nag_ode_ivp_rk_interp (d02pxc)

1. Purpose

nag_ode_ivp_rk_interp (d02pxc) is a function to compute the solution of a system of ordinary differential equations using interpolation anywhere on an integration step taken by nag_ode_ivp_rk_onestep (d02pdc).

2. Specification

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

void nag_ode_ivp_rk_interp(Integer neq, double twant, Nag_SolDeriv request, Integer
nwant,

double ywant[], double ypwant[], void (*f) (Integer neq, double t, double y[], double yp[], Nag_User *comm), Nag_ODE_RK *opt, Nag_User *comm, NagError *fail)

3. Description

This function and its associated functions (nag_ode_ivp_rk_setup (d02pvc), nag_ode_ivp_rk_onestep (d02pdc), nag_ode_ivp_rk_reset_tend (d02pwc), nag_ode_ivp_rk_errass (d02pzc)) 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 (Brankin *et al*, 1991) integrate

y' = f(t, y) given $y(t_0) = y_0$

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

nag_ode_ivp_rk_onestep (d02pdc) computes the solution at the end of an integration step. Using the information computed on that step nag_ode_ivp_rk_interp computes the solution by interpolation at any point on that step. It cannot be used if **method** = **Nag_RK_7_8** was specified in the call to set-up function nag_ode_ivp_rk_setup (d02pvc).

4. Parameters

neq

Input: the number of ordinary differential equations in the system. Constraint: $\mathbf{neq} \geq 1.$

twant

Input: the value of the independent variable, t, where a solution is desired.

request

Input: determines whether the solution and/or its first derivative are computed as follows:

 $request = Nag_Sol$ - compute approximate solution only

 $\mathbf{request} = \mathbf{Nag_Der}$ - compute approximate first derivative of the solution only

 $request = Nag_SolDer$ - compute both approximate solution and first derivative.

Constraint: request = Nag_Sol or Nag_Der or Nag_SolDer.

nwant

Input: the number of components of the solution to be computed. The first **nwant** components are evaluated.

Constraint: $1 \leq$ **nwant** \leq **neq**.

ywant[nwant]

Output: an approximation to the first **nwant** components of the solution at **twant** when specified by **request**.

ypwant[nwant]

Output: an approximation to the first **nwant** components of the first derivative of the solution at **twant** when specified by **request**.

f

This function must evaluate the functions f_i (that is the first derivatives y'_i) for given values of the arguments t, y_i . It must be the same procedure as supplied to nag_ode_ivp_rk_onestep (d02pdc).

void f (Integer neq, double t, double y[], double yp[], Nag_User *comm) nea Input: the number of differential equations. \mathbf{t} Input: the current value of the independent variable, t. y[neq] Input: the current values of the dependent variables, y_i for i = 1, 2, ..., neq. yp[neq] Output: the values of f_i for $i = 1, 2, \ldots,$ neq. comm Input/Output: pointer to a structure of type Nag-User with the following member: **p** - Pointer Input/Output: 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.)

opt

Input: the structure of type Nag_ODE_RK as output from nag_ode_ivp_rk_onestep (d02pdc). This structure must not be changed by the user.

Output: some members of **opt** are changed internally.

comm

Input/Output: pointer to a structure of type Nag_User with the following member:

p - Pointer

Input/Output: the pointer \mathbf{p} , of type Pointer, allows the user to communicate information to and from the user-defined function $\mathbf{f}()$. An object of the required type should be declared by the user, e.g. a structure, and its address assigned to the pointer \mathbf{p} by means of a cast to Pointer in the calling program, e.g. comm. $\mathbf{p} = (Pointer)\&s$. The type pointer will be void * with a C compiler that defines void * and char * otherwise.

fail

The NAG error parameter, see the Essential Introduction to the NAG C Library.

5. Error Indications and Warnings

NE_PREV_CALL

The previous call to a function had resulted in a severe error. You must call nag_ode_ivp_rk_setup (d02pvc) to start another problem.

NE_RK_INVALID_CALL

The function to be called as specified in the setup function nag_ode_ivp_rk_setup (d02pvc) was nag_ode_ivp_rk_range (d02pcc). However the actual call was made to nag_ode_ivp_rk_interp. This is not permitted.

NE_MISSING_CALL

Previous call to nag_ode_ivp_rk_onestep (d02pdc) has not been made, hence nag_ode_ivp_rk_interp must not be called.

NE_PREV_CALL_INI

The previous call to the function nag_ode_ivp_rk_onestep (d02pdc) resulted in a severe error. You must call nag_ode_ivp_rk_setup (d02pvc) to start another problem.

NE_NEQ

The value of neq supplied is not the same as that given to the setup function nag_ode_ivp_rk_setup (d02pvc). neq = $\langle value \rangle$ but the value given to nag_ode_ivp_rk_setup (d02pvc) was $\langle value \rangle$.

NE_BAD_PARAM

On entry parameter **request** had an illegal value.

NE_2_INT_ARG_GT

On entry $nwant = \langle value \rangle$ while $neq = \langle value \rangle$. These parameters must satisfy $neq \leq nwant$. INT ABC IT

NE_INT_ARG_LT

On entry, **nwant** must not be less than 1: **nwant** = $\langle value \rangle$.

NE_ALLOC_FAIL

Memory allocation failed.

NE_RK_PX_METHOD

Interpolation is not available with **method** = **Nag_RK_7_8**. Either use **method** = **Nag_RK_2_3** or **Nag_RK_4_5** for which interpolation is available. Alternatively use nag_ode_ivp_rk_reset_tend (d02pwc) to make nag_ode_ivp_rk_onestep (d02pdc) step exactly to the points where you want output.

NE_MEMORY_FREED

Internally allocated memory has been freed by a call to nag_ode_ivp_rk_free (d02ppc) without a subsequent call to the set up function nag_ode_ivp_rk_setup (d02pvc).

6. Further Comments

None.

6.1. Accuracy

The computed values will be of a similar accuracy to that computed by nag_ode_ivp_rk_onestep (d02pdc).

6.2. References

Brankin R W, Gladwell I and Shampine L F (1991) RKSUITE: a suite of Runge-Kutta codes for the initial value problem for ODEs SoftReport 91-S1, Department of Mathematics, Southern Methodist University, Dallas, TX 75275, U.S.A.

7. See Also

nag_ode_ivp_rk_onestep (d02pdc) nag_ode_ivp_rk_setup (d02pvc) nag_ode_ivp_rk_reset_tend (d02pwc) nag_ode_ivp_rk_errass (d02pzc)

8. Example

We solve the equation

y'' = -y, y(0) = 0, 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. nag_ode_ivp_rk_onestep (d02pdc) is used to integrate the problem one step at a time and nag_ode_ivp_rk_interp is used to compute the first component of the solution and its derivative at intervals of length $\pi/8$ across the range whenever these points lie in one of those integration steps. We use a moderate order Runge-Kutta method (**method = Nag_RK_4.5**) with tolerances **tol =** 1.0e-3 and **tol =** 1.0e-4 in turn so that we may compare the solutions. The value of π is obtained by using X01AAC.

```
8.1. Program Text
```

```
/* nag_ode_ivp_rk_interp(d02pxc) Example Program
 * Copyright 1994 Numerical Algorithms Group.
 * Mark 3, 1994.
 */
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nagd02.h>
#include <nagx01.h>
#ifdef NAG_PROTO
static void f(Integer neq, double t1, double y[], double yp[], Nag_User *comm);
#else
static void f();
#endif
#define NEQ 2
#define NWANT 1
#define ZERO 0.0
#define ONE 1.0
#define TWO 2.0
#define FOUR 4.0
main()
ſ
  Integer neq, nwant;
  double hstart, pi, tnow, tend, tol, tstart, tinc, twant;
  Integer i, j, nout;
double thres[NEQ], ynow[NEQ], ypnow[NEQ], ystart[NEQ], ywant[NWANT];
  double ypwant[NWANT];
  Nag_RK_method method;
  Nag_ErrorAssess errass;
  Nag_ODE_RK opt;
  Nag_User comm;
  Vprintf("d02pxc Example Program Results\n");
  /* Set initial conditions and input for d02pvc */
  neq = NEQ;
  method = Nag_RK_4_5;
  pi = X01AAC;
  tstart = ZERO;
  ystart[0] = ZERO;
  ystart[1] = ONE;
  tend = TWO*pi;
  for (i=0; i<neq; i++)</pre>
   thres[i] = 1.0e-8;
  errass = Nag_ErrorAssess_off;
 hstart = ZERO;
  /*
   * Set control for output
   */
  nwant = NWANT;
  nout = 16;
  tinc = tend/nout;
  for (i=1; i<=2; i++)</pre>
    Ł
      if (i==1) tol = 1.0e-3;
      if (i==2) tol = 1.0e-4;
      d02pvc(neq, tstart, ystart, tend, tol, thres, method,
             Nag_RK_onestep, errass, hstart, &opt, NAGERR_DEFAULT);
```

```
Vprintf("\nCalculation with tol = %8.1e\n\n",tol);
           Vprintf ("
                                                  y2\n\n");
                         t
                                     y1
                                        %8.4f\n", tstart, ystart[0], ystart[1]);
           Vprintf("%8.3f
                              %8.4f
           j = nout - 1;
           twant = tend - j*tinc;
           do
             {
               d02pdc(neq, f, &tnow, ynow, ypnow, &opt, &comm, NAGERR_DEFAULT);
               while (twant<=tnow)
                 {
                   d02pxc(neq, twant, Nag_SolDer, nwant, ywant, ypwant, f,
                          &opt, &comm, NAGERR_DEFAULT);
                   Vprintf("%8.3f
                                      %8.4f
                                                %8.4f\n'', twant, ywant[0],
                   ypwant[0]);
j = j - 1;
                   twant = tend - j*tinc;
                 }
             } while (tnow<tend);</pre>
           Vprintf("\nCost of the integration in evaluations of f is %ld\n\n",
                   opt.totfcn);
           d02ppc(&opt);
         }
       exit(EXIT_SUCCESS);
     }
     #ifdef NAG_PROTO
     static void f(Integer neq, double t, double y[], double yp[], Nag_User *comm)
     #else
          static void f(neq, t, y, yp, comm)
          Integer neq;
          double t;
          double y[], yp[];
          Nag_User *comm;
     #endif
     {
       yp[0] = y[1];
      yp[1] = -y[0];
8.2. Program Data
     None.
8.3. Program Results
     d02pxc Example Program Results
     Calculation with tol = 1.0e-03
         t
                    y1
                                 y2
        0.000
                   0.0000
                                1.0000
                   0.3827
        0.393
                                0.9239
        0.785
                   0.7071
                                0.7071
                   0.9239
        1.178
                                0.3826
        1.571
                   1.0000
                                -0.0001
        1.963
                   0.9238
                               -0.3828
        2.356
                   0.7070
                               -0.7073
       2.749
                  0.3825
                               -0.9240
        3.142
                  -0.0002
                               -0.9999
                  -0.3829
                               -0.9238
        3.534
       3.927
                  -0.7072
                               -0.7069
        4.320
                  -0.9239
                               -0.3823
       4.712
                  -0.9999
                                0.0004
       5.105
                  -0.9236
                                0.3830
       5.498
                  -0.7068
                                0.7073
        5.890
                  -0.3823
                                0.9239
                  0.0004
        6.283
                                0.9998
```

Cost of the integration in evaluations of f is $68\,$

Calculation with tol = 1.0e-04

| t | y1 | y2 |
|-------|---------|---------|
| t | y1 | y2 |
| 0.000 | 0.0000 | 1.0000 |
| 0.393 | 0.3827 | 0.9239 |
| 0.785 | 0.7071 | 0.7071 |
| 1.178 | 0.9239 | 0.3827 |
| 1.571 | 1.0000 | 0.0000 |
| 1.963 | 0.9239 | -0.3827 |
| 2.356 | 0.7071 | -0.7071 |
| 2.749 | 0.3827 | -0.9239 |
| 3.142 | 0.0000 | -1.0000 |
| 3.534 | -0.3827 | -0.9239 |
| 3.927 | -0.7071 | -0.7071 |
| 4.320 | -0.9239 | -0.3827 |
| 4.712 | -1.0000 | 0.0000 |
| 5.105 | -0.9238 | 0.3827 |
| 5.498 | -0.7071 | 0.7071 |
| 5.890 | -0.3826 | 0.9239 |
| 6.283 | 0.0000 | 1.0000 |
| 0.200 | 0.0000 | 1.0000 |

Cost of the integration in evaluations of f is $105\,$