NAG Library Function Document

nag_ode_ivp_rkts_reset_tend (d02prc)

1 Purpose

nag_ode_ivp_rkts_reset_tend (d02prc) resets the end point in an integration performed by nag_ode_ivp_rkts_onestep (d02pfc).

2 Specification

```
#include <nag.h>
#include <nagd02.h>
void nag_ode_ivp_rkts_reset_tend (double tendnu, Integer iwsav[],
     double rwsav[], NagError *fail)
```

3 Description

nag_ode_ivp_rkts_reset_tend (d02prc) and its associated functions (nag_ode_ivp_rkts_onestep (d02pfc), nag_ode_ivp_rkts_setup (d02pqc), nag_ode_ivp_rkts_interp (d02psc), nag_ode_ivp_rkts_diag (d02ptc) and nag_ode_ivp_rkts_errass (d02puc)) solve the 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_reset_tend (d02prc) is used to reset the final value of the independent variable, t_f, when the integration is already underway. It can be used to extend or reduce the range of integration. The new value must be beyond the current value of the independent variable (as returned in **tnow** by nag_ode_ivp_rkts_onestep (d02pfc)) in the current direction of integration. It is much more efficient to use nag_ode_ivp_rkts_reset_tend (d02prc) for this purpose than to use nag_ode_ivp_rkts_setup (d02pqc) which involves the overhead of a complete restart of the integration.

If you want to change the direction of integration then you must restart by a call to nag_ode_ivp_rkts_setup (d02pqc).

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 Arguments

1: **tendnu** – double *Input*

On entry: the new value for t_f.

Constraint: sign(**tendnu** − **tnow**) = sign(**tend** − **tstart**), where **tstart** and **tend** are as supplied in the previous call to nag_ode_ivp_rkts_setup (d02pqc) and **tnow** is returned by the preceding call to nag_ode_ivp_rkts_onestep (d02pfc) (i.e., integration must proceed in the same direction as before). **tendnu** must be distinguishable from **tnow** for the method and the ***machine precision*** being used.

2: **iwsav**[**130**] – Integer *Communication Array*
3: **rwsav**[**350**] – double *Communication Array*

Note: the communication array **rwsav** used by the other functions in the suite must be used here however, only the first 350 elements will be referenced.

On entry: these must be the same arrays supplied in a previous call to nag_ode_ivp_rkts_onestep (d02pfc). They must remain unchanged between calls.

On exit: information about the integration for use on subsequent calls to nag_ode_ivp_rkts_onestep (d02pfc) or other associated functions.

4: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE_BAD_PARAM

On entry, argument ⟨*value*⟩ had an illegal value.

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_MISSING_CALL

You cannot call this function before you have called the step integrator.

NE_PREV_CALL

On entry, a previous call to the setup function has not been made or the communication arrays have become corrupted, or a catastrophic error has already been detected elsewhere. You cannot continue integrating the problem.

NE_PREV_CALL_INI

You cannot call this function after the integrator has returned an error.

NE_RK_DIRECTION_NEG

On entry, **tendnu** is not beyond **tnow** (step integrator) in the direction of integration.
The direction is negative, **tendnu** = ⟨*value*⟩ and **tnow** = ⟨*value*⟩.

NE_RK_DIRECTION_POS

On entry, **tendnu** is not beyond **tnow** (step integrator) in the direction of integration.
The direction is positive, **tendnu** = ⟨*value*⟩ and **tnow** = ⟨*value*⟩.

NE_RK_INVALID_CALL

You cannot call this function when the range integrator has been used.

NE_RK_STEP

On entry, **tendnu** is too close to **tnow** (step integrator). Their difference is ⟨*value*⟩, but this quantity must be at least ⟨*value*⟩.

7 Accuracy

Not applicable.

8 Parallelism and Performance

Not applicable.

9 Further Comments

None.

10 Example

This example integrates a two body problem. The equations for the coordinates $(x(t), y(t))$ of one body as functions of time t in a suitable frame of reference are

$$x'' = -\frac{x}{r^3}$$

$$y'' = -\frac{y}{r^3}, \quad r = \sqrt{x^2 + y^2}.$$

The initial conditions

$$\begin{aligned} x(0) &= 1 - \epsilon, \quad & x'(0) &= 0 \\ y(0) &= 0, & y'(0) &= \sqrt{\frac{1+\epsilon}{1-\epsilon}} \end{aligned}$$

lead to elliptic motion with $0 < \epsilon < 1$. $\epsilon = 0.7$ is selected and the system of ODEs is reposed as

$$y_1' = y_3$$

$$y_2' = y_4$$

$$y_3' = -\frac{y_1}{r^3}$$

$$y_4' = -\frac{y_2}{r^3}$$

over the range $[0, 6\pi]$. Relative error control is used with threshold values of 1.0e−10 for each solution component and compute the solution at intervals of length π across the range using nag_ode_ivp_rkts_reset_tend (d02prc) to reset the end of the integration range. A high-order Runge–Kutta method (**method** = Nag_RK_7_8) is also used with tolerances **tol** = 1.0e−4 and **tol** = 1.0e−5 in turn so that the solutions may be compared.

10.1 Program Text

```
/* nag_ode_ivp_rkts_reset_tend (d02prc) Example Program.
 *
 * Copyright 2013 Numerical Algorithms Group.
 *
 * Mark 24, 2013.
 */
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagd02.h>

#ifdef __cplusplus
extern "C" {
#endif
static void NAG_CALL f(double  t, Integer  n, const double *y,
                       double *yp, Nag_Comm *comm);
#ifdef __cplusplus
}
#endif
```

```
#define N 4

int main(void)
{
  /* Scalars */
  double          tol0 = 1.0e-3;
  Integer         npts = 6, exit_status = 0;
  Integer         liwsav, lrwsav, n;
  double          hnext, hstart, tendnu, tfinal, tinc, tgot, tol, tstart,
                  waste;
  Integer         fevals, i, j, k, stepcost, stepsok;
  /* Arrays */
  static double ruser[1] = {-1.0};
  double          *rwsav = 0, *thresh = 0, *ygot = 0, *yinit = 0, *ypgot = 0;
  Integer         *iwsav = 0;
  char            nag_enum_arg[40];
  /* NAG types */
  NagError        fail;
  Nag_RK_method   method;
  Nag_ErrorAssess errass;
  Nag_Comm        comm;

  INIT_FAIL(fail);

  printf("nag_ode_ivp_rkts_reset_tend (d02prc) Example Program Results\n\n");

  /* For communication with user-supplied functions: */
  comm.user = ruser;

  n = N;
  liwsav = 130;
  lrwsav = 350 + 32 * n;
  if (
      !(thresh = NAG_ALLOC(n, double)) ||
      !(ygot = NAG_ALLOC(n, double)) ||
      !(yinit = NAG_ALLOC(n, double)) ||
      !(ypgot = NAG_ALLOC(n, double)) ||
      !(iwsav = NAG_ALLOC(liwsav, Integer)) ||
      !(rwsav = NAG_ALLOC(lrwsav, double))
    )
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }

  /* Skip heading in data file*/
  scanf("%*[^\n] ");

  /* Set initial conditions for ODE and parameters for the integrator. */
  scanf(" %39s%*[^\n] ", nag_enum_arg);
  /* nag_enum_name_to_value (x04nac) Converts NAG enum member name to value. */
  method = (Nag_RK_method) nag_enum_name_to_value(nag_enum_arg);
  scanf(" %39s%*[^\n] ", nag_enum_arg);
  errass = (Nag_ErrorAssess)  nag_enum_name_to_value(nag_enum_arg);
  scanf("%lf%lf%*[^\n] ", &tstart, &tfinal);

  for (j = 0; j < n; j++)
    scanf("%lf", &yinit[j]);
  scanf("%*[^\n] ");
  scanf("%lf%*[^\n] ", &hstart);
  for (j = 0; j < n; j++)
    scanf("%lf", &thresh[j]);
  scanf("%*[^\n] ");

  tinc = (tfinal - tstart)/(double) (npts);
  tol = tol0;
  for (i = 1; i <= 2; i++)
    {
      tol = tol * 0.1;
      tendnu = tstart + tinc;
```

```
/* Initialize Runge-Kutta method for integrating ODE using
 * nag_ode_ivp_rkts_setup (d02pqc).
 */
nag_ode_ivp_rkts_setup(n, tstart, tendnu, yinit, tol, thresh, method,
                       errass, hstart, iwsav, rwsav, &fail);
if (fail.code != NE_NOERROR)
  {
    printf("Error from nag_ode_ivp_rkts_setup (d02pqc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }

printf(" Calculation with tol = %8.1e\n", tol);
printf("    t         y1        y2        y3        y4\n");
printf("%6.3f", tstart);
for (k = 0; k < n; k++)
  printf("   %7.3f", yinit[k]);
printf("\n");

tgot = tstart;
while (tgot < tfinal)
  {
    /* Solve ODE by Runge-Kutta method by a sequence of single steps using
     * nag_ode_ivp_rkts_onestep (d02pfc).
     */
    nag_ode_ivp_rkts_onestep(f, n, &tgot, ygot, ypgot, &comm,
                             iwsav, rwsav, &fail);
    if (fail.code != NE_NOERROR)
      {
        printf("Error from nag_ode_ivp_rkts_onestep (d02pfc).\n%s\n",
               fail.message);
        exit_status = 2;
        goto END;
      }

    /* When incremental stage in t has been reached:
     * print solution and reset end time for next stage.
     */
    if (tgot == tendnu)
      {
        printf("%6.3f", tgot);
        for (k = 0; k < n; k++)
          printf("   %7.3f", ygot[k]);
        printf("\n");

        /* Reset end-time for integration by adding increment tinc using
         * nag_ode_ivp_rkts_reset_tend (d02prc): resets end of range for
         * nag_ode_ivp_rkts_onestep (d02pfc).
         */
        tendnu = tendnu + tinc;
        nag_ode_ivp_rkts_reset_tend(tendnu, iwsav, rwsav, &fail);
        if (fail.code != NE_NOERROR)
          {
            printf(
              "Error from nag_ode_ivp_rkts_reset_tend (d02prc).\n%s\n",
              fail.message);
            exit_status = 3;
            goto END;
          }
      }
  }
/* Get diagnostics on whole integration using
 * nag_ode_ivp_rkts_diag (d02ptc).
 */
nag_ode_ivp_rkts_diag(&fevals, &stepcost, &waste, &stepsok, &hnext,
                      iwsav, rwsav, &fail);
if (fail.code != NE_NOERROR)
  {
    printf("Error from nag_ode_ivp_rkts_diag (d02ptc).\n%s\n",
           fail.message);
          exit_status = 4;
          goto END;
        }
      printf("Cost of the integration in evaluations of f is %6ld\n\n",
             fevals);
    }
 END:
  NAG_FREE(thresh);
  NAG_FREE(yinit);
  NAG_FREE(ygot);
  NAG_FREE(ypgot);
  NAG_FREE(rwsav);
  NAG_FREE(iwsav);
  return exit_status;
}

static void NAG_CALL f(double t, Integer n, const double *y, double *yp,
                       Nag_Comm *comm)
{
  /* Scalars */
  double r;

  if (comm->user[0] == -1.0)
    {
      printf("(User-supplied callback f, first invocation.)\n");
      comm->user[0] = 0.0;
    }
  r = sqrt(y[0]*y[0] + y[1]*y[1]);
  yp[0] = y[2];
  yp[1] = y[3];
  yp[2] = -y[0]/ pow(r, 3);
  yp[3] = -y[1]/ pow(r, 3);
}
```

10.2 Program Data

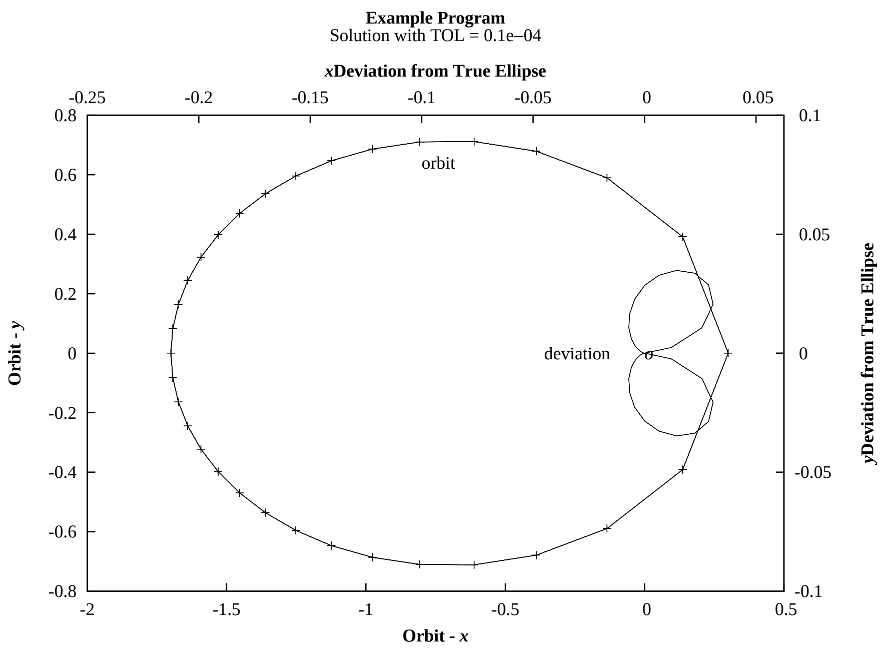
```
nag_ode_ivp_rkts_reset_tend (d02prc) Example Program Data
   Nag_RK_7_8                                            : method
   Nag_ErrorAssess_off                                   : errass
   0.0                       18.8495559215387594307     : tstart, tfinal
   0.3      0.0      0.0      2.38047614284761666599    : yinit
   0.0                                                   : hstart
   1.0E-10  1.0E-10  1.0E-10  1.0E-10                   : thresh
```

10.3 Program Results

```
nag_ode_ivp_rkts_reset_tend (d02prc) Example Program Results

 Calculation with tol =  1.0e-04
    t         y1        y2        y3        y4
 0.000     0.300     0.000     0.000     2.380
(User-supplied callback f, first invocation.)
 3.142    -1.700     0.000    -0.000    -0.420
 6.283     0.300    -0.000     0.000     2.380
 9.425    -1.700     0.000    -0.000    -0.420
12.566     0.300    -0.000     0.002     2.380
15.708    -1.700     0.000    -0.000    -0.420
18.850     0.300    -0.001     0.004     2.380
Cost of the integration in evaluations of f is    571

 Calculation with tol =  1.0e-05
    t         y1        y2        y3        y4
 0.000     0.300     0.000     0.000     2.380
 3.142    -1.700    -0.000     0.000    -0.420
 6.283     0.300     0.000    -0.000     2.380
 9.425    -1.700     0.000    -0.000    -0.420
12.566     0.300    -0.000     0.000     2.380
15.708    -1.700     0.000    -0.000    -0.420
18.850     0.300    -0.000     0.001     2.380
Cost of the integration in evaluations of f is    748
```


Example Program
Solution with TOL = 0.1e–04
xDeviation from True Ellipse
-0.25
-0.2
-0.15
-0.1
-0.05
0
0.05
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0.1
0.05
0
-0.05
-0.1
orbit
deviation
Orbit - y
yDeviation from True Ellipse
-2
-1.5
-1
-0.5
0
0.5
Orbit - x