

## Chapter 16. Integration of Ordinary Differential Equations

### 16.0 Introduction

Problems involving ordinary differential equations (ODEs) can always be reduced to the study of sets of first-order differential equations. For example the second-order equation

$$\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x) \quad (16.0.1)$$

can be rewritten as two first-order equations

$$\begin{aligned} \frac{dy}{dx} &= z(x) \\ \frac{dz}{dx} &= r(x) - q(x)z(x) \end{aligned} \quad (16.0.2)$$

where  $z$  is a new variable. This exemplifies the procedure for an arbitrary ODE. The usual choice for the new variables is to let them be just derivatives of each other (and of the original variable). Occasionally, it is useful to incorporate into their definition some other factors in the equation, or some powers of the independent variable, for the purpose of mitigating singular behavior that could result in overflows or increased roundoff error. Let common sense be your guide: If you find that the original variables are smooth in a solution, while your auxiliary variables are doing crazy things, then figure out why and choose different auxiliary variables.

The generic problem in ordinary differential equations is thus reduced to the study of a set of  $N$  coupled *first-order* differential equations for the functions  $y_i$ ,  $i = 1, 2, \dots, N$ , having the general form

$$\frac{dy_i(x)}{dx} = f_i(x, y_1, \dots, y_N), \quad i = 1, \dots, N \quad (16.0.3)$$

where the functions  $f_i$  on the right-hand side are known.

A problem involving ODEs is not completely specified by its equations. Even more crucial in determining how to attack the problem numerically is the nature of the problem's boundary conditions. Boundary conditions are algebraic conditions on the values of the functions  $y_i$  in (16.0.3). In general they can be satisfied at

discrete specified points, but do not hold between those points, i.e., are not preserved automatically by the differential equations. Boundary conditions can be as simple as requiring that certain variables have certain numerical values, or as complicated as a set of nonlinear algebraic equations among the variables.

Usually, it is the nature of the boundary conditions that determines which numerical methods will be feasible. Boundary conditions divide into two broad categories.

- In *initial value problems* all the  $y_i$  are given at some starting value  $x_s$ , and it is desired to find the  $y_i$ 's at some final point  $x_f$ , or at some discrete list of points (for example, at tabulated intervals).
- In *two-point boundary value problems*, on the other hand, boundary conditions are specified at more than one  $x$ . Typically, some of the conditions will be specified at  $x_s$  and the remainder at  $x_f$ .

This chapter will consider exclusively the initial value problem, deferring two-point boundary value problems, which are generally more difficult, to Chapter 17.

The underlying idea of any routine for solving the initial value problem is always this: Rewrite the  $dy$ 's and  $dx$ 's in (16.0.3) as finite steps  $\Delta y$  and  $\Delta x$ , and multiply the equations by  $\Delta x$ . This gives algebraic formulas for the change in the functions when the independent variable  $x$  is "stepped" by one "stepsize"  $\Delta x$ . In the limit of making the stepsize very small, a good approximation to the underlying differential equation is achieved. Literal implementation of this procedure results in *Euler's method* (16.1.1, below), which is, however, *not* recommended for any practical use. Euler's method is conceptually important, however; one way or another, practical methods all come down to this same idea: Add small increments to your functions corresponding to derivatives (right-hand sides of the equations) multiplied by stepsizes.

In this chapter we consider three major types of practical numerical methods for solving initial value problems for ODEs:

- Runge-Kutta methods
- Richardson extrapolation and its particular implementation as the Bulirsch-Stoer method
- predictor-corrector methods.

A brief description of each of these types follows.

1. *Runge-Kutta* methods propagate a solution over an interval by combining the information from several Euler-style steps (each involving one evaluation of the right-hand  $f$ 's), and then using the information obtained to match a Taylor series expansion up to some higher order.

2. *Richardson extrapolation* uses the powerful idea of extrapolating a computed result to the value that *would* have been obtained if the stepsize had been very much smaller than it actually was. In particular, extrapolation to zero stepsize is the desired goal. The first practical ODE integrator that implemented this idea was developed by Bulirsch and Stoer, and so extrapolation methods are often called Bulirsch-Stoer methods.

3. *Predictor-corrector* methods store the solution along the way, and use those results to extrapolate the solution one step advanced; they then correct the extrapolation using derivative information at the new point. These are best for very smooth functions.

Runge-Kutta is what you use when (i) you don't know any better, or (ii) you have an intransigent problem where Bulirsch-Stoer is failing, or (iii) you have a trivial

problem where computational efficiency is of no concern. Runge-Kutta succeeds virtually always; but it is not usually fastest, except when evaluating  $f_i$  is cheap and moderate accuracy ( $\lesssim 10^{-5}$ ) is required. Predictor-corrector methods, since they use past information, are somewhat more difficult to start up, but, for many smooth problems, they are computationally more efficient than Runge-Kutta. In recent years Bulirsch-Stoer has been replacing predictor-corrector in many applications, but it is too soon to say that predictor-corrector is dominated in all cases. However, it appears that only rather sophisticated predictor-corrector routines are competitive. Accordingly, we have chosen *not* to give an implementation of predictor-corrector in this book. We discuss predictor-corrector further in §16.7, so that you can use a canned routine should you encounter a suitable problem. In our experience, the relatively simple Runge-Kutta and Bulirsch-Stoer routines we give are adequate for most problems.

Each of the three types of methods can be organized to monitor internal consistency. This allows numerical errors which are inevitably introduced into the solution to be controlled by automatic, (*adaptive*) changing of the fundamental stepsize. We always recommend that adaptive stepsize control be implemented, and we will do so below.

In general, all three types of methods can be applied to any initial value problem. Each comes with its own set of debits and credits that must be understood before it is used.

We have organized the routines in this chapter into three nested levels. The lowest or “nitty-gritty” level is the piece we call the *algorithm* routine. This implements the basic formulas of the method, starts with dependent variables  $y_i$  at  $x$ , and returns new values of the dependent variables at the value  $x + h$ . The algorithm routine also yields up some information about the quality of the solution after the step. The routine is dumb, however, and it is unable to make any adaptive decision about whether the solution is of acceptable quality or not.

That quality-control decision we encode in a *stepper* routine. The stepper routine calls the algorithm routine. It may reject the result, set a smaller stepsize, and call the algorithm routine again, until compatibility with a predetermined accuracy criterion has been achieved. The stepper’s fundamental task is to take the largest stepsize consistent with specified performance. Only when this is accomplished does the true power of an algorithm come to light.

Above the stepper is the *driver* routine, which starts and stops the integration, stores intermediate results, and generally acts as an interface with the user. There is nothing at all canonical about our driver routines. You should consider them to be examples, and you can customize them for your particular application.

Of the routines that follow, `rk4`, `rkck`, `mmid`, `stoerm`, and `simpr` are algorithm routines; `rkqs`, `bsstep`, `stiff`, and `stifbs` are steppers; `rkdumb` and `odeint` are drivers.

Section 16.6 of this chapter treats the subject of *stiff equations*, relevant both to ordinary differential equations and also to partial differential equations (Chapter 19).

#### CITED REFERENCES AND FURTHER READING:

- Gear, C.W. 1971, *Numerical Initial Value Problems in Ordinary Differential Equations* (Englewood Cliffs, NJ: Prentice-Hall).
- Acton, F.S. 1970, *Numerical Methods That Work*; 1990, corrected edition (Washington: Mathematical Association of America), Chapter 5.
- Stoer, J., and Bulirsch, R. 1980, *Introduction to Numerical Analysis* (New York: Springer-Verlag), Chapter 7.
- Lambert, J. 1973, *Computational Methods in Ordinary Differential Equations* (New York: Wiley).
- Lapidus, L., and Seinfeld, J. 1971, *Numerical Solution of Ordinary Differential Equations* (New York: Academic Press).

## 16.1 Runge-Kutta Method

The formula for the Euler method is

$$y_{n+1} = y_n + hf(x_n, y_n) \quad (16.1.1)$$

which advances a solution from  $x_n$  to  $x_{n+1} \equiv x_n + h$ . The formula is unsymmetrical: It advances the solution through an interval  $h$ , but uses derivative information only at the beginning of that interval (see Figure 16.1.1). That means (and you can verify by expansion in power series) that the step’s error is only one power of  $h$  smaller than the correction, i.e.  $O(h^2)$  added to (16.1.1).

There are several reasons that Euler’s method is not recommended for practical use, among them, (i) the method is not very accurate when compared to other, fancier, methods run at the equivalent stepsize, and (ii) neither is it very stable (see §16.6 below).

Consider, however, the use of a step like (16.1.1) to take a “trial” step to the midpoint of the interval. Then use the value of both  $x$  and  $y$  at that midpoint to compute the “real” step across the whole interval. Figure 16.1.2 illustrates the idea. In equations,

$$\begin{aligned} k_1 &= hf(x_n, y_n) \\ k_2 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right) \\ y_{n+1} &= y_n + k_2 + O(h^3) \end{aligned} \quad (16.1.2)$$

As indicated in the error term, this symmetrization cancels out the first-order error term, making the method *second order*. [A method is conventionally called  $n$ th order if its error term is  $O(h^{n+1})$ .] In fact, (16.1.2) is called the *second-order Runge-Kutta* or *midpoint* method.

We needn’t stop there. There are many ways to evaluate the right-hand side  $f(x, y)$  that all agree to first order, but that have different coefficients of higher-order error terms. Adding up the right combination of these, we can eliminate the error terms order by order. That is the basic idea of the Runge-Kutta method. Abramowitz and Stegun [1], and Gear [2], give various specific formulas that derive from this basic

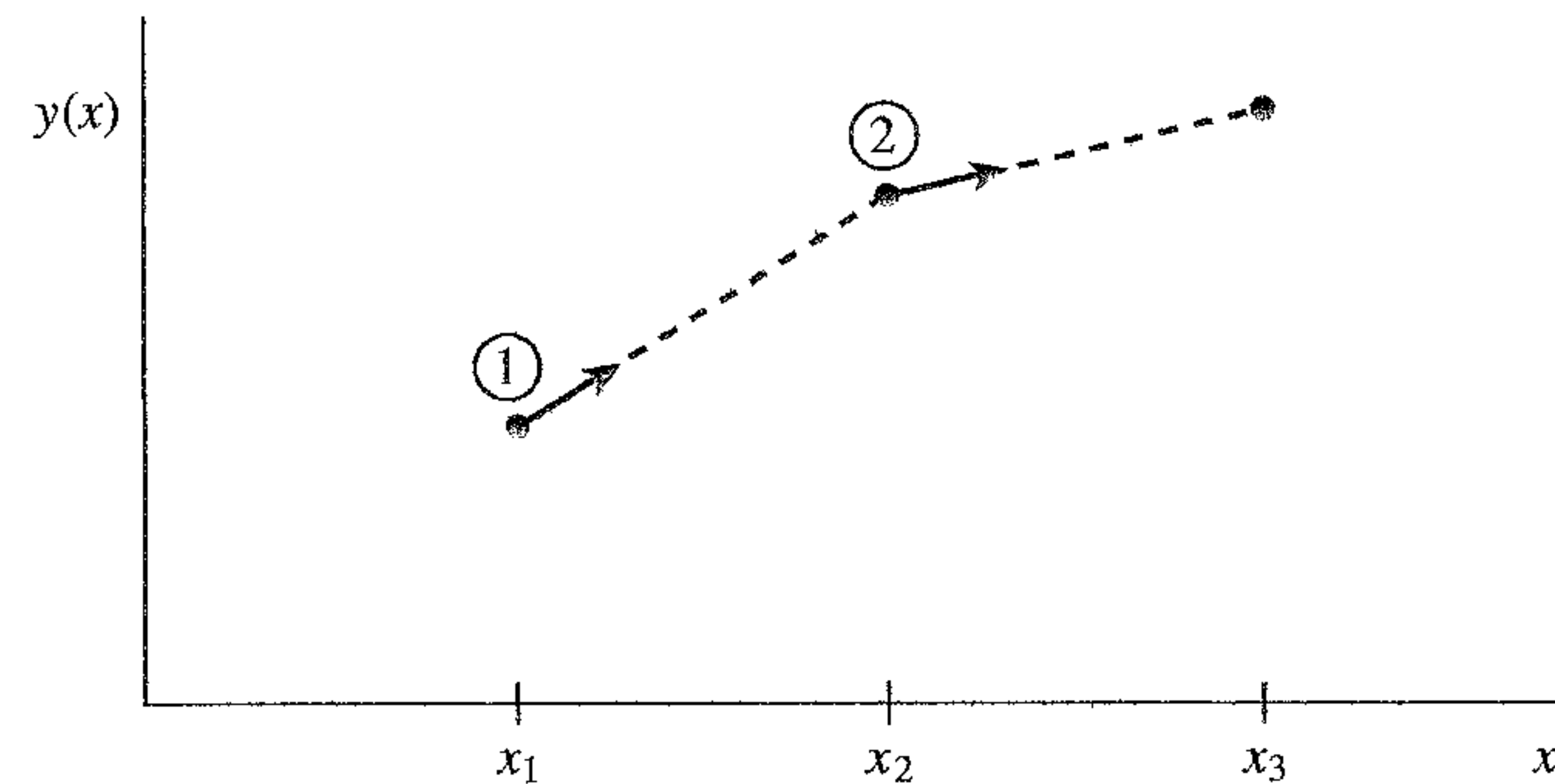


Figure 16.1.1. Euler's method. In this simplest (and least accurate) method for integrating an ODE, the derivative at the starting point of each interval is extrapolated to find the next function value. The method has first-order accuracy.

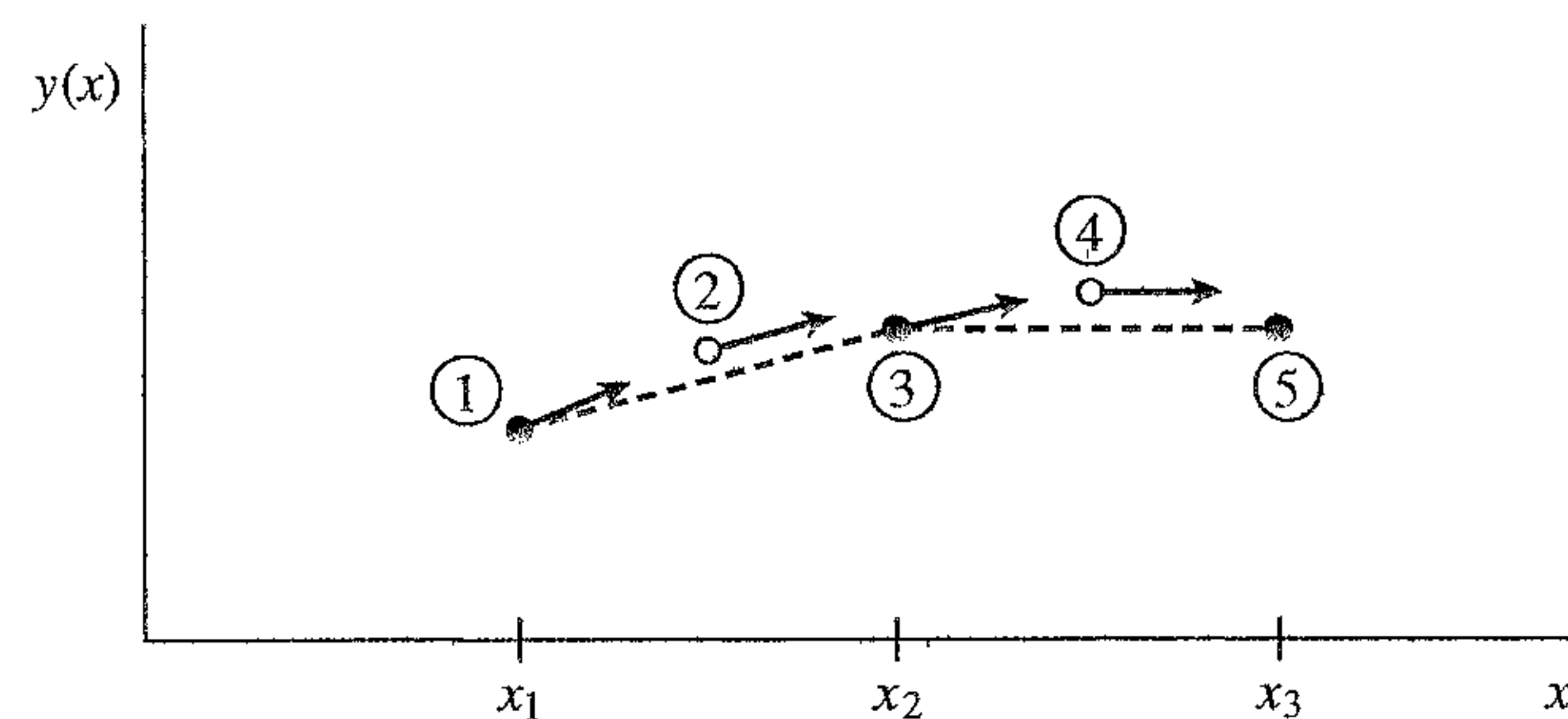


Figure 16.1.2. Midpoint method. Second-order accuracy is obtained by using the initial derivative at each step to find a point halfway across the interval, then using the midpoint derivative across the full width of the interval. In the figure, filled dots represent final function values, while open dots represent function values that are discarded once their derivatives have been calculated and used.

idea. By far the most often used is the classical *fourth-order Runge-Kutta formula*, which has a certain sleekness of organization about it:

$$\begin{aligned}
 k_1 &= hf(x_n, y_n) \\
 k_2 &= hf\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right) \\
 k_3 &= hf\left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right) \\
 k_4 &= hf(x_n + h, y_n + k_3) \\
 y_{n+1} &= y_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} + O(h^5)
 \end{aligned} \tag{16.1.3}$$

The fourth-order Runge-Kutta method requires four evaluations of the right-hand side per step  $h$  (see Figure 16.1.3). This will be superior to the midpoint method (16.1.2) if at least twice as large a step is possible with (16.1.3) for the same accuracy. Is that so? The answer is: often, perhaps even usually, but surely not always! This takes us back to a central theme, namely that *high order* does not always mean *high accuracy*. The statement "fourth-order Runge-Kutta is generally superior to second-order" is a true one, but you should recognize it as a statement about the

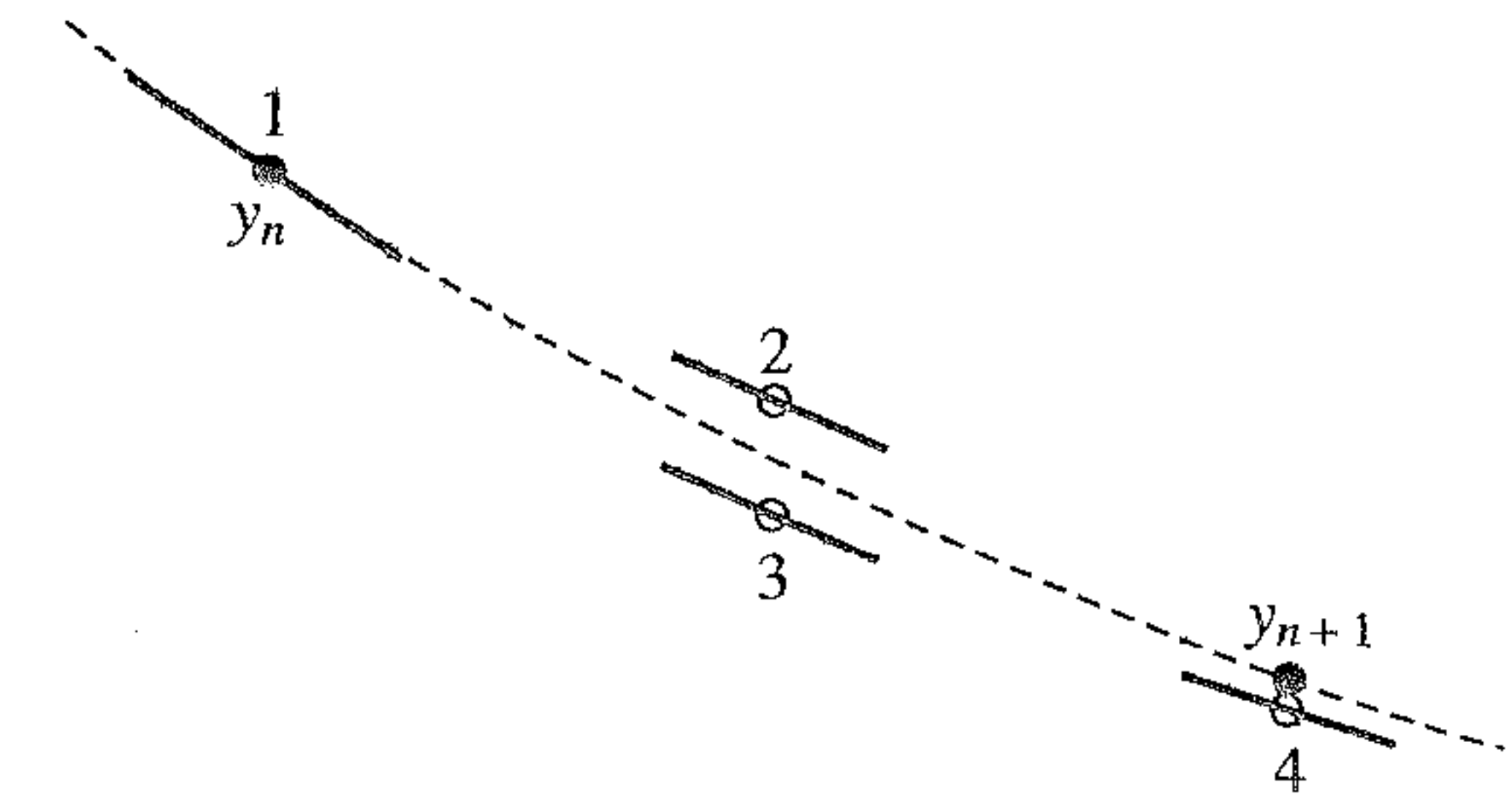


Figure 16.1.3. Fourth-order Runge-Kutta method. In each step the derivative is evaluated four times: once at the initial point, twice at trial midpoints, and once at a trial endpoint. From these derivatives the final function value (shown as a filled dot) is calculated. (See text for details.)

contemporary practice of science rather than as a statement about strict mathematics. That is, it reflects the nature of the problems that contemporary scientists like to solve.

For many scientific users, fourth-order Runge-Kutta is not just the first word on ODE integrators, but the last word as well. In fact, you can get pretty far on this old workhorse, especially if you combine it with an adaptive stepsize algorithm. Keep in mind, however, that the old workhorse's last trip may well be to take you to the poorhouse: Bulirsch-Stoer or predictor-corrector methods can be very much more efficient for problems where very high accuracy is a requirement. Those methods are the high-strung racehorses. Runge-Kutta is for ploughing the fields. However, even the old workhorse is more nimble with new horseshoes. In §16.2 we will give a modern implementation of a Runge-Kutta method that is quite competitive as long as very high accuracy is not required. An excellent discussion of the pitfalls in constructing a good Runge-Kutta code is given in [3].

Here is the routine for carrying out one classical Runge-Kutta step on a set of  $n$  differential equations. You input the values of the independent variables, and you get out new values which are stepped by a stepsize  $h$  (which can be positive or negative). You will notice that the routine requires you to supply not only function `derivs` for calculating the right-hand side, but also values of the derivatives at the starting point. Why not let the routine call `derivs` for this first value? The answer will become clear only in the next section, but in brief is this: This call may not be your only one with these starting conditions. You may have taken a previous step with too large a stepsize, and this is your replacement. In that case, you do not want to call `derivs` unnecessarily at the start. Note that the routine that follows has, therefore, only three calls to `derivs`.

```

SUBROUTINE rk4(y,dydx,n,x,h,yout,derivs)
INTEGER n,NMAX
REAL h,x,dydx(n),y(n),yout(n)
EXTERNAL derivs
PARAMETER (NMAX=50)          Set to the maximum number of functions.
    Given values for the variables y(1:n) and their derivatives dydx(1:n) known at x, use
    the fourth-order Runge-Kutta method to advance the solution over an interval h and return
    the incremented variables as yout(1:n), which need not be a distinct array from y. The
    user supplies the subroutine derivs(x,y,dydx), which returns derivatives dydx at x.
INTEGER i
REAL h6,hh,xh,dym(NMAX),dym(NMAX),yt(NMAX)
hh=h*0.5
h6=h/6.
xh=x+hh

```

```

do 11 i=1,n           First step.
  yt(i)=y(i)+hh*dydx(i)
enddo 11
call derivs(xh,yt,dyt) Second step.
do 12 i=1,n
  yt(i)=y(i)+hh*dyt(i)
enddo 12
call derivs(xh,yt,dym) Third step.
do 13 i=1,n
  yt(i)=y(i)+h*dym(i)
  dym(i)=dyt(i)+dym(i)
enddo 13
call derivs(x+h,yt,dyt) Fourth step.
do 14 i=1,n           Accumulate increments with proper weights.
  yout(i)=y(i)+h6*(dydx(i)+dyt(i)+2.*dym(i))
enddo 14
return
END

```

The Runge-Kutta method treats every step in a sequence of steps in identical manner. Prior behavior of a solution is not used in its propagation. This is mathematically proper, since any point along the trajectory of an ordinary differential equation can serve as an initial point. The fact that all steps are treated identically also makes it easy to incorporate Runge-Kutta into relatively simple “driver” schemes.

We consider adaptive stepsize control, discussed in the next section, an essential for serious computing. Occasionally, however, you just want to tabulate a function at equally spaced intervals, and without particularly high accuracy. In the most common case, you want to produce a graph of the function. Then all you need may be a simple driver program that goes from an initial  $x_s$  to a final  $x_f$  in a specified number of steps. To check accuracy, double the number of steps, repeat the integration, and compare results. This approach surely does not minimize computer time, and it can fail for problems whose nature *requires* a variable stepsize, but it may well minimize user effort. On small problems, this may be the paramount consideration.

Here is such a driver, self-explanatory, which tabulates the integrated functions in a common block path.

```

SUBROUTINE rk4(vstart,nvar,x1,x2,nstep,derivs)
  INTEGER nstep,nvar,NMAX,NSTPMX
  PARAMETER (NMAX=50,NSTPMX=200)           Maximum number of functions and
  REAL x1,x2,vstart(nvar),xx(NSTPMX),y(NMAX,NSTPMX) maximum number of values to
  EXTERNAL derivs                          be stored.
  COMMON /path/ xx,y                        Storage of results.
  USES rk4
  Starting from initial values vstart(1:nvar) known at x1 use fourth-order Runge-Kutta to
  advance nstep equal increments to x2. The user-supplied subroutine derivs(x,v,dvdx)
  evaluates derivatives. Results are stored in the common block path. Be sure to dimension
  the common block appropriately.
  INTEGER i,k
  REAL h,x,dv(NMAX),v(NMAX)
  do 11 i=1,nvar           Load starting values.
    v(i)=vstart(i)
    y(i,1)=v(i)
  enddo 11
  xx(1)=x1
  x=x1
  h=(x2-x1)/nstep
  do 13 k=1,nstep         Take nstep steps.
    call derivs(x,v,dv)

```

```

call rk4(v,dv,nvar,x,h,v,derivs)
if(x+h.eq.x)pause 'stepsize not significant in rk4'
x=x+h
xx(k+1)=x           Store intermediate steps.
do 12 i=1,nvar
  y(i,k+1)=v(i)
enddo 12
enddo 13
return
END

```

#### CITED REFERENCES AND FURTHER READING:

- Abramowitz, M., and Stegun, I.A. 1964, *Handbook of Mathematical Functions*, Applied Mathematics Series, Volume 55 (Washington: National Bureau of Standards; reprinted 1968 by Dover Publications, New York), §25.5. [1]
- Gear, C.W. 1971, *Numerical Initial Value Problems in Ordinary Differential Equations* (Englewood Cliffs, NJ: Prentice-Hall), Chapter 2. [2]
- Shampine, L.F., and Watts, H.A. 1977, in *Mathematical Software III*, J.R. Rice, ed. (New York: Academic Press), pp. 257–275; 1979, *Applied Mathematics and Computation*, vol. 5, pp. 93–121. [3]
- Rice, J.R. 1983, *Numerical Methods, Software, and Analysis* (New York: McGraw-Hill), §9.2.

## 16.2 Adaptive Stepsize Control for Runge-Kutta

A good ODE integrator should exert some adaptive control over its own progress, making frequent changes in its stepsize. Usually the purpose of this adaptive stepsize control is to achieve some predetermined accuracy in the solution with minimum computational effort. Many small steps should tiptoe through treacherous terrain, while a few great strides should speed through smooth uninteresting countryside. The resulting gains in efficiency are not mere tens of percents or factors of two; they can sometimes be factors of ten, a hundred, or more. Sometimes accuracy may be demanded not directly in the solution itself, but in some related conserved quantity that can be monitored.

Implementation of adaptive stepsize control requires that the stepping algorithm return information about its performance, most important, an estimate of its truncation error. In this section we will learn how such information can be obtained. Obviously, the calculation of this information will add to the computational overhead, but the investment will generally be repaid handsomely.

With fourth-order Runge-Kutta, the most straightforward technique by far is *step doubling* (see, e.g., [1]). We take each step twice, once as a full step, then, independently, as two half steps (see Figure 16.2.1). How much overhead is this, say in terms of the number of evaluations of the right-hand sides? Each of the three separate Runge-Kutta steps in the procedure requires 4 evaluations, but the single and double sequences share a starting point, so the total is 11. This is to be compared not to 4, but to 8 (the two half-steps), since — stepsize control aside — we are achieving the accuracy of the smaller (half) stepsize. The overhead cost is therefore a factor 1.375. What does it buy us?