.  
*Constraint:* **tol** > 0.0.

8: **err\_c** – Nag\_ErrorControl*Input*

*On entry:* the type of error control. At each step in the numerical solution an estimate of the local error, *est*, is made. For the current step to be accepted the following condition must be satisfied:

$$est = \sqrt{\frac{1}{neq} \sum_{i=1}^{neq} (e_i / (\tau_r \times |y_i| + \tau_a))^2} \leq 1.0$$

where  $\tau_r$  and  $\tau_a$  are defined by

<b>err_c</b>	$\tau_r$	$\tau_a$
Nag_Relative	<b>tol</b>	$\epsilon$
Nag_Absolute	0.0	<b>tol</b>
Nag_Mixed	<b>tol</b>	<b>tol</b>

where  $\epsilon$  is a small machine-dependent number and  $e_i$  is an estimate of the local error at  $y_i$ , computed internally. If the appropriate condition is not satisfied, the step size is reduced and the solution is recomputed on the current step. If you wish to measure the error in the computed solution in terms of the number of correct decimal places, then **err\_c** should be set to Nag\_Absolute on entry, whereas if the error requirement is in terms of the number of correct significant digits, then **err\_c** should be set to Nag\_Relative. If you prefer a mixed error test, then **err\_c** should be set to Nag\_Mixed. The recommended value for **err\_c** is Nag\_Relative.

*Constraint:* **err\_c** = Nag\_Absolute, Nag\_Mixed or Nag\_Relative.

9: **output** – function, supplied by the user*External Function*

**output** permits access to intermediate values of the computed solution (for example to print or plot them), at successive user-specified points. It is initially called by nag\_ode\_ivp\_bdf\_gen (d02ejc) with **xsol** = **x** (the initial value of  $x$ ). You must reset **xsol** to the next point (between the current **xsol** and **xend**) where **output** is to be called, and so on at each call to **output**. If, after a call to **output**, the reset point **xsol** is beyond **xend**, nag\_ode\_ivp\_bdf\_gen (d02ejc) will integrate to **xend** with no further calls to **output**; if a call to **output** is required at the point **xsol** = **xend**, then **xsol** must be given precisely the value **xend**.

The specification of **output** is:

```
void output (Integer neq, double *xsol, const double y[],
            Nag_User *comm)
```

1: **neq** – Integer

*Input*

*On entry:* the number of differential equations.

2: **xsol** – double \*

*Input/Output*

*On entry:* the value of the independent variable  $x$ .

*On exit:* you must set **xsol** to the next value of  $x$  at which **output** is to be called.

3: **y[neq]** – const double

*Input*

*On entry:*  $y[i-1]$  holds the value of the variable  $y_i$ , for  $i = 1, 2, \dots, neq$ .

4: **comm** – Nag\_User \*

Pointer to a structure of type Nag\_User with the following member:

**p** – Pointer

*On entry/exit:* the pointer **comm**→**p** should be cast to the required type, e.g.,  

```
struct user *s = (struct user *)comm → p,
```

to obtain the original object's address with appropriate type. (See the argument **comm** below.)

If you do not wish to access intermediate output, the actual argument **output** must be the NAG defined null function pointer `NULLFN`.

- 10: **g** – function, supplied by the user *External Function*  
**g** must evaluate  $g(x, y)$  for specified values  $x, y$ . It specifies the function  $g$  for which the first position  $x$  where  $g(x, y) = 0$  is to be found.

The specification of **g** is:

```
double g (Integer neq, double x, const double y[], Nag_User *comm)
```

1: **neq** – Integer *Input*

*On entry:* the number of differential equations.

2: **x** – double *Input*

*On entry:* the value of the independent variable  $x$ .

3: **y[neq]** – const double *Input*

*On entry:*  $y[i - 1]$  holds the value of the variable  $y_i$ , for  $i = 1, 2, \dots, \mathbf{neq}$ .

4: **comm** – Nag\_User \*

Pointer to a structure of type Nag\_User with the following member:

**p** – Pointer

*On entry/exit:* the pointer **comm**→**p** should be cast to the required type, e.g.,  
`struct user *s = (struct user *)comm → p`, to obtain the original object's address with appropriate type. (See the argument **comm** below.)

If you do not require the root finding option, the actual argument **g** must be the NAG defined null double function pointer `NULLDFN`.

- 11: **comm** – Nag\_User \*

Pointer to a structure of type Nag\_User with the following member:

**p** – Pointer

*On entry/exit:* the pointer **comm**→**p**, of type Pointer, allows you to communicate information to and from **fcn**, **pedery**, **output** and **g**. An object of the required type should be declared, e.g., a structure, and its address assigned to the pointer **comm**→**p** by means of a cast to Pointer in the calling program, e.g., `comm.p = (Pointer)&s`. The type pointer will be `void *` with a C compiler that defines `void *` and `char *` otherwise.

- 12: **fail** – NagError \* *Input/Output*

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

## 6 Error Indicators and Warnings

### NE\_2\_REAL\_ARG\_EQ

On entry,  $\mathbf{x} = \langle \text{value} \rangle$  while  $\mathbf{xend} = \langle \text{value} \rangle$ . These arguments must satisfy  $\mathbf{x} \neq \mathbf{xend}$ .

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

**NE\_BAD\_PARAM**

On entry, argument **err\_c** had an illegal value.

**NE\_INT\_ARG\_LT**

On entry, **neq** =  $\langle value \rangle$ .  
Constraint: **neq**  $\geq 1$ .

**NE\_INTERNAL\_ERROR**

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

**NE\_NO\_SIGN\_CHANGE**

No change in sign of the function  $g(x, y)$  was detected in the integration range.

**NE\_REAL\_ARG\_LE**

On entry, **tol** must not be less than or equal to 0.0: **tol** =  $\langle value \rangle$ .

**NE\_TOL\_PROGRESS**

The value of **tol**,  $\langle value \rangle$ , is too small for the function to make any further progress across the integration range. Current value of **x** =  $\langle value \rangle$ .

**NE\_TOL\_TOO\_SMALL**

The value of **tol**,  $\langle value \rangle$ , is too small for the function to take an initial step.

**NE\_XSOL\_INCONSIST**

On call  $\langle value \rangle$  to the supplied print function **xsol** was set to a value behind the previous value of **xsol** in the direction of integration.  
Previous **xsol** =  $\langle value \rangle$ , **xend** =  $\langle value \rangle$ , new **xsol** =  $\langle value \rangle$ .

**NE\_XSOL\_NOT\_RESET**

On call  $\langle value \rangle$  to the supplied print function **xsol** was not reset.

**NE\_XSOL\_SET\_WRONG**

**xsol** was set to a value behind **x** in the direction of integration by the first call to the supplied print function.  
The integration range is  $(\langle value \rangle, \langle value \rangle)$ , **xsol** =  $\langle value \rangle$ .

## 7 Accuracy

The accuracy of the computation of the solution vector **y** may be controlled by varying the local error tolerance **tol**. In general, a decrease in local error tolerance should lead to an increase in accuracy. You are advised to choose **err\_c** = Nag\_Relative unless you have a good reason for a different choice. It is particularly appropriate if the solution decays.

If the problem is a root-finding one, then the accuracy of the root determined will depend strongly on  $\frac{\partial g}{\partial x}$  and  $\frac{\partial g}{\partial y_i}$ , for  $i = 1, 2, \dots, \mathbf{neq}$ . Large values for these quantities may imply large errors in the root.

## 8 Parallelism and Performance

nag\_ode\_ivp\_bdf\_gen (d02ejc) is not threaded in any implementation.

## 9 Further Comments

If more than one root is required, then to determine the second and later roots `nag_ode_ivp_bdf_gen` (d02ejc) may be called again starting a short distance past the previously determined roots.

If it is easy to code, you should supply the function `pederv`. However, it is important to be aware that if `pederv` is coded incorrectly, a very inefficient integration may result and possibly even a failure to complete the integration (`fail.code` = NE\_TOL\_PROGRESS).

## 10 Example

We illustrate the solution of five different problems. In each case the differential system is the well-known stiff Robertson problem.

$$\begin{aligned} y_1' &= -0.04y_1 + 10^4 y_2 y_3 \\ y_2' &= 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2 \\ y_3' &= 3 \times 10^7 y_2^2 \end{aligned}$$

with initial conditions  $y_1 = 1.0$ ,  $y_2 = y_3 = 0.0$  at  $x = 0.0$ . We solve each of the following problems with local error tolerances  $1.0e-3$  and  $1.0e-4$ .

- (i) To integrate to  $x = 10.0$  producing output at intervals of 2.0 until a point is encountered where  $y_1 = 0.9$ . The Jacobian is calculated numerically.
- (ii) As (i) but with the Jacobian calculated analytically.
- (iii) As (i) but with no intermediate output.
- (iv) As (i) but with no root-finding termination condition.
- (v) Integrating the equations as in (i) but with no intermediate output and no root-finding termination condition.

### 10.1 Program Text

```

/* nag_ode_ivp_bdf_gen (d02ejc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#include <nag.h>
#include <math.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nagd02.h>

#ifdef __cplusplus
extern "C"
{
#endif
    static void NAG_CALL fcn(Integer neq, double x, const double y[],
                             double f[], Nag_User *comm);
    static void NAG_CALL pederv(Integer neq, double x, const double y[],
                                 double pw[], Nag_User *comm);
    static double NAG_CALL g(Integer neq, double x, const double y[],
                              Nag_User *comm);
    static void NAG_CALL out(Integer neq, double *tsol, const double y[],
                              Nag_User *comm);
#ifdef __cplusplus
}
#endif

struct user

```

```

{
  double xend, h;
  Integer k;
  Integer *use_comm;
};

#define NEQ 3
int main(void)
{
  static Integer use_comm[4] = { 1, 1, 1, 1 };
  Integer exit_status = 0, j, neq;
  NagError fail;
  Nag_User comm;
  double tol, x, *y = 0;
  struct user s;

  INIT_FAIL(fail);

  printf("nag_ode_ivp_bdf_gen (d02ejc) Example Program Results\n");

  /* For communication with user-supplied functions
   * assign address of user defined structure
   * to comm.p.
   */
  s.use_comm = use_comm;
  comm.p = (Pointer) &s;

  neq = NEQ;
  if (neq >= 1) {
    if (!(y = NAG_ALLOC(neq, double)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }
  }
  else {
    exit_status = 1;
    return exit_status;
  }
  s.xend = 10.0;
  printf("\nCase 1: calculating Jacobian internally\n");
  printf(" intermediate output, root-finding\n\n");

  for (j = 3; j <= 4; ++j) {
    tol = pow(10.0, -(double) j);
    printf("\n Calculation with tol = %10.1e\n", tol);
    x = 0.0;
    y[0] = 1.0;
    y[1] = 0.0;
    y[2] = 0.0;
    s.k = 4;
    s.h = (s.xend - x) / (double) (s.k + 1);
    printf("      X      Y(1)      Y(2)      Y(3)\n");
    /* nag_ode_ivp_bdf_gen (d02ejc).
     * Ordinary differential equations solver, stiff, initial
     * value problems using the Backward Differentiation
     * Formulae
     */
    nag_ode_ivp_bdf_gen(neq, fcn, NULLFN, &x, y, s.xend, tol, Nag_Relative,
                        out, g, &comm, &fail);
    if (fail.code != NE_NOERROR) {
      printf("Error from nag_ode_ivp_bdf_gen (d02ejc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
    printf(" Root of Y(1)-0.9 at %5.3f\n", x);
    printf(" Solution is ");
    printf("%7.4f %8.5f %7.4f\n", y[0], y[1], y[2]);
  }
  printf("\nCase 2: calculating Jacobian by pederv\n");
}

```

```

printf(" intermediate output, root-finding\n\n");

for (j = 3; j <= 4; ++j) {
    tol = pow(10.0, -(double) j);
    printf("\n Calculation with tol = %10.1e\n", tol);
    x = 0.0;
    y[0] = 1.0;
    y[1] = 0.0;
    y[2] = 0.0;
    s.k = 4;
    s.h = (s.xend - x) / (double) (s.k + 1);
    printf("      X          Y(1)          Y(2)          Y(3)\n");
    /* nag_ode_ivp_bdf_gen (d02ejc), see above. */
    nag_ode_ivp_bdf_gen(neq, fcn, pederv, &x, y, s.xend, tol, Nag_Relative,
                        out, g, &comm, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_ode_ivp_bdf_gen (d02ejc).\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }
    printf(" Root of Y(1)-0.9 at %5.3f\n", x);
    printf(" Solution is ");
    printf("%7.4f %8.5f %7.4f\n", y[0], y[1], y[2]);
}
printf("\nCase 3: calculating Jacobian internally\n");
printf(" no intermediate output, root-finding\n\n");
for (j = 3; j <= 4; ++j) {
    tol = pow(10.0, -(double) j);
    printf("\n Calculation with tol = %10.1e\n", tol);
    x = 0.0;
    y[0] = 1.0;
    y[1] = 0.0;
    y[2] = 0.0;

    /* nag_ode_ivp_bdf_gen (d02ejc), see above. */
    nag_ode_ivp_bdf_gen(neq, fcn, NULLFN, &x, y, s.xend, tol, Nag_Relative,
                        NULLFN, g, &comm, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_ode_ivp_bdf_gen (d02ejc).\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }

    printf(" Root of Y(1)-0.9 at %5.3f\n", x);
    printf(" Solution is ");
    printf("%7.4f %8.5f %7.4f\n", y[0], y[1], y[2]);
}
printf("\nCase 4: calculating Jacobian internally\n");
printf(" intermediate output, no root-finding\n\n");

for (j = 3; j <= 4; ++j) {
    tol = pow(10.0, -(double) j);
    printf("\n Calculation with tol = %10.1e\n", tol);
    x = 0.0;
    y[0] = 1.0;
    y[1] = 0.0;
    y[2] = 0.0;
    s.k = 4;
    s.h = (s.xend - x) / (double) (s.k + 1);
    printf("      X          Y(1)          Y(2)          Y(3)\n");
    /* nag_ode_ivp_bdf_gen (d02ejc), see above. */
    nag_ode_ivp_bdf_gen(neq, fcn, NULLFN, &x, y, s.xend, tol, Nag_Relative,
                        out, NULLDFN, &comm, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_ode_ivp_bdf_gen (d02ejc).\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }
    printf("%8.2f", x);
    printf("%13.4f%13.5f%13.4f\n", y[0], y[1], y[2]);
}

```

```

printf("\nCase 5: calculating Jacobian internally\n");
printf(" no intermediate output, no root-finding (integrate to xend)\n\n");

for (j = 3; j <= 4; ++j) {
    tol = pow(10.0, -(double) j);
    printf("\n Calculation with tol = %10.1e\n", tol);
    x = 0.0;
    y[0] = 1.0;
    y[1] = 0.0;
    y[2] = 0.0;
    printf("          X          Y(1)          Y(2)          Y(3)\n");
    printf("%8.2f", x);
    printf("%13.4f%13.5f%13.4f\n", y[0], y[1], y[2]);
    /* nag_ode_ivp_bdf_gen (d02ejc), see above. */
    nag_ode_ivp_bdf_gen(neq, fcn, NULLFN, &x, y, s.xend, tol, Nag_Relative,
                       NULLFN, NULLDFN, &comm, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_ode_ivp_bdf_gen (d02ejc).\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }
    printf("%8.2f", x);
    printf("%13.4f%13.5f%13.4f\n", y[0], y[1], y[2]);
}
END:
    NAG_FREE(y);
    return exit_status;
}

static void NAG_CALL fcn(Integer neq, double x, const double y[], double f[],
                        Nag_User *comm)
{
    struct user *s = (struct user *) comm->p;

    if (s->use_comm[0]) {
        printf("(User-supplied callback fcn, first invocation.)\n");
        s->use_comm[0] = 0;
    }

    f[0] = y[0] * -0.04 + y[1] * 1e4 * y[2];
    f[1] = y[0] * 0.04 - y[1] * 1e4 * y[2] - y[1] * 3e7 * y[1];
    f[2] = y[1] * 3e7 * y[1];
}

static void NAG_CALL pederv(Integer neq, double x, const double y[],
                            double pw[], Nag_User *comm)
{
#define PW(I, J) pw[((I) - 1)*neq + (J) - 1]
    struct user *s = (struct user *) comm->p;

    if (s->use_comm[1]) {
        printf("(User-supplied callback pederv, first invocation.)\n");
        s->use_comm[1] = 0;
    }

    PW(1, 1) = -0.04;
    PW(1, 2) = y[2] * 1e4;
    PW(1, 3) = y[1] * 1e4;
    PW(2, 1) = 0.04;
    PW(2, 2) = y[2] * -1e4 - y[1] * 6e7;
    PW(2, 3) = y[1] * -1e4;
    PW(3, 1) = 0.0;
    PW(3, 2) = y[1] * 6e7;
    PW(3, 3) = 0.0;
}

static double NAG_CALL g(Integer neq, double x, const double y[],
                        Nag_User *comm)
{
    struct user *s = (struct user *) comm->p;

```

```

    if (s->use_comm[2]) {
        printf("(User-supplied callback g, first invocation.)\n");
        s->use_comm[2] = 0;
    }

    return y[0] - 0.9;
}

static void NAG_CALL out(Integer neq, double *xsol, const double y[],
                        Nag_User *comm)
{
    struct user *s = (struct user *) comm->p;

    printf("%8.2f", *xsol);
    printf("%13.4f%13.5f%13.4f\n", y[0], y[1], y[2]);

    *xsol = s->xend - (double) s->k * s->h;
    s->k--;
}

```

## 10.2 Program Data

None.

## 10.3 Program Results

nag\_ode\_ivp\_bdf\_gen (d02ejc) Example Program Results

Case 1: calculating Jacobian internally  
intermediate output, root-finding

```

Calculation with tol = 1.0e-03
  X      Y(1)      Y(2)      Y(3)
  0.00    1.0000    0.00000    0.0000
(User-supplied callback g, first invocation.)
(User-supplied callback fcn, first invocation.)
  2.00    0.9416    0.00003    0.0583
  4.00    0.9055    0.00002    0.0945
Root of Y(1)-0.9 at 4.377
Solution is 0.9000 0.00002 0.1000

```

```

Calculation with tol = 1.0e-04
  X      Y(1)      Y(2)      Y(3)
  0.00    1.0000    0.00000    0.0000
  2.00    0.9416    0.00003    0.0584
  4.00    0.9055    0.00002    0.0945
Root of Y(1)-0.9 at 4.377
Solution is 0.9000 0.00002 0.1000

```

Case 2: calculating Jacobian by pederv  
intermediate output, root-finding

```

Calculation with tol = 1.0e-03
  X      Y(1)      Y(2)      Y(3)
(User-supplied callback pederv, first invocation.)
  0.00    1.0000    0.00000    0.0000
  2.00    0.9416    0.00003    0.0583
  4.00    0.9055    0.00002    0.0945
Root of Y(1)-0.9 at 4.377
Solution is 0.9000 0.00002 0.1000

```

```

Calculation with tol = 1.0e-04
  X      Y(1)      Y(2)      Y(3)
  0.00    1.0000    0.00000    0.0000
  2.00    0.9416    0.00003    0.0584
  4.00    0.9055    0.00002    0.0945
Root of Y(1)-0.9 at 4.377

```

Solution is 0.9000 0.00002 0.1000

Case 3: calculating Jacobian internally  
no intermediate output, root-finding

Calculation with tol = 1.0e-03  
Root of Y(1)-0.9 at 4.377  
Solution is 0.9000 0.00002 0.1000

Calculation with tol = 1.0e-04  
Root of Y(1)-0.9 at 4.377  
Solution is 0.9000 0.00002 0.1000

Case 4: calculating Jacobian internally  
intermediate output, no root-finding

X	Y(1)	Y(2)	Y(3)
0.00	1.0000	0.00000	0.0000
2.00	0.9416	0.00003	0.0583
4.00	0.9055	0.00002	0.0945
6.00	0.8793	0.00002	0.1207
8.00	0.8586	0.00002	0.1414
10.00	0.8414	0.00002	0.1586
10.00	0.8414	0.00002	0.1586

X	Y(1)	Y(2)	Y(3)
0.00	1.0000	0.00000	0.0000
2.00	0.9416	0.00003	0.0584
4.00	0.9055	0.00002	0.0945
6.00	0.8793	0.00002	0.1207
8.00	0.8585	0.00002	0.1414
10.00	0.8414	0.00002	0.1586
10.00	0.8414	0.00002	0.1586

Case 5: calculating Jacobian internally  
no intermediate output, no root-finding (integrate to xend)

X	Y(1)	Y(2)	Y(3)
0.00	1.0000	0.00000	0.0000
10.00	0.8414	0.00002	0.1586

X	Y(1)	Y(2)	Y(3)
0.00	1.0000	0.00000	0.0000
10.00	0.8414	0.00002	0.1586

---