Donald Greenspan

Numerical Solution of Ordinary Differential Equations

for Classical, Relativistic and Nano Systems

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Contents

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Preface

The study and application of ordinary differential equations has been a major part of the history of mathematics. In recent years, new applications in such areas as molecular mechanics and nanophysics have simply added to their significance.

This book is intended to be used as either a handbook or a text for a one-semester, introductory course in the numerical solution of ordinary differential equations. Theory, methodology, intuition, and applications are interwoven throughout. The choice of methods is guided by applied, rather than theoretical, interests. Throughout, nonlinearity and determinism are emphasized.

Chapter 1 develops Euler's method and fundamental convergence theory. Chapter 2 develops Runge–Kutta formulas through the highest order available, that is, order 10. Chapter 3 develops Taylor expansion methodology of arbitrary orders. Chapter 4 develops conservative numerical methodology. Chapter 5 is concerned with very large systems of differential equations, such as those used in molecular mechanics. Chapter 6 studies practical aspects of instability. Chapters 7 and 8 are concerned with boundary value problems. Chapter 9 presents, in an entirely self-contained fashion, fundamentals of special relativistic dynamics, in which the differential equations and the related constraints are truly unique. Chapter 10 is a survey with references of the many other topics available in the literature.

Flexibility is incorporated by providing programs generically. Computer technology is in such a rapid state of growth that the use of a specific programming language can become outdated in a very short time. In addition, the individual who wishes to use a graphics routine is free to use whichever is most readily available to him or her.

Relatively difficult sections are marked with an asterisk and may be omitted without disturbing the book's continuity.

Finally, it should be noted that this book contains materials of interest in engineering and science which are not available elsewhere. For example, Chap-

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ter 5 develops numerical methodology which conserves exactly the same energy, linear momentum and angular momentum as does a conservative continuous system.

I wish to thank the Institute of Mathematics and Its Applications for permission to reproduce Table 2.2.

Donald Greenspan

Arlington, Texas, 2005

1
Euler's Method

1.1
Introduction

In this chapter, we will consider a numerical method for a basic initial value problem, that is, for

$$y' = F(x, y), \quad y(0) = \alpha. \tag{1.1}$$

We will use a simplistic numerical method called Euler's method. Because of the simplicity of both the problem and the method, the related theory is relatively transparent and will be provided in detail. Though we will not do so, the theory developed in this chapter does extend to the more advanced methods to be introduced later, but only with increased complexity.

With respect to (1.1), we assume that a unique solution exists, but that analytical attempts to construct it have failed.

1.2
Euler's Method

Consider the problem of approximating a continuous function $y = f(x)$ on $x \geq 0$ which satisfies the differential equation

$$y' = F(x, y) \tag{1.2}$$

on $x > 0$, and the initial condition

$$y(0) = \alpha, \tag{1.3}$$

in which α is a given constant. In 1768 (see the Collected Works of L. Euler, vols. 11 (1913), 12 (1914)), L. Euler developed a method to prove that the initial value problem (1.2), (1.3) had a solution. The method was numerical in

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nature and today it is implemented on modern computers and is called Euler's method. The basic idea is as follows. By the definition of a derivative,

$$y'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}. \tag{1.4}$$

For small $h > 0$, then, (1.4) implies that a reasonable difference quotient approximation for $y'(x)$ is

$$y'(x) = \frac{f(x+h) - f(x)}{h}. \tag{1.5}$$

Substitution of (1.5) into (1.2) yields the difference equation

$$\frac{f(x+h) - f(x)}{h} = F(x,y) \tag{1.6}$$

which approximates the differential equation (1.2). However, (1.6) can be rewritten as

$$f(x+h) = f(x) + hF(x,y)$$

or, equivalently, as

$$y(x+h) = y(x) + hF(x, y(x)), \tag{1.7}$$

which enables one to approximate $y(x+h)$ in terms of $y(x)$ and $F(x, y(x))$. Equation (1.7) is the cornerstone of Euler's method, which is described precisely as follows.

Since a computer cannot calculate indefinitely, let $x \geq 0$ be replaced by $0 \leq x \leq L$, in which L is a positive constant. The value of L is usually determined by the physics of the phenomenon under consideration. If the phenomenon occurs over a short period of time, then L can be chosen to be relatively small. If the phenomenon is long lasting, then L must be relatively large. In either case, L is a fixed, positive constant. The interval $0 \leq x \leq L$ is then divided into n equal parts, each of length h, by the points $x_i = ih$, $i = 0, 1, 2, \ldots, n$. The value $h = L/n$ is called the grid size. The points x_i are called grid points. Let $y_i = y(x_i)$, $i = 0, 1, 2, \ldots, n$, so that initial condition (1.3) implies $y_0 = \alpha$. Next, at each of the grid points x_0, x_1, x_2, $\ldots$, x_{n-1}, approximate the differential equation by (3.6) in the notation

$$\frac{y_{i+1} - y_i}{h} = F(x_i, y_i), \quad i = 0, 1, 2, \ldots, n-1, \tag{1.8}$$

or, in explicit recursive form

$$y_{i+1} = y_i + hF(x_i, y_i), \quad i = 0, 1, 2, \ldots, n-1. \tag{1.9}$$

Then, beginning with

$$y_0 = \alpha, \tag{1.10}$$

set $i = 0$ in (1.9) and determine y_1. Knowing y_1, set $i = 1$ in (1.9) and determine y_2. Knowing y_2, set $i = 2$ in (1.9) and determine y_3, and so forth, until, finally, y_n is generated. The resulting discrete function $y_0, y_1, y_2, \dots, y_n$ is called the numerical solution.

Example 1.1 Consider the initial value problem

$$y' + y = x, \quad y(0) = 1. \tag{1.11}$$

This is a linear problem and can be solved exactly to yield the solution

$$Y(x) = x - 1 + 2e^{-x}. \tag{1.12}$$

Hence, there is no need to solve (1.11) numerically. We will proceed numerically for illustrative purposes only. For Euler's method, fix $L = 1$ and $h = 0.2$. Then, $x_0 = 0.0$, $x_1 = 0.2$, $x_2 = 0.4$, $x_3 = 0.6$, $x_4 = 0.8$, $x_5 = 1.0$ and differential equation (1.11) is approximated by the difference equation

$$\frac{y_{i+1} - y_i}{0.2} + y_i = x_i, \quad i = 0, 1, 2, 3, 4,$$

or, equivalently, by

$$y_{i+1} = (0.8)y_i + (0.2)x_i, \quad i = 0, 1, 2, 3, 4. \tag{1.13}$$

Since $y_0 = 1$, (1.13) yields, to three decimal places

$$\begin{aligned}
y_1 &= (0.8)y_0 + (0.2)x_0 = (0.8)(1.000) + (0.2)(0.0) = 0.800\\
y_2 &= (0.8)y_1 + (0.2)x_1 = (0.8)(0.800) + (0.2)(0.2) = 0.680\\
y_3 &= (0.8)y_2 + (0.2)x_2 = (0.8)(0.680) + (0.2)(0.4) = 0.624\\
y_4 &= (0.8)y_3 + (0.2)x_3 = (0.8)(0.624) + (0.2)(0.6) = 0.619\\
y_5 &= (0.8)y_4 + (0.2)x_4 = (0.8)(0.619) + (0.2)(0.8) = 0.655.
\end{aligned}$$

Thus, the numerical approximation with $h = 0.2$ is

$$\begin{aligned}
y(0.0) &= 1.000\\
y(0.2) &= 0.800\\
y(0.4) &= 0.680\\
y(0.6) &= 0.624\\
y(0.8) &= 0.619\\
y(1.0) &= 0.655.
\end{aligned}$$

However, from (1.12), the exact solution, rounded to three decimal places, at the grid points is given by

$$Y(0.0) = 1.000$$
$$Y(0.2) = 0.837$$
$$Y(0.4) = 0.741$$
$$Y(0.6) = 0.698$$
$$Y(0.8) = 0.699$$
$$Y(1.0) = 0.736.$$

Comparison of the numerical and the exact solutions then yields the precise amount of error that results at each grid point when employing Euler's method.

Now, unlike the above example, numerical methodology will be applied only when the exact solution of (1.2), (1.3) is *not* known. Thus, in practice the error at each grid point will not be known. It is essential then to know, *a priori*, that the unknown error at each grid point is arbitrarily small if h is arbitrarily small, that is, that the error at each grid point decreases to zero as h decreases to zero. If this were valid, then one would have the assurance that the error generated by Euler's method is negligible for all sufficiently small grid sizes h. That this is correct *when all calculations are exact* will be established next.

A generic algorithm for Euler's method is given as follows.

Algorithm 1 Euler

Step 1. Set a counter $k = 1$.
Step 2. Set a time step h.
Step 3. Set an initial time x.
Step 4. Set initial value y.
Step 5. Calculate
$K_0 = y$
$K_1 = hF(x, y)$.
Step 6. Calculate y at $x + h$ by
$y(x + h) = (K_0 + K_1)$.
Step 7. Increase the counter from k to $k + 1$.
Step 8. Set $y = y(x + h)$, $x = x + h$.
Step 9. Repeat Steps 5–8.
Step 10. Continue until $k = 100$.

1.3 Convergence of Euler's Method*

We wish to show now that, for Euler's method, *the error at each grid point decreases to zero as h decreases to zero*. The associated theory is called convergence theory. In developing convergence theory, we will require some preliminary results.

Lemma 1.1 *If the numbers* $|E_i|, \quad i = 0, 1, 2, 3, \ldots, n$, *satisfy*

$$|E_{i+1}| \le A\,|E_i| + B, \quad i = 0, 1, 2, 3, \ldots, n-1 \tag{1.14}$$

where A and B are nonnegative constants and $A \neq 1$, then

$$|E_i| \le A^i\,|E_0| + \frac{A^i - 1}{A - 1}B, \quad i = 1, 2, 3 \ldots, n \tag{1.15}$$

Proof. For $i = 0$, (1.14) yields

$$|E_1| \le A\,|E_0| + B = A\,|E_0| + \frac{A-1}{A-1}B,$$

so that (1.15) is valid for $i = 1$. The proof is now completed by induction. Assume that for fixed i, (1.15) is valid, that is,

$$|E_i| \le A^i\,|E_0| + \frac{A^i - 1}{A - 1}B.$$

Then we must prove that

$$|E_{i+1}| \le A^{i+1}\,|E_0| + \frac{A^{i+1} - 1}{A - 1}B.$$

Since, by (1.14),

$$|E_{i+1}| \le A\,|E_i| + B,$$

then

$$|E_{i+1}| \le A\left[A^i\,|E_0| + \frac{A^i - 1}{A - 1}B\right] + B = A^{i+1}\,|E_0| + \frac{A^{i+1} - 1}{A - 1}B,$$

and the proof is complete. □

The value of Lemma 1.1 is as follows. If each term of a sequence $|E_0|, |E_1|, |E_2|, |E_3|, |E_4|, \ldots, |E_n|, \ldots$, is related to the previous term by (1.14), then Lemma 1.1 enables one to relate each term directly to $|E_0|$ only, that is, to the very first term of the sequence.

Theorem 1.1 *Let I be the open interval $0 < x < L$ and $\bar{I}$ the closed interval $0 \leq x \leq L$. Assume the initial value problem*

$$y' = F(x,y),\ y(0) = \alpha \tag{1.16}$$

has the unique solution $Y(x)$ on $\bar{I}$. Then, on I,

$$Y'(x) \equiv F(x, Y(x)) \tag{1.17}$$

and

$$Y(0) = \alpha. \tag{1.18}$$

Assume that $Y'(x)$ and $Y''(x)$ are continuous and that there exist positive constants M, N such that

$$\left|Y''(x)\right| \leq N, \quad 0 \leq x \leq L \tag{1.19}$$

$$\left|\frac{\partial F}{\partial y}\right| \leq M, \quad 0 \leq x \leq L, \quad -\infty < y < \infty. \tag{1.20}$$

Next, let $\bar{I}$ be subdivided into n equal parts by the grid points $x_0 < x_1 < x_2 < \ldots < x_n$, where $x_0 = 0$, $x_n = L$. The grid size h is given by

$$h = L/n. \tag{1.21}$$

Let y_k be the numerical solution of (1.16) *by Euler's method on the grid points, so that*

$$y_{k+1} = y_k + hF(x_k, y_k), \quad k = 0, 1, 2, \ldots, n-1 \tag{1.22}$$

$$y_0 = \alpha. \tag{1.23}$$

Finally, define the error E_k at each grid point x_k by

$$E_k = Y_k - y_k, \quad k = 0, 1, 2, 3, \ldots, n. \tag{1.24}$$

Then,

$$|E_k| \leq \frac{\left[(1+Mh)^k - 1\right] Nh}{2M}, \quad k = 0, 1, 2, 3, \ldots, n. \tag{1.25}$$

Proof. Consider

$$|E_{k+1}| = |Y_{k+1} - y_{k+1}|.$$

Then

$$|E_{k+1}| = |Y_{k+1} - y_{k+1}| = |Y(x_k + h) - (y_k + hF(x_k, y_k))|.$$

Introducing a Taylor expansion for $Y(x_k + h)$ implies

$$\begin{aligned}|E_{k+1}| &= \left|\left(Y(x_k) + hY'(x_k) + \frac{1}{2}h^2 Y''(\xi)\right) - (y_k + hF(x_k, y_k))\right| \\ &= \left|Y_k - y_k + h\left[Y'(x_k) - F(x_k, y_k)\right] + \frac{1}{2}h^2 Y''(\xi)\right|.\end{aligned}$$

From (1.17), then

$$|E_{k+1}| = \left| Y_k - y_k + h\left[F(x_k, Y_k) - F(x_k, y_k)\right] + \frac{1}{2}h^2 Y''(\xi) \right|,$$

which, by the mean value theorem for a function of two variables, implies

$$\begin{aligned} |E_{k+1}| &= \left| Y_k - y_k + h\left[(Y_k - y_k)\frac{\partial F}{\partial y}(x_k, \eta)\right] + \frac{1}{2}h^2 Y''(\xi) \right| \\ &= \left| (Y_k - y_k)\left(1 + h\frac{\partial F}{\partial y}\right) + \frac{1}{2}h^2 Y''(\xi) \right|. \end{aligned}$$

Hence, by the rules for absolute values,

$$|E_{k+1}| \le |Y_k - y_k| \left(1 + h\left|\frac{\partial F}{\partial y}\right|\right) + \frac{1}{2}h^2 \left|Y''(\xi)\right|,$$

which, by (1.19), (1.20) yields

$$|E_{k+1}| \le |Y_k - y_k|\,(1 + Mh) + \frac{1}{2}h^2 N.$$

Thus, since $|Y_k - y_k| = |E_k|$, one has

$$|E_{k+1}| \le |E_k|\,(1 + Mh) + \frac{1}{2}h^2 N. \tag{1.26}$$

Application of Lemma 1.1 to (1.26) with $A = (1 + Mh)$, $B = \frac{1}{2}h^2 N$ then implies

$$|E_k| \le (1 + Mh)^k\,|E_0| + \frac{(1 + Mh)^k - 1}{(1 + Mh) - 1}\left(\frac{1}{2}h^2 N\right). \tag{1.27}$$

However, since $Y(0) = y(0) = \alpha$, one has $E_0 = 0$, so that (1.27) simplifies to

$$|E_k| \le \frac{\left[(1 + Mh)^k - 1\right] Nh}{2M}, \quad k = 0, 1, 2, 3, \ldots, n, \tag{1.28}$$

and the theorem is proved. □

Theorem 1.2 *Under the assumptions of Theorem 1.1, one has that at each grid point*

$$\lim_{h \to 0} |E_k| = 0, \quad k = 0, 1, 2, 3, \ldots, n.$$

Proof. Since $(1 + Mh) > 1$, the largest value of $(1 + Mh)^k$ results when $k = n$. Thus, from (1.28),

$$|E_k| \le \frac{\left[(1 + Mh)^n - 1\right] Nh}{2M}, \tag{1.29}$$

which, by (1.21), implies

$$|E_k| \leq \frac{\left[(1+Mh)^{L/h}-1\right]Nh}{2M}. \tag{1.30}$$

By the laws of exponents, then,

$$|E_k| \leq \frac{\left\{\left[(1+Mh)^{\frac{1}{Mh}}\right]^{ML}-1\right\}Nh}{2M}. \tag{1.31}$$

Note now that if $Mh = \gamma$, then

$$\lim_{h\to 0} Mh = \lim_{\gamma\to 0} \gamma = 0.$$

Thus,

$$\lim_{h\to 0}\left[(1+Mh)^{\frac{1}{Mh}}\right]^{ML} = \lim_{\gamma\to 0}\left[(1+\gamma)^{\frac{1}{\gamma}}\right]^{ML}.$$

But, $\lim_{\gamma\to 0}\left[(1+\gamma)^{\frac{1}{\gamma}}\right] = e$. Thus,

$$\lim_{h\to 0}\frac{\left\{\left[(1+Mh)^{\frac{1}{Mh}}\right]^{ML}-1\right\}Nh}{2M} = \lim_{h\to 0}\frac{\left\{e^{ML}-1\right\}Nh}{2M} = 0.$$

Thus, from (1.31), $\lim_{h\to 0}|E_k| = 0$ for all values of k, and the theorem is proved. □

1.4
Remarks

In practice, as will be shown soon, numerical methods which are more economical and more accurate than Euler's method can be developed easily. However, convergence proofs for these methods are more complex than for Euler's method.

Note that the essence of Theorem 1.2 is that if one wishes arbitrarily high accuracy, one need only choose h sufficiently small. Unfortunately, such remarks are purely qualitative. Indeed, if one has a prescribed accuracy, Theorems 1.1 and 1.2 do not allow one to determine the precise h, *a priori*, since the constant N in (1.19) is rarely known exactly and the practical matter of roundoff error in actual calculations has not been included in the theorems. The determination of accuracy is often estimated in an *a posteriori* manner as follows. One calculates for both h and $\frac{1}{2}h$ and takes those figures which are in agreement for the two calculations. For example, if at a point x and for $h = 0.1$ one finds

$y = 0.876\,532$ while for $h = 0.05$ one finds at the same point that $y = 0.876\,513$, then one assumes that the result $y = 0.8765$ is *an* accurate result.

As noted above, Theorems 1.1 and 1.2 do not consider roundoff error, which is always present in computer calculations. At the present time there is no universally accepted method to analyze roundoff error after a large number of time steps. The three main methods for analyzing roundoff accumulation are the analytical method (Henrici (1962), (1963)), the probabilistic method (Henrici (1962), (1963)) and the interval arithmetic method (Moore (1979)), each of which has both advantages and disadvantages.

1.5 Exercises

1.1 With $h = 0.1$, find the numerical solution on $0 \le x \le 1$ by Euler's method for

$$y' = y^2 + 2x - x^4, \quad y(0) = 0.$$

and compare your results with the exact solution $y = x^2$.

1.2 With $h = 0.1$, find the numerical solution on $0 \le x \le 2$ by Euler's method for

$$y' = y^3 - 8x^3 + 2, \quad y(0) = 0$$

and compare your results with the exact solution $y = 2x$.

1.3 With $h = 0.05$, find the numerical solution on $0 \le x \le 1$ by Euler's method for

$$y' = xy^2 - 2y, \quad y(0) = 1.$$

Find the exact solution and compare the numerical results with it.

1.4 With $h = 0.01$, find the numerical solution on $0 \le x \le 2$ by Euler's method for

$$y' = -2xy^2, \quad y(0) = 1,$$

and compare your results with the exact solution $y = \frac{1}{1+x^2}$.

1.5 With $h = 0.05$, find the numerical solution on $0 \le x \le 1$ by Euler's method for

$$y' = e^y - e^{x^2} + 2x, \quad y(0) = 0,$$

and compare your results with the exact solution $y = x^2$.