

## 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) and nag\_ode\_ivp\_rk\_step\_revcomm (d02pgc).

#### 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\_rk\_step\_revcomm (d02pgc), nag\_ode\_ivp\_rk\_interp\_setup (d02phc), nag\_ode\_ivp\_rk\_in\_interp\_eval (d02pj), 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) or nag\_ode\_ivp\_rk\_step\_revcomm (d02pgc)) 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:*  $\text{sign}(\mathbf{tendnu} - \mathbf{tnow}) = \text{sign}(\mathbf{tend} - \mathbf{tstart})$ , 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) or nag\_ode\_ivp\_rk\_step\_revcomm (d02pgc) (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) or `nag_ode_ivp_rk_step_revcomm` (d02pgc). 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 `nag_ode_ivp_rk_step_revcomm` (d02pgc) or other associated functions.

- 4: **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\_ALLOC\_FAIL

Dynamic memory allocation failed.

See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

### 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.

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

See Section 2.7.6 in How to Use the NAG Library and its Documentation for further information.

### NE\_MISSING\_CALL

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

### NE\_NO\_LICENCE

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

See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

### 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** =  $\langle value \rangle$  and **tnow** =  $\langle value \rangle$ .

**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  $\langle value \rangle$ , but this quantity must be at least  $\langle value \rangle$ .

**7 Accuracy**

Not applicable.

**8 Parallelism and Performance**

nag\_ode\_ivp\_rkts\_reset\_tend (d02prc) is not threaded in any implementation.

**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

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

The initial conditions

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

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

$$\begin{aligned}y'_1 &= y_3 \\y'_2 &= y_4 \\y'_3 &= -\frac{y_1}{r^3} \\y'_4 &= -\frac{y_2}{r^3}\end{aligned}$$

over the range  $[0, 6\pi]$ . Relative error control is used with threshold values of  $1.0\text{e}-10$  for each solution component and compute the solution at intervals of length  $\pi$  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** =  $1.0\text{e}-4$  and **tol** =  $1.0\text{e}-5$  in turn so that the solutions may be compared.

## 10.1 Program Text

```

/* nag_ode_ivp_rkts_reset_tend (d02prc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */
#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 */
#ifdef _WIN32

```

```

    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif

    /* Set initial conditions for ODE and parameters for the integrator. */

#ifdef _WIN32
    scanf_s(" %39s%*[\n] ", nag_enum_arg, (unsigned)_countof(nag_enum_arg));
#else
    scanf(" %39s%*[\n] ", nag_enum_arg);
#endif
    /* 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);

#ifdef _WIN32
    scanf_s(" %39s%*[\n] ", nag_enum_arg, (unsigned)_countof(nag_enum_arg));
#else
    scanf(" %39s%*[\n] ", nag_enum_arg);
#endif
    errass = (Nag_ErrorAssess) nag_enum_name_to_value(nag_enum_arg);

#ifdef _WIN32
    scanf_s("%lf%lf%*[\n] ", &tstart, &tfinal);
#else
    scanf("%lf%lf%*[\n] ", &tstart, &tfinal);
#endif

    for (j = 0; j < n; j++)
#ifdef _WIN32
        scanf_s("%lf", &yinit[j]);
#else
        scanf("%lf", &yinit[j]);
#endif
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif

#ifdef _WIN32
    scanf_s("%lf%*[\n] ", &hstart);
#else
    scanf("%lf%*[\n] ", &hstart);
#endif
    for (j = 0; j < n; j++)
#ifdef _WIN32
        scanf_s("%lf", &thresh[j]);
#else
        scanf("%lf", &thresh[j]);
#endif
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif

    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 %6" NAG_IFMT
      "\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

