

## NAG Library Function Document

### nag\_ode\_ivp\_adams\_interp (d02qzc)

## 1 Purpose

nag\_ode\_ivp\_adams\_interp (d02qzc) interpolates components of the solution of a non-stiff system of first order ordinary differential equations from information provided by nag\_ode\_ivp\_adams\_roots (d02qfc). Normally this function will be used in conjunction with the integration function, nag\_ode\_ivp\_adams\_roots (d02qfc), operating in one-step mode.

## 2 Specification

```
#include <nag.h>
#include <nagd02.h>
void nag_ode_ivp_adams_interp (Integer neqf, double twant, Integer nwant,
                               double ywant[], double ypwant[], Nag_ODE_Adams *opt, NagError *fail)
```

## 3 Description

nag\_ode\_ivp\_adams\_interp (d02qzc) evaluates the first **nwant** components of the solution of a non-stiff system of first order ordinary differential equations at any point using the method of Watts and Shampine (1986) and information generated by nag\_ode\_ivp\_adams\_roots (d02qfc). nag\_ode\_ivp\_adams\_interp (d02qzc) should not normally be used to extrapolate outside the current range of the values produced by the integration function.

## 4 References

Watts H A and Shampine L F (1986) Smoother interpolants for Adams codes *SIAM J. Sci. Statist. Comput.* 7 334–345

## 5 Arguments

- |    |  |              |
|----|--|--------------|
| 1: | <b>neqf</b> – Integer  | <i>Input</i> |
|    | <i>On entry</i> : the number of differential equations.  |              |
|    | <i>Constraint</i> : <b>neqf</b> $\geq 1$ .   |              |
| 2: | <b>twant</b> – double  | <i>Input</i> |
|    | <i>On entry</i> : the point at which components of the solution and derivative are to be evaluated. <b>twant</b> should not normally be an extrapolation point, that is <b>twant</b> should satisfy<br>$\mathbf{opt}\rightarrow\mathbf{tcurr} - \mathbf{opt}\rightarrow\mathbf{hlast} \leq \mathbf{twant} \leq \mathbf{opt}\rightarrow\mathbf{tcurr}$ .<br>or if integration is proceeding in the negative direction<br>$\mathbf{opt}\rightarrow\mathbf{tcurr} - \mathbf{opt}\rightarrow\mathbf{hlast} \geq \mathbf{twant} \geq \mathbf{opt}\rightarrow\mathbf{tcurr}$ . |              |
|    | Extrapolation is permitted but not recommended and a <b>fail</b> value of NW_EXTRAPOLATION is returned whenever extrapolation is attempted.  |              |
| 3: | <b>nwant</b> – Integer   | <i>Input</i> |
|    | <i>On entry</i> : the number of components of the solution and derivative whose values, at <b>twant</b> , are required. The first <b>nwant</b> components are evaluated.   |              |
|    | <i>Constraint</i> : $1 \leq \mathbf{nwant} \leq \mathbf{neqf}$ .   |              |

4:	<b>ywant[nwant]</b> – double	<i>Output</i>
<i>On exit: ywant[i – 1] contains the calculated value of the <math>i</math>th component of the solution at <b>twant</b>, for <math>i = 1, 2, \dots, \text{nwant}</math>.</i>		
5:	<b>ypwant[nwant]</b> – double	<i>Output</i>
<i>On exit: ypwant[i – 1] contains the calculated value of the <math>i</math>th component of the derivative at <b>twant</b>, for <math>i = 1, 2, \dots, \text{nwant}</math>.</i>		
6:	<b>opt</b> – Nag_ODE_Adams *	<i>Input</i>
<i>On entry: the structure of type Nag_ODE_Adams as output from the integration function nag_ode_ivp_adams_roots (d02qfc). The structure <b>must</b> be passed unchanged. (See Section 9 for comments about deallocation of memory from <b>opt</b>.)</i>		
7:	<b>fail</b> – NagError *	<i>Input/Output</i>
<i>The NAG error argument (see Section 3.6 in the Essential Introduction).</i>		

## 6 Error Indicators and Warnings

### NE\_INT\_ARG\_LT

On entry, **nwant** =  $\langle\text{value}\rangle$ .  
Constraint: **nwant**  $\geq 1$ .

### NE\_NEQF

The value of **neqf** supplied is not the same as that given to the setup function nag\_ode\_ivp\_adams\_setup (d02qwc). **neqf** =  $\langle\text{value}\rangle$  but the value given to nag\_ode\_ivp\_adams\_setup (d02qwc) was  $\langle\text{value}\rangle$ .

### NE\_NO\_INTEGRATE

The integrator function nag\_ode\_ivp\_adams\_roots (d02qfc) has not been called.

### NE\_NO\_STEPS

No successful integration steps were taken in the call(s) to the integration function nag\_ode\_ivp\_adams\_roots (d02qfc).

### NE\_NWANT\_GT

**nwant** is greater than the value of **neqf** given to the setup function nag\_ode\_ivp\_adams\_setup (d02qwc). **nwant** =  $\langle\text{value}\rangle$ , **neqf** =  $\langle\text{value}\rangle$ .

### NW\_EXTRAPOLATION

Extrapolation requested, **twant** =  $\langle\text{value}\rangle$ .

## 7 Accuracy

The error in interpolation is of a similar order to the error arising from the integration. The same order of accuracy can be expected when extrapolating using nag\_ode\_ivp\_adams\_interp (d02qzc). However, the actual error in extrapolation will, in general, be much larger than for interpolation.

## 8 Parallelism and Performance

Not applicable.

## 9 Further Comments

When interpolation for only a few components is required then it is more efficient to order the components of interest so that they are numbered first.

The structure **opt** will contain pointers which have been allocated memory during a call to nag\_ode\_ivp\_adams\_setup (d02qwc). This allocated memory is used by nag\_ode\_ivp\_adams\_roots (d02qfc) and nag\_ode\_ivp\_adams\_interp (d02qzc). When all calls to these functions have been completed the function nag\_ode\_ivp\_adams\_free (d02qyc) may be called to free the allocated memory from the structure.

## 10 Example

This example solves the equation

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

reposed as

$$\begin{aligned} y'_1 &= y_2 \\ y'_2 &= -y_1 \end{aligned}$$

over the range  $[0, \pi/2]$  with initial conditions  $y_1 = 0$  and  $y_2 = 1$  using vector error control (**vectol** = Nag\_TRUE) and nag\_ode\_ivp\_adams\_roots (d02qfc) in one-step mode (**one\_step** = Nag\_TRUE). nag\_ode\_ivp\_adams\_interp (d02qzc) is used to provide solution values at intervals of  $\pi/16$ .

### 10.1 Program Text

```
/* nag_ode_ivp_adams_interp (d02qzc) Example Program.
*
* Copyright 1991 Numerical Algorithms Group.
*
* Mark 2, 1991.
* Mark 6 revised, 2000.
* Mark 7 revised, 2001.
* Mark 8 revised, 2004.
*/
#include <nag.h>
#include <stdio.h>
#include <nag_stlib.h>
#include <nagd02.h>
#include <nagx01.h>

#ifndef __cplusplus
extern "C" {
#endif
static void NAG_CALL ftry03(Integer neqf, double x, const double y[],
                           double yp[], Nag_User *comm);
#ifndef __cplusplus
}
#endif

#define NEQF    2
#define TSTART 0.0

int main(void)
{
    static Integer use_comm[1] = {1};
    Nag_Boolean alter_g, crit, one_step, sophist, vectol;
    Integer exit_status = 0, i, j, max_step, neqf, neqg, nwant;
    NagError fail;
    Nag_ODE_Adams opt;
    Nag_Start state;
    Nag_User comm;
```

```

double      *atol = 0, hmax, pi, *rtol = 0, t, tcrit, tinc, tout, twant,
*y = 0;
double      *ypwant = 0, *ywant = 0;

INIT_FAIL(fail);

printf("nag_ode_ivp_adams_interp (d02qzc) Example Program Results\n");

/* For communication with user-supplied functions: */
comm.p = (Pointer)

/* nag_pi (x01aac).
 * pi
 */
pi = nag_pi;
state = Nag_NewStart;
neqf = NEQF;
if (neqf >= 1)
{
    if (!(atol = NAG_ALLOC(neqf, double)) ||
        !(rtol = NAG_ALLOC(neqf, double)) ||
        !(y = NAG_ALLOC(neqf, double)) ||
        !(ywant = NAG_ALLOC(neqf, double)) ||
        !(ypwant = NAG_ALLOC(neqf, double)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
}
else
{
    exit_status = 1;
    return exit_status;
}

neqq = 0;
sophist = Nag_FALSE;
vectol = Nag_TRUE;
for (i = 0; i < 2; ++i)
{
    atol[i] = 1e-08;
    rtol[i] = 0.0001;
}
one_step = Nag_TRUE;
crit = Nag_TRUE;
tinc = pi * 0.0625;
tcrit = tinc * 8.0;
tout = tcrit;
max_step = 500;
hmax = 2.0;
t = TSTART;
twant = TSTART + tinc;
nwant = 2;
y[0] = 0.0;
y[1] = 1.0;
printf("\n   T       Y(1)      Y(2)\n");
printf(" %6.4f  %7.4f %7.4f \n", t, y[0], y[1]);

/* nag_ode_ivp_adams_setup (d02qwc).
 * Setup function for nag_ode_ivp_adams_roots (d02qfc)
 */
nag_ode_ivp_adams_setup(&state, neqf, vectol, atol, rtol, one_step, crit,
                       tcrit, hmax, max_step, neqq, &alter_g, sophist, &opt,
                       &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_ode_ivp_adams_setup (d02qwc).%s\n",
           fail.message);
    exit_status = 1;
}

```

```

        goto END;
    }

j = 1;

while (t < tout && fail.code == NE_NOERROR)
{
    /* nag_ode_ivp_adams_roots (d02qfc).
     * Ordinary differential equation solver using Adams method
     * (sophisticated use)
     */
    nag_ode_ivp_adams_roots(neqf, ftry03, &t, y, tout, NULLDFN,
                            &comm, &opt, &fail);
    if (fail.code != NE_NOERROR)
    {
        printf("Error from nag_ode_ivp_adams_roots (d02qfc).\n%s\n",
               fail.message);
        exit_status = 1;
        goto END;
    }

    while (twant <= t && fail.code == NE_NOERROR)
    {
        /* nag_ode_ivp_adams_interp (d02qzc).
         * Interpolation function for use with
         * nag_ode_ivp_adams_roots (d02qfc)
         */
        nag_ode_ivp_adams_interp(neqf, twant, nwant, ywant, ypwant, &opt,
                                &fail);
        if (fail.code != NE_NOERROR)
        {
            printf(
                "Error from nag_ode_ivp_adams_interp (d02qzc).\n%s\n",
                fail.message);
            exit_status = 1;
            goto END;
        }

        printf(" %6.4f    %7.4f %7.4f  \n", twant, ywant[0], ywant[1]);
        ++j;
        twant = (double) j*tinc + 0.0;
    }
}

/* Free the memory which was allocated by
 * nag_ode_ivp_adams_setup (d02qwc) to the pointers inside opt.
 */
/* nag_ode_ivp_adams_free (d02qyc).
 * Freeing function for use with nag_ode_ivp_adams_roots
 * (d02qfc)
 */
nag_ode_ivp_adams_free(&opt);

END:
NAG_FREE(atol);
NAG_FREE(rtol);
NAG_FREE(y);
NAG_FREE(ywant);
NAG_FREE(ypwant);
return exit_status;
}

static void NAG_CALL ftry03(Integer neqf, double x, const double y[], double
                           yp[], Nag_User *comm)
{
    Integer *use_comm = (Integer *)comm->p;

    if (use_comm[0])
    {
        printf("(User-supplied callback ftry03, first invocation.)\n");
        use_comm[0] = 0;
    }
}

```

```
    }  
    yp[0] = y[1];  
    yp[1] = -y[0];  
} /* ftry03 */
```

## 10.2 Program Data

None.

### 10.3 Program Results

```
nag_ode_ivp_adams_interp (d02qzc) Example Program Results
```

T	Y(1)	Y(2)
0.0000	0.0000	1.0000
(User-supplied callback ftry03, first invocation.)		
0.1963	0.1951	0.9808
0.3927	0.3827	0.9239
0.5890	0.5556	0.8315
0.7854	0.7071	0.7071
0.9817	0.8315	0.5556
1.1781	0.9239	0.3827
1.3744	0.9808	0.1951
1.5708	1.0000	-0.0000

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