NAG Toolbox for MATLAB d02nd

1 Purpose

d02nd is a forward communication function for integrating stiff systems of explicit ordinary differential equations when the Jacobian is a sparse matrix.

2 Syntax

```
[t, y, ydot, rwork, inform, ysav, wkjac, jacpvt, ifail] = d02nd(neq, t,
tout, y, rwork, rtol, atol, itol, inform, fcn, ysav, jac, wkjac, jacpvt,
monitr, itask, itrace, 'sdysav', sdysav, 'nwkjac', nwkjac, 'njcpvt',
njcpvt)
```

3 Description

d02nd is a general purpose function for integrating the initial value problem for a stiff system of explicit ordinary differential equations,

$$y' = g(t, y).$$

It is designed specifically for the case where the Jacobian $\frac{\partial g}{\partial y}$ is a sparse matrix.

Both interval and step oriented modes of operation are available and also modes designed to permit intermediate output within an interval oriented mode.

An outline of a typical program calling d02nd is given below. It calls the sparse matrix linear algebra setup function d02nu, and the Backward Differentiation Formula (BDF) integrator setup function d02nv, its diagnostic counterpart d02ny, and the sparse linear algebra diagnostic function d02nx.

```
.
.
[...] = d02nv(...);
[...] = d02nu(...);
[..., ifail] = d02nd(...);
if (ifail ~= 1 and ifail < 14)
    [...] = d02nx(...);
    [...] = d02ny(...);
end
.
.</pre>
```

The linear algebra setup function d02nu and one of the integrator setup functions, d02nv or d02nw, must be called prior to the call of d02nd. Either or both of the integrator diagnostic function d02ny, or the sparse matrix linear algebra diagnostic function d02nx, may be called after the call to d02nd. There is also a function, d02nz, designed to permit you to change step size on a continuation call to d02nd without restarting the integration process.

4 References

See the D02M/N Sub-chapter Introduction.

5 Parameters

5.1 Compulsory Input Parameters

1: neq - int32 scalar

The number of differential equations to be solved.

Constraint: $neq \ge 1$.

2: t – double scalar

t, the value of the independent variable. The input value of t is used only on the first call as the initial point of the integration.

3: tout – double scalar

The next value of t at which a computed solution is desired. For the initial t, the input value of **tout** is used to determine the direction of integration. Integration is permitted in either direction (see also **itask**).

Constraint: **tout** \neq **t**.

4: y(ldysav) - double array

ldysav, the first dimension of the array, must be at least neq.

The values of the dependent variables (solution). On the first call the first \mathbf{neq} elements of \mathbf{y} must contain the vector of initial values.

5: $rwork(50 + 4 \times ldysav) - double array$

6: rtol(*) - double array

Note: the dimension of the array **rtol** must be at least 1 if itol = 1 or itol = 2, and at least **neq** otherwise.

The relative local error tolerance.

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

7: atol(*) - double array

Note: the dimension of the array atol must be at least 1 if itol = 1 or itol = 3, and at least neq otherwise.

The absolute local error tolerance.

Constraint: **atol**(i) ≥ 0.0 for all relevant i (see **itol**).

8: itol – int32 scalar

A value to indicate the form of the local error test. **itol** indicates to d02nd whether to interpret either or both of **rtol** or **atol** as a vector or a 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	$rtol(1) \times y_i + atol(1)$
2	scalar	vector	$rtol(1) \times y_i + atol(i)$
3	vector	scalar	$\mathbf{rtol}(i) \times y_i + \mathbf{atol}(1)$
4	vector	vector	$rtol(i) \times y_i + atol(i)$

 e_i is an estimate of the local error in y_i , computed internally, and the choice of norm to be used is defined by a previous call to an integrator setup function.

Constraint: $1 \leq itol \leq 4$.

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9: inform(23) - int32 array

10: fcn – string containing name of m-file

fcn must evaluate the derivative vector for the explicit ordinary differential equation system, defined by y' = g(t, y).

Its specification is:

$$[f, ires] = fcn(neq, t, y, ires)$$

Input Parameters

1: neq - int32 scalar

The number of differential equations being solved.

2: t – double scalar

t, the current value of the independent variable.

y(neq) - double array

The value of y_i , for $i = 1, 2, \dots, neq$.

4: ires – int32 scalar

ires = 1.

You may set ires as follows to indicate certain conditions in fcn to the integrator:

ires = 1

Indicates a normal return from **fcn**, that is **ires** is not altered by you and integration continues.

ires = 2

Indicates to the integrator that control should be passed back immediately to the calling (sub)program with the error indicator set to **ifail** = 11.

ires = 3

Indicates to the integrator that an error condition has occurred in the solution vector, its time derivative or in the value of t. The integrator will use a smaller time step to try to avoid this condition. If this is not possible, the integrator returns to the calling (sub)program with the error indicator set to **ifail** = 7.

ires = 4

Indicates to the integrator to stop its current operation and to enter the (sub)program **monitr** immediately with parameter **imon** = -2.

Output Parameters

1: f(neq) - double array

The value y_i' , given by $y_i' = g_i(t, y)$, for i = 1, 2, ..., neq.

2: ires – int32 scalar

ires = 1.

You may set ires as follows to indicate certain conditions in fcn to the integrator:

ires = 1

Indicates a normal return from **fcn**, that is **ires** is not altered by you and integration continues

ires = 2

Indicates to the integrator that control should be passed back immediately to the calling (sub)program with the error indicator set to **ifail** = 11.

ires = 3

Indicates to the integrator that an error condition has occurred in the solution vector, its time derivative or in the value of t. The integrator will use a smaller time step to try to avoid this condition. If this is not possible, the integrator returns to the calling (sub)program with the error indicator set to **ifail** = 7.

ires = 4

Indicates to the integrator to stop its current operation and to enter the (sub)program **monitr** immediately with parameter **imon** = -2.

11: ysav(ldysav,sdysav) – double array

ldysav, the first dimension of the array, must be at least neq.

An appropriate value for **sdysav** is described in the specifications of the integrator setup functions d02nv and d02nw. This value must be the same as that supplied to the integrator setup function.

12: jac – string containing name of m-file

jac must evaluate the Jacobian of the system. If this option is not required, the actual argument for **jac** must be the string 'd02ndz'. **d02ndz** is included in the NAG Fortran Library and so need not be supplied by you. You must indicate to the integrator whether this option is to be used by setting the parameter **jceval** appropriately in a call to the sparse matrix linear algebra setup function d02nu.

First we must define the system of nonlinear equations which is solved internally by the integrator. The time derivative, y', generated internally has the form

$$y' = (y - z)/(hd),$$

where h is the current step size and d is a parameter that depends on the integration method in use. The vector y is the current solution and the vector z depends on information from previous time steps. This means that $\frac{d}{dy}(\) = \frac{1}{(hd)} \frac{d}{dy}(\)$. The system of nonlinear equations that is solved has the form

$$y' - g(t, y) = 0$$

but is solved in the form

$$r(t, y) = 0,$$

where the function r is defined by

$$r(t, y) = hd((y-z)/(hd) - g(t, y)).$$

It is the Jacobian matrix $\frac{\partial r}{\partial y}$ that you must supply in **jac** as follows:

$$\frac{\partial r_i}{\partial y_j} = 1 - (hd) \frac{\partial g_i}{\partial y_j}, \text{ if } i = j;$$

$$\frac{\partial r_i}{\partial y_i} = -(hd)\frac{\partial g_i}{\partial y_i}$$
, otherwise.

Its specification is:

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[pdj] = jac(neq, t, y, h, d, j, pdj)

Input Parameters

1: neq - int32 scalar

The number of differential equations being solved.

2: t - double scalar

t, the current value of the independent variable.

y(neq) – double array

The current solution component y_i , for i = 1, 2, ..., neq.

4: h – double scalar

The current step size.

5: **d – double scalar**

The parameter d which depends upon the integration method.

6: j - int32 scalar

The column of the Jacobian that jac must return in the array pdj.

7: pdj(neq) - double array

Is set to zero.

 $\mathbf{pdj}(i)$ should be set to the (i,j)th element of the Jacobian, where j is given by \mathbf{j} . Only nonzero elements of this array need be set, since it is preset to zero before the call to \mathbf{jac} .

Output Parameters

1: pdj(neq) - double array

Is set to zero.

 $\mathbf{pdj}(i)$ should be set to the (i,j)th element of the Jacobian, where j is given by \mathbf{j} . Only nonzero elements of this array need be set, since it is preset to zero before the call to \mathbf{jac} .

13: wkjac(nwkjac) – double array

The actual size depends on whether the sparsity structure is supplied or whether it is to be estimated. An appropriate value for **nwkjac** is described in the specification of the linear algebra setup function d02nu. This value must be the same as that supplied to d02nu.

14: **jacpvt(njcpvt) – int32 array**

The actual size depends on whether the sparsity structure is supplied or whether it is to be estimated. An appropriate value for **njcpvt** is described in the specification of the linear algebra setup function d02nu. This value must be the same as that supplied to d02nu.

15: monitr – string containing name of m-file

monitr performs tasks requested by you. If this option is not required, then the actual argument for monitr must be the string 'd02nby'. d02nby is included in the NAG Fortran Library.

Its specification is:

```
[hnext, y, imon, inln, hmin, hmax] = monitr(neq, ldysav, t, hlast, hnext, y, ydot, ysav, r, acor, imon, hmin, hmax, nqu)
```

Input Parameters

1: neq - int32 scalar

The number of differential equations being solved.

2: ldysav – int32 scalar

An upper bound on the number of differential equations to be solved.

3: t – double scalar

The current value of the independent variable.

4: hlast – double scalar

The last step size successfully used by the integrator.

5: hnext – double scalar

The step size that the integrator proposes to take on the next step.

The next step size to be used. If this is different from the input value, then **imon** must be set to 4.

6: y(ldysav) - double array

ldysav, the first dimension of the array, must be at least neq.

y, the values of the dependent variables evaluated at t.

These values must not be changed unless **imon** is set to 2.

7: ydot(ldysav) – double array

ldysav, the first dimension of the array, must be at least neq.

The time derivatives y' of the vector y.

8: ysav(ldysav, sdysav) - double array

ldysav, the first dimension of the array, must be at least neq.

Workspace to enable you to carry out interpolation using either of the functions d02xj or d02xk.

9: r(ldysav) - double array

ldysav, the first dimension of the array, must be at least neq.

If **imon** = 0 and **inln** = 3, the first **neq** elements contain the residual vector y' - g(t, y).

10: **acor(ldysav,2) – double array**

ldysav, the first dimension of the array, must be at least neq.

With **imon** = 1, $\mathbf{acor}(i, 1)$ contains the weight used for the *i*th equation when the norm is evaluated, and $\mathbf{acor}(i, 2)$ contains the estimated local error for the *i*th equation. The scaled local error at the end of a timestep may be obtained by calling the double function d02za as follows:

```
[errloc, ifail] = d02za(acor(1:neq,2), acor(1:neq,1));
% Check ifail before proceeding
```

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11: imon – int32 scalar

A flag indicating under what circumstances monitr was called.

imon = -2

Entry from the integrator after ires = 4 (set in the user-supplied (sub)program fcn) caused an early termination (this facility could be used to locate discontinuities).

imon = -1

The current step failed repeatedly.

imon = 0

Entry after a call to the internal nonlinear equation solver (see inln).

imon = 1

The current step was successful.

May be reset to determine subsequent action in d02nd.

imon = -2

Integration is to be halted. A return will be made from the integrator to the calling (sub)program with **ifail** = 12.

imon = -1

Allow the integrator to continue with its own internal strategy. The integrator will try up to three restarts unless **imon** is set $\neq -1$ on exit.

imon = 0

Return to the internal nonlinear equation solver, where the action taken is determined by the value of **inln**.

imon = 1

Normal exit to the integrator to continue integration.

imon = 2

Restart the integration at the current time point. The integrator will restart from order 1 when this option is used. The **monitr** provided solution **y** will be used for the initial conditions.

imon = 3

Try to continue with the same step size and order as was to be used before the call to **monitr**. **hmin** and **hmax** may be altered if desired.

imon = 4

Continue the integration but using a new value of **hnext** and possibly new values of **hmin** and **hmax**.

12: hmin – double scalar

The minimum step size to be taken on the next step.

The minimum step size to be used. If this is different from the input value, then **imon** must be set to 3 or 4.

13: hmax – double scalar

The maximum step size to be taken on the next step.

The maximum step size to be used. If this is different from the input value, then **imon** must be set to 3 or 4. If **hmax** is set to zero, no limit is assumed.

14: nqu – int32 scalar

The order of the integrator used on the last step. This is supplied to enable you to carry out interpolation using either of the functions d02xj or d02xk.

Output Parameters

1: hnext – double scalar

The step size that the integrator proposes to take on the next step.

The next step size to be used. If this is different from the input value, then **imon** must be set to 4.

2: y(ldysav) - double array

y, the values of the dependent variables evaluated at t.

These values must not be changed unless **imon** is set to 2.

3: imon – int32 scalar

A flag indicating under what circumstances monitr was called.

imon = -2

Entry from the integrator after ires = 4 (set in the user-supplied (sub)program fcn) caused an early termination (this facility could be used to locate discontinuities).

imon = -1

The current step failed repeatedly.

imon = 0

Entry after a call to the internal nonlinear equation solver (see inln).

imon = 1

The current step was successful.

May be reset to determine subsequent action in d02nd.

imon = -2

Integration is to be halted. A return will be made from the integrator to the calling (sub)program with **ifail** = 12.

imon = -1

Allow the integrator to continue with its own internal strategy. The integrator will try up to three restarts unless **imon** is set $\neq -1$ on exit.

 $\mathbf{imon} = 0$

Return to the internal nonlinear equation solver, where the action taken is determined by the value of **inln**.

imon = 1

Normal exit to the integrator to continue integration.

imon = 2

Restart the integration at the current time point. The integrator will restart from order 1 when this option is used. The **monitr** provided solution **y** will be used for the initial conditions.

imon = 3

Try to continue with the same step size and order as was to be used before the call to **monitr**. **hmin** and **hmax** may be altered if desired.

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imon = 4

Continue the integration but using a new value of **hnext** and possibly new values of **hmin** and **hmax**.

4: inln – int32 scalar

The action to be taken by the internal nonlinear equation solver when **monitr** is exited with $\mathbf{imon} = 0$. By setting $\mathbf{inln} = 3$ and returning to the integrator, the residual vector is evaluated and placed in the array \mathbf{r} , and then **monitr** is called again. At present this is the only option available: \mathbf{inln} must not be set to any other value.

5: hmin – double scalar

The minimum step size to be taken on the next step.

The minimum step size to be used. If this is different from the input value, then **imon** must be set to 3 or 4.

6: hmax – double scalar

The maximum step size to be taken on the next step.

The maximum step size to be used. If this is different from the input value, then **imon** must be set to 3 or 4. If **hmax** is set to zero, no limit is assumed.

16: itask – int32 scalar

The task to be performed by the integrator.

itask = 1

Normal computation of output values of y(t) at t =tout (by overshooting and interpolating).

itask = 2

Take one step only and return.

itask = 3

Stop at the first internal integration point at or beyond t = tout and return.

itask = 4

Normal computation of output values of y(t) at $t = \mathbf{tout}$ but without overshooting $t = \mathbf{tcrit}$ (e.g., see d02mv). **tcrit** must be specified as an option in one of the integrator setup functions prior to the first call to the integrator, or specified in the optional input function prior to a continuation call. **tcrit** may be equal to or beyond **tout**, but not before it, in the direction of integration.

itask = 5

Take one step only and return, without passing **tcrit** (e.g., see d02mv). **tcrit** must be specified as under **itask** = 4.

Constraint: $1 \leq itask \leq 5$.

17: itrace – int32 scalar

The level of output that is printed by the integrator. **itrace** may take the value -1, 0, 1, 2 or 3.

itrace < -1

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

itrace = -1

No output is generated.

itrace = 0

Only warning messages are printed on the current error message unit (see x04aa).

itrace > 0

Warning messages are printed as above, and on the current advisory message unit (see x04ab) output is generated which details Jacobian entries, the nonlinear iteration and the time integration. The advisory messages are given in greater detail the larger the value of **itrace**.

5.2 Optional Input Parameters

1: sdysav – int32 scalar

Default: The second dimension of the array ysav.

An appropriate value for sdysav is described in the specifications of the integrator setup functions d02nv and d02nw. This value must be the same as that supplied to the integrator setup function.

2: nwkjac – int32 scalar

Default: The dimension of the array wkjac.

The actual size depends on whether the sparsity structure is supplied or whether it is to be estimated. An appropriate value for **nwkjac** is described in the specification of the linear algebra setup function d02nu. This value must be the same as that supplied to d02nu.

3: njcpvt – int32 scalar

Default: The dimension of the array jacpvt.

The actual size depends on whether the sparsity structure is supplied or whether it is to be estimated. An appropriate value for **njcpvt** is described in the specification of the linear algebra setup function d02nu. This value must be the same as that supplied to d02nu.

5.3 Input Parameters Omitted from the MATLAB Interface

ldysav

5.4 Output Parameters

1: t - double scalar

The value at which the computed solution y is returned (usually at **tout**).

2: y(ldysav) - double array

The computed solution vector, evaluated at t (usually $t = \mathbf{tout}$).

3: ydot(ldysav) – double array

The time derivatives y' of the vector y at the last integration point.

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- 4: $rwork(50 + 4 \times ldysav) double array$
- 5: inform(23) int32 array
- 6: ysav(ldysav,sdysav) double array
- 7: wkjac(nwkjac) double array
- 8: jacpvt(njcpvt) int32 array
- 9: ifail int32 scalar

0 unless the function detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail = 1

An illegal input was detected on entry, or after an internal call to (sub)program **monitr**. If **itrace** > -1, then the form of the error will be detailed on the current error message unit (see x04aa).

ifail = 2

The maximum number of steps specified has been taken (see the description of optional inputs in the integrator setup functions and the optional input continuation function, d02nz).

ifail = 3

With the given values of **rtol** and **atol** no further progress can be made across the integration range from the current point **t**. The components $y(1), y(2), \ldots, y(neq)$ contain the computed values of the solution at the current point **t**.

ifail = 4

There were repeated error test failures on an attempted step, before completing the requested task, but the integration was successful as far as **t**. The problem may have a singularity, or the local error requirements may be inappropriate.

ifail = 5

There were repeated convergence test failures on an attempted step, before completing the requested task, but the integration was successful as far as t. This may be caused by an inaccurate Jacobian matrix or one which is incorrectly computed.

ifail = 6

Some error weight w_i became zero during the integration (see the description of **itol**). Pure relative error control (**atol**(i) = 0.0) was requested on a variable (the ith) which has now vanished. The integration was successful as far as **t**.

ifail = 7

The user-supplied (sub)program fcn set its error flag (ires = 3) continually despite repeated attempts by the integrator to avoid this.

ifail = 8

Not used for the integrator.

ifail = 9

A singular Jacobian $\frac{\partial r}{\partial y}$ has been encountered. This error exit is unlikely to be taken when solving explicit ordinary differential equations. You should check the problem formulation and Jacobian calculation.

ifail = 10

An error occurred during Jacobian formulation or back-substitution (a more detailed error description may be directed to the current error message unit, see x04aa).

ifail = 11

The user-supplied (sub)program **fcn** signalled the integrator to halt the integration and return (**ires** = 2). Integration was successful as far as \mathbf{t} .

ifail = 12

The (sub)program **monitr** set **imon** = -2 and so forced a return but the integration was successful as far as t.

ifail = 13

The requested task has been completed, but it is estimated that a small change in **rtol** and **atol** 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 = 14

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

ifail = 15

The linear algebra setup function d02nu was not called prior to calling d02nd.

7 Accuracy

The accuracy of the numerical solution may be controlled by a careful choice of the parameters **rtol** and **atol**, and to a much lesser extent by the choice of norm. You are advised to use scalar error control unless the components of the solution are expected to be poorly scaled. For the type of decaying solution typical of many stiff problems, relative error control with a small absolute error threshold will be most appropriate (that is, you are advised to choose **itol** = 1 with **atol**(1) small but positive).

8 Further Comments

Since numerical stability and memory are often conflicting requirements when solving ordinary differential systems where the Jacobian matrix is sparse, we provide a diagnostic function, d02nx, whose aim is to inform you how much memory is required to solve the problem and to give you some indication of numerical stability.

In general, you are advised to choose the backward differentiation formula option (setup function d02nv) but if efficiency is of great importance and especially if it is suspected that $\frac{\partial g}{\partial y}$ has complex eigenvalues near the imaginary axis for some part of the integration, you should try the BLEND option (setup function d02nw).

9 Example

d02nd_fcn.m

d02nd.12 [NP3663/21]

```
function [f, ires] = fcn(neq, t, y, ires)
    f = zeros(3,1);
    f(1) = -0.04d0*y(1) + 1.0d4*y(2)*y(3);
    f(2) = 0.04d0*y(1) - 1.0d4*y(2)*y(3) - 3.0d7*y(2)*y(2);
    f(3) = 3.0d7*y(2)*y(2);
```

```
d02nd_jac.m

function p = jac(neq, t, y, h, d)
    p = zeros(neq, neq);
    hxd = h*d;
    p(1,1) = 1.0d0 - hxd*(-0.04d0);
    p(1,2) = -hxd*(1.0d4*y(3));
    p(1,3) = -hxd*(1.0d4*y(2));
    p(2,1) = -hxd*(0.04d0);
    p(2,2) = 1.0d0 - hxd*(-1.0d4*y(3)-6.0d7*y(2));
    p(2,3) = -hxd*(-1.0d4*y(2));
    p(3,2) = -hxd*(6.0d7*y(2));
    p(3,3) = 1.0d0 - hxd*(0.0d0);
```

```
d02nd_monitr.m

function [hnext, y, imon, inln, hmin, hmax] = ...
    monitr(neq, neqmax, t, hlast, hnext, y, ydot, ysave, r, acor, imon, hmin, hmax, nqu)
    inln=int32(0);
```

```
neq = int32(3);
t = 0;
tout = 10;
y = [1;
     0;
     0];
rwork = zeros(62,1);
rtol = [0.0001];
atol = [1e-07];
itol = int32(1);
inform = zeros(23, 1, 'int32');
ysave = zeros(3, 6);
wkjac = zeros(100, 1);
itask = int32(1);
itrace = int32(0);
[const, rwork, ifail] = ...
   d02nv(int32(3), int32(6), int32(5), 'Newton', false, zeros(6), ...
    0, 1e-10, 10, 0, int32(200), int32(5), 'Average-L2', rwork);
int32(0), ..
   int32(150), 0, 0.1, 1e-4, true, rwork);
[tOut, yOut, ydot, rworkOut, informOut, ysaveOut, wkjacOut, jacpvtOut,
ifail] = ...
    d02nd(neq, t, tout, y, rwork, rtol, atol, itol, inform, ...
'd02nd_fcn', ysave, 'd02nd_jac', wkjac, jacpvt, 'd02nd_monitr', ...
    itask, itrace)
tOut =
   10
yOut =
   0.8414
    0.0000
    0.1586
ydot =
   -0.0075
   -0.0000
    0.0075
```

```
rworkOut =
   array elided
informOut =
       55
       136
        16
        4
        4
        78
        0
         3
        0
       100
       150
        29
        71
        16
        7
         3
        73
      1108
         1
         0
         0
         0
         0
ysaveOut =
   0.8355 -0.0067
                          -0.0000
                  0.0002
                                   0.0000
                                           -0.0000
   0.0000 -0.0000
                 0.0000
                          -0.0000
                                  0.0000
                                          -0.0000
   0.0000
wkjacOut =
array elided
jacpvtOut =
   array elided
ifail =
         0
```

d02nd.14 (last) [NP3663/21]