NAG Toolbox

nag_ode_ivp_rkts_onestep (d02pf)

1 Purpose

nag_ode_ivp_rkts_onestep (d02pf) is a one-step function for solving an initial value problem for a first-order system of ordinary differential equations using Runge–Kutta methods.

2 Syntax

```
[tnow, ynow, ypnow, user, iwsav, rwsav, ifail] = nag_ode_ivp_rkts_onestep(f, n, iwsav, rwsav, 'user', user)
[tnow, ynow, ypnow, user, iwsav, rwsav, ifail] = d02pf(f, n, iwsav, rwsav, 'user', user)
```

3 Description

nag_ode_ivp_rkts_onestep (d02pf) and its associated functions (nag_ode_ivp_rkts_setup (d02pq), nag_ode_ivp_rkts_reset_tend (d02pr), nag_ode_ivp_rkts_interp (d02ps), nag_ode_ivp_rkts_diag (d02pt) and nag_ode_ivp_rkts_errass (d02pu)) solve an initial value problem for a first-order system of ordinary differential equations. The functions, based on Runge–Kutta methods and derived from RKSUITE (see Brankin *et al.* (1991)), integrate

$$y' = f(t, y) \quad \text{given} \quad y(t_0) = y_0$$

where y is the vector of n solution components and t is the independent variable.

nag_ode_ivp_rkts_onestep (d02pf) is designed to be used in complicated tasks when solving systems of ordinary differential equations. You must first call nag_ode_ivp_rkts_setup (d02pq) to specify the problem and how it is to be solved. Thereafter you (repeatedly) call nag_ode_ivp_rkts_onestep (d02pf) to take one integration step at a time from **tstart** in the direction of **tend** (as specified in nag_ode_ivp_rkts_setup (d02pq)). In this manner nag_ode_ivp_rkts_onestep (d02pf) returns an approximation to the solution **ynow** and its derivative **ypnow** at successive points **tnow**. If nag_ode_ivp_rkts_onestep (d02pf) encounters some difficulty in taking a step, the integration is not advanced and the function returns with the same values of **tnow**, **ynow** and **ypnow** as returned on the previous successful step. nag_ode_ivp_rkts_onestep (d02pf) tries to advance the integration as far as possible subject to passing the test on the local error and not going past **tend**.

In the call to nag_ode_ivp_rkts_setup (d02pq) you can specify either the first step size for nag_ode_ivp_rkts_onestep (d02pf) to attempt or that it computes automatically an appropriate value. Thereafter nag_ode_ivp_rkts_onestep (d02pf) estimates an appropriate step size for its next step. This value and other details of the integration can be obtained after any call to nag_ode_ivp_rkts_onestep (d02pf) by a call to nag_ode_ivp_rkts_diag (d02pt). The local error is controlled at every step as specified in nag_ode_ivp_rkts_setup (d02pq). If you wish to assess the true error, you must set **method** to a positive value in the call to nag_ode_ivp_rkts_setup (d02pq). This assessment can be obtained after any call to nag_ode_ivp_rkts_onestep (d02pf) by a call to nag_ode_ivp_rkts_errass (d02pu).

If you want answers at specific points there are two ways to proceed:

(i) The more efficient way is to step past the point where a solution is desired, and then call nag_ode_ivp_rkts_interp (d02ps) to get an answer there. Within the span of the current step, you can get all the answers you want at very little cost by repeated calls to nag_ode_ivp_rkts_interp (d02ps). This is very valuable when you want to find where something happens, e.g., where a particular solution component vanishes. You cannot proceed in this way with **method** $= 3$ or -3.

(ii) The other way to get an answer at a specific point is to set **tend** to this value and integrate to **tend**. nag_ode_ivp_rkts_onestep (d02pf) will not step past **tend**, so when a step would carry it past, it will reduce the step size so as to produce an answer at **tend** exactly. After getting an answer there

(**tnow** = **tend**), you can reset **tend** to the next point where you want an answer, and repeat. **tend** could be reset by a call to nag_ode_ivp_rkts_setup (d02pq), but you should not do this. You should use nag_ode_ivp_rkts_reset_tend (d02pr) instead because it is both easier to use and much more efficient. This way of getting answers at specific points can be used with any of the available methods, but it is the only way with **method** = 3 or −3. It can be inefficient. Should this be the case, the code will bring the matter to your attention.

4 References

Brankin R W, Gladwell I and Shampine L F (1991) RKSUITE: A suite of Runge–Kutta codes for the initial value problems for ODEs *SoftReport 91-S1* Southern Methodist University

5 Parameters

5.1 Compulsory Input Parameters

1: **f** – SUBROUTINE, supplied by the user.

f must evaluate the functions f_i (that is the first derivatives y_i') for given values of the arguments t, y_i.

```
[yp, user] = f(t, n, y, user)
```

Input Parameters

1: **t** – REAL (KIND=nag_wp)

t, the current value of the independent variable.

2: **n** – INTEGER

n, the number of ordinary differential equations in the system to be solved.

3: **y**(**n**) – REAL (KIND=nag_wp) array

The current values of the dependent variables, y_i, for $i = 1, 2, \ldots, n$.

4: **user** – INTEGER array

f is called from nag_ode_ivp_rkts_onestep (d02pf) with the object supplied to nag_ode_ivp_rkts_onestep (d02pf).

Output Parameters

1: **yp**(**n**) – REAL (KIND=nag_wp) array

The values of f_i, for $i = 1, 2, \ldots, n$.

2: **user** – INTEGER array

2: **n** – INTEGER

n, the number of ordinary differential equations in the system to be solved.

Constraint: **n** ≥ 1.

3: **iwsav**(**130**) – INTEGER array

4: **rwsav**(**32** × **n** + **350**) – REAL (KIND=nag_wp) array

These must be the same arrays supplied in a previous call to nag_ode_ivp_rkts_setup (d02pq). They must remain unchanged between calls.

5.2 Optional Input Parameters

1: **user** – INTEGER array

user is not used by nag_ode_ivp_rkts_onestep (d02pf), but is passed to **f**. Note that for large objects it may be more efficient to use a global variable which is accessible from the m-files than to use **user**.

5.3 Output Parameters

1: **tnow** – REAL (KIND=nag_wp)

t, the value of the independent variable at which a solution has been computed.

2: **ynow**(**n**) – REAL (KIND=nag_wp) array

An approximation to the solution at **tnow**. The local error of the step to **tnow** was no greater than permitted by the specified tolerances (see nag_ode_ivp_rkts_setup (d02pq)).

3: **ypnow**(**n**) – REAL (KIND=nag_wp) array

An approximation to the first derivative of the solution at **tnow**.

4: **user** – INTEGER array

5: **iwsav**(**130**) – INTEGER array

6: **rwsav**(**32** × **n** + **350**) – REAL (KIND=nag_wp) array

Information about the integration for use on subsequent calls to nag_ode_ivp_rkts_onestep (d02pf) or other associated functions.

7: **ifail** – INTEGER

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

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail = 1

A call to this function cannot be made after it has returned an error.
The setup function must be called to start another problem.

On entry, **n** = ⟨*value*⟩, but the value passed to the setup function was .

On entry, the communication arrays have become corrupted, or a catastrophic error has already been detected elsewhere. You cannot continue integrating the problem.

tend, as specified in the setup function, has already been reached.
To start a new problem, you will need to call the setup function.
To continue integration beyond **tend** then
nag_ode_ivp_rkts_reset_tend (d02pr) must first be called to reset **tend** to a new end value.

ifail = 2 (*warning*)

More than 100 output points have been obtained by integrating to **tend** (as specified in the setup function). They have been so clustered that it would probably be (much) more efficient to use the interpolation function (if |**method**| = 3, switch to |**method**| = 2 at setup).
However, you can continue integrating the problem.

ifail $= 3$ (*warning*)

Approximately ⟨*value*⟩ function evaluations have been used to compute the solution since the integration started or since this message was last printed.
However, you can continue integrating the problem.

ifail $= 4$ (*warning*)

Approximately ⟨*value*⟩ function evaluations have been used to compute the solution since the integration started or since this message was last printed. Your problem has been diagnosed as stiff. If the situation persists, it will cost roughly ⟨*value*⟩ times as much to reach **tend** (setup) as it has cost to reach the current time. You should probably call functions intended for stiff problems. However, you can continue integrating the problem.

ifail $= 5$ (*warning*)

In order to satisfy your error requirements the solver has to use a step size of ⟨*value*⟩ at the current time, ⟨*value*⟩. This step size is too small for the ***machine precision***, and is smaller than ⟨*value*⟩.

ifail $= 6$ (*warning*)

The global error assessment algorithm failed at start of integration.
The integration is being terminated.

The global error assessment may not be reliable for times beyond ⟨*value*⟩.
The integration is being terminated.

ifail $= -99$

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

ifail $= -399$

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

ifail $= -999$

Dynamic memory allocation failed.

7 Accuracy

The accuracy of integration is determined by the arguments **tol** and **thresh** in a prior call to nag_ode_ivp_rkts_setup (d02pq) (see the function document for nag_ode_ivp_rkts_setup (d02pq) for further details and advice). Note that only the local error at each step is controlled by these arguments. The error estimates obtained are not strict bounds but are usually reliable over one step. Over a number of steps the overall error may accumulate in various ways, depending on the properties of the differential system.

8 Further Comments

If nag_ode_ivp_rkts_onestep (d02pf) returns with **ifail** $= 5$ and the accuracy specified by **tol** and **thresh** is really required then you should consider whether there is a more fundamental difficulty. For example, the solution may contain a singularity. In such a region the solution components will usually be large in magnitude. Successive output values of **ynow** should be monitored with the aim of trapping the solution before the singularity. In any case numerical integration cannot be continued through a singularity, and analytical treatment may be necessary.

Performance statistics are available after any return from nag_ode_ivp_rkts_onestep (d02pf) (except when **ifail** $= 1$) by a call to nag_ode_ivp_rkts_diag (d02pt). If **method** > 0 in the call to nag_ode_ivp_rkts_setup (d02pq), global error assessment is available after any return from nag_ode_ivp_rkts_onestep (d02pf) (except when **ifail** $= 1$) by a call to nag_ode_ivp_rkts_errass (d02pu).

After a failure with **ifail** $= 5$ or 6 each of the diagnostic functions nag_ode_ivp_rkts_diag (d02pt) and nag_ode_ivp_rkts_errass (d02pu) may be called only once.

If nag_ode_ivp_rkts_onestep (d02pf) returns with **ifail** $= 4$ then it is advisable to change to another code more suited to the solution of stiff problems. nag_ode_ivp_rkts_onestep (d02pf) will not return with **ifail** $= 4$ if the problem is actually stiff but it is estimated that integration can be completed using less function evaluations than already computed.

9 Example

This example solves the equation

$$y'' = -y, \quad y(0) = 0, \quad y'(0) = 1$$

reposed as

$$y_1' = y_2$$
$$y_2' = -y_1$$

over the range $[0, 2\pi]$ with initial conditions $y_1 = 0.0$ and $y_2 = 1.0$. We use relative error control with threshold values of 1.0e−8 for each solution component and print the solution at each integration step across the range. We use a medium order Runge–Kutta method (**method** $= 2$) with tolerances **tol** $=$ 1.0e−4 and **tol** $=$ 1.0e−5 in turn so that we may compare the solutions.

9.1 Program Text

```
     function d02pf_example

fprintf('d02pf example results\n\n');

% Set initial conditions and input
method = nag_int(2);
tstart = 0;
tend = 2*pi;
yinit = [0;1];
hstart = 0;
thresh = [1e-08; 1e-08];
n = nag_int(2);
tol0 =  1.0E-4;
ynow = zeros(20, n);
tnow = zeros(20, 1);
err1 = zeros(20, 2);
err2 = zeros(20, 2);

% Set control for output
tol = 10.0*tol0;

% Run through the calculation twice with two tolerance values
for i = 1:2

  tol = tol*0.1;

  % Call setup function
  [iwsav, rwsav, ifail] = d02pq(tstart, tend, yinit, tol, thresh, method);

  tnow(1) = tstart;
  ynow(1,:) = yinit;
  j=1;
  while tnow(j) < tend
    j=j+1;
    [tnow(j), ynow(j, :), ypnow, user, iwsav, rwsav, ifail] = ...
      d02pf(@f, n, iwsav, rwsav);

    err1(j, i) =  ynow(j, 1)-sin(tnow(j));
    err2(j, i) =  ynow(j, 2)-cos(tnow(j));

  end
```

```
  fprintf('\nCalculation with TOL = %8.1e:\n\n', tol);
  [fevals, stepcost, waste, stepsok, hnext, iwsav, ifail] = d02pt(iwsav, rwsav);
  fprintf('  Number of evaluations of f = %d\n', fevals);

  % Store the t values for use in plotting errors
  if i == 1
    tnow1 = tnow;
  end

  % Store value of j
  npts(i) = j;
end

% Plot results
fig1 = figure;
title({['First-order ODEs solution by single stepping'],...
          ['Medium-order Runge-Kutta Method, Two Tolerances']});
hold on;
axis([0 10 -1.2 1.2]);
xlabel('t');
ylabel('Solution (y, y'')');
plot(tnow(1:npts(2)), ynow(1:npts(2), 1), '-xr');
text(ceil(tnow(npts(2))), ynow(npts(2), 1), 'y', 'Color', 'r');
plot(tnow(1:npts(2)), ynow(1:npts(2), 2), '-xg');
text(ceil(tnow(npts(2))), ynow(npts(2), 2), 'y''', 'Color', 'g');
% Plot errors with a different (log) scale
ax1 = gca;
ax2 = axes('Position',get(ax1,'Position'),...
           'XAxisLocation','bottom','YAxisLocation','right',...
           'YScale','log','Color','none','XColor','k','YColor','k');
hold on;
axis([0 10 1e-9 1e-4]);
ylabel('abs(Error)');
plot(ax2, tnow1(1:npts(1)), abs(err1(1:npts(1), 1)), '-*b');
text(ceil(tnow1(npts(1))), err1(npts(1), 1) - 1e-5, ...
     'y-error (tol=0.001)', 'Color', 'b');
plot(ax2, tnow, abs(err1(:, 2)), '-sm');
text(ceil(tnow(npts(2))), err1(npts(2), 2), 'y-error (tol=0.0001)', ...
     'Color', 'm');

hold off;

function [yp, user] = f(t, n, y, user)
  yp = [y(2); -y(1)];
```

9.2 Program Results

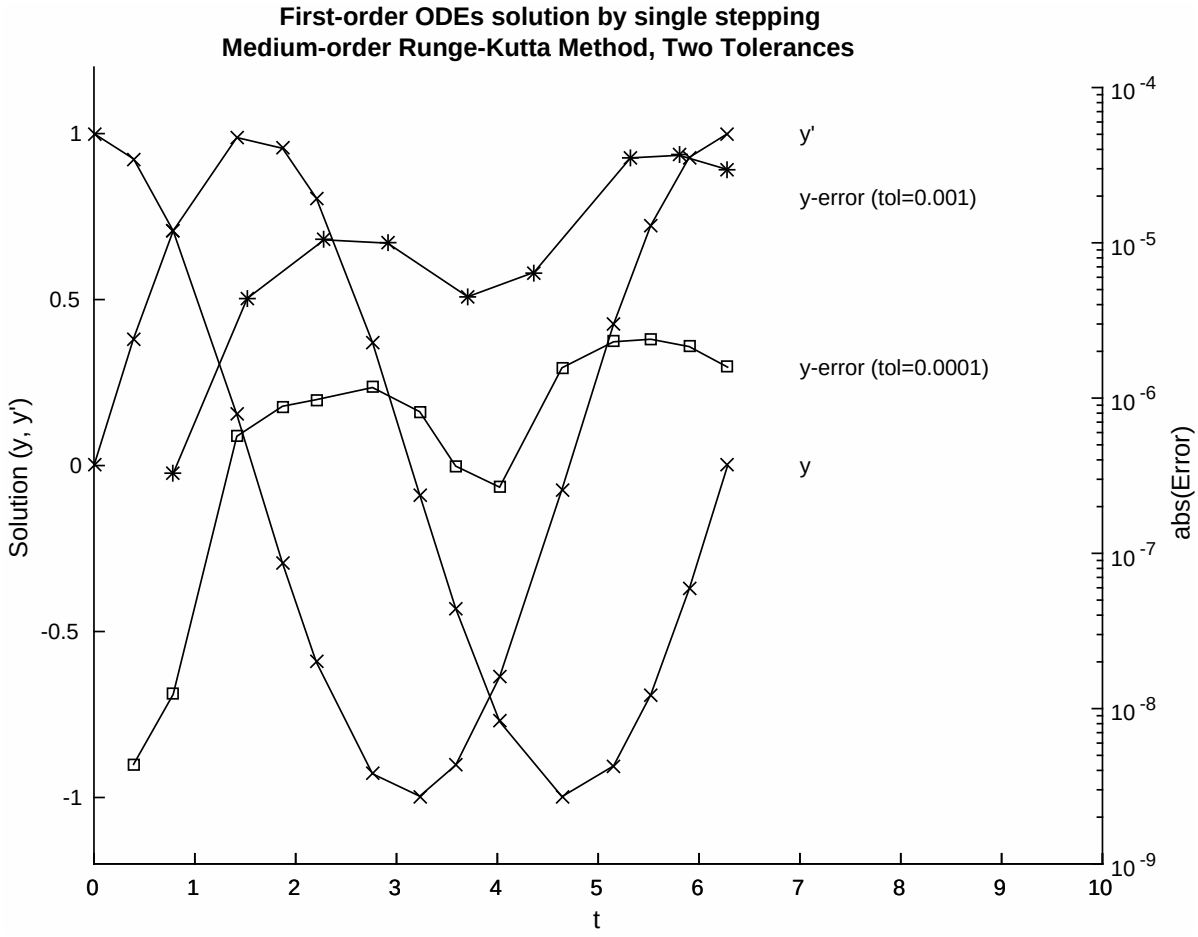
```
     d02pf example results

Calculation with TOL =  1.0e-04:

  Number of evaluations of f = 204

Calculation with TOL =  1.0e-05:

  Number of evaluations of f = 314
```


First-order ODEs solution by single stepping
Medium-order Runge-Kutta Method, Two Tolerances
Solution (y, y')
abs(Error)
t
y'
y-error (tol=0.001)
y-error (tol=0.0001)
y
1
0.5
0
-0.5
-1
0
1
2
3
4
5
6
7
8
9
10
10 -4
10 -5
10 -6
10 -7
10 -8
10 -9