

## 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>$\mathbf{opt}\rightarrow\mathbf{tcurr} - \mathbf{opt}\rightarrow\mathbf{hlast} \leq \mathbf{twant} \leq \mathbf{opt}\rightarrow\mathbf{tcurr}.$ |              |
|    | 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> [ $i - 1$ ] contains the calculated value of the $i$ th component of the solution at <b>twant</b> , for $i = 1, 2, \dots, \text{nwant}$ .  |                               |                     |
| 5:   | <b>ypwant[nwant]</b> – double | <i>Output</i>       |
| <i>On exit: ypwant</i> [ $i - 1$ ] contains the calculated value of the $i$ th component of the derivative at <b>twant</b> , for $i = 1, 2, \dots, \text{nwant}$ .   |                               |                     |
| 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 must be passed unchanged. (See Section 9 for comments about deallocation of memory from opt.)</i> |                               |                     |
| 7:   | <b>fail</b> – NagError *      | <i>Input/Output</i> |
| The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).  |                               |                     |

## 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

nag\_ode\_ivp\_adams\_interp (d02qzc) is not threaded in any implementation.

## 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.
*
* NAGPRODCODE Version.
*
* Copyright 2016 Numerical Algorithms Group.
*
* Mark 26, 2016.
*/
#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, neqq, 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) &use_comm;

/* 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).\\n%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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