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INTRODUCTION

It is probably no exaggeration to say that differential equations are the most common and important mathematical model in science and engineering. Whenever we want to model a system where the state variables vary with time and/or space, differential equations are the natural tool for describing its behavior. The construction of a differential equation model demands a thorough understanding of what takes place in the process we want to describe.

However, setting up a differential equation model is not enough, we must also solve the equations. The process of finding useful solutions of a differential equation is much a symbiosis of modeling, mathematics and choosing a method, analytical or numerical. Therefore, when you are requested to solve a differential equation problem from some application, it is useful to know facts about its modeling background, its mathematical properties, and its numerical treatment. The last part involves choosing appropriate numerical methods, adequate Software, and appealing ways of visualizing the result.

The interaction among modeling, mathematics, numerical methods, and programming is nowadays referred to as *scientific computing* and its purpose is to perform *simulations* of processes in science and engineering.

1.1 WHAT IS A DIFFERENTIAL EQUATION?

A differential equation is a relation between a function and its derivatives. If the function u depends on only one variable t, i.e., $u = u(t)$, the differential equation is called

Introduction to Computation and Modeling for Differential Equations, Second Edition. Lennart Edsberg.

ordinary. If u depends on at least two variables t and x, i.e., $u = u(x, t)$, the differential equation is called *partial*.

1.2 EXAMPLES OF AN ORDINARY AND A PARTIAL DIFFERENTIAL EQUATION

An example of an elementary ordinary differential equation (ODE) is

$$\frac{du}{dt} = au \tag{1.1}$$

where a is a *parameter*, in this case a real constant. It is frequently used to model, e.g., the growth of a population ($a > 0$) or the decay of a radioactive substance ($a < 0$). The ODE (1.1) is a special case of differential equations called *linear with constant coefficients* (see Chapter 2).

The differential equation (1.1) can be solved analytically, i.e., the solution can be written explicitly as an *algebraic formula*. Any function of the form

$$u(t) = Ce^{at} \tag{1.2}$$

where C is an arbitrary constant satisfies (1.1) and is a solution. The expression (1.2) is called the *general* solution. If C is known to have a certain value, however, we get a unique solution, which, when plotted in the (t, u)-plane, gives a trajectory (solution curve). This solution is called a *particular* solution.

The constant C can be determined, e.g., by selecting a point (t_0, u_0) in the (t, u)-plane through which the solution curve shall pass. Such a point is called an *initial point* and the demand that the solution shall go through this point is called the *initial condition*. A differential equation together with an initial condition is called an *initial value problem* (IVP) (Figure 1.1).

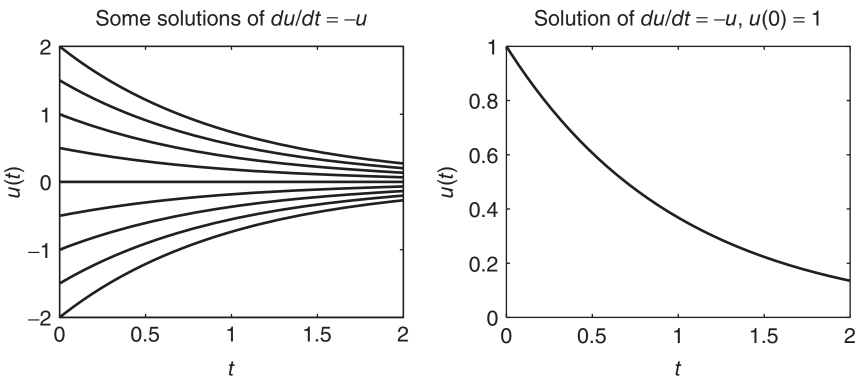

Figure 1.1 General and particular solution

Observe that the differential equation alone does not define a unique solution, we also need an initial condition or other conditions. A plot of all trajectories, i.e., all solutions of the ODE (1.1) in the (t, u)-plane will result in a graph that is totally black as there are infinitely many solution curves filling up the whole plane.

In general, it is not possible to find analytical solutions of a differential equation. The “simple” differential equation

$$\frac{du}{dt} = t^2 + u^2 \tag{1.3}$$

cannot be solved analytically. If we want to plot some of its trajectories, we have to use numerical methods.

An example of an elementary partial differential equation (PDE) is

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \tag{1.4}$$

where a is a *parameter*, in this case a real constant. The solution of (1.4) is a function of two variables $u = u(x, t)$. This differential equation is called the *1D* (one space dimension, x) *advection equation*. Physically it describes the evolution of a scalar quantity, e.g., temperature $u(x, t)$ carried along the x-axis by a flow with constant velocity a. It is also known as the linear convection equation and is an example of a *hyperbolic* PDE (see Chapter 5).

The *general* solution of this differential equation is (see Exercise 1.2.4)

$$u(x, t) = F(x - at) \tag{1.5}$$

where F is any arbitrary differentiable function of one variable. This is indeed a large family of solutions! The three functions

$$u(x, t) = x - at, \quad u(x, t) = e^{-(x-at)^2}, \quad u(x, t) = sin(x - at)$$

are just three solutions out of the infinitely many solutions of this PDE.

To obtain a unique solution for $t > 0$ we need an *initial condition*. If the differential equation is valid for all x, i.e., $-\infty < x < \infty$ and $u(x, t)$ is known for $t = 0$, i.e., $u(x, 0) = u_0(x)$ where $u_0(x)$ is a given function, the initial value function, we get the *particular* solution (Figure 1.2)

$$u(x, t) = u_0(x - at) \tag{1.6}$$

Physically, (1.6) corresponds to the propagation of the initial function $u_0(x)$ along the x-axis with velocity $|a|$. The propagation is to the right if $a > 0$ and to the left if $a < 0$.

The graphical representation can alternatively be done in 3D (Figure 1.3).

When a PDE is formulated on a semi-infinite or finite x-interval, *boundary conditions* are needed in addition to initial conditions to specify a unique solution.

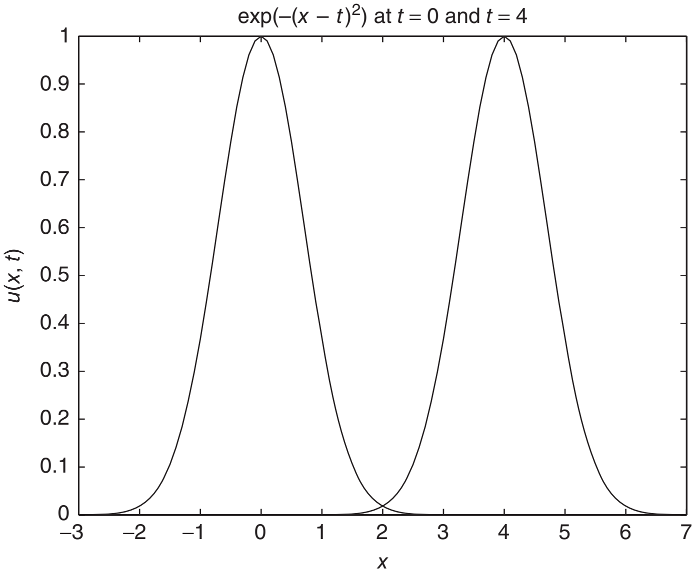

Figure 1.2 Propagation of a solution of the advection equation

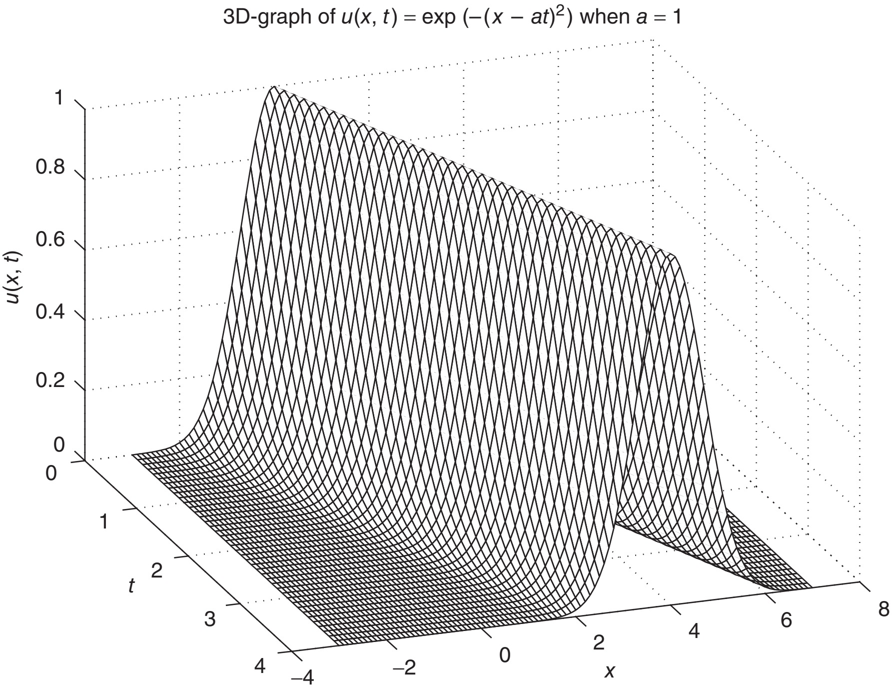

Figure 1.3 3D graph of a propagating solution

Most PDEs can only be solved with numerical methods. Only for very special classes of PDE problems it is possible to find an analytic solution, often in the form of an infinite series.

Exercise 1.2.1. If a is a complex constant $a = \mu + i\omega$ what is the real and imaginary part of e^{at}?

Exercise 1.2.2. What conditions are necessary to impose on μ and ω if $Re(e^{at})$ for $t > 0$ is to be

a) exponentially decreasing,
b) exponentially increasing,
c) oscillating with constant amplitude,
d) oscillating with increasing amplitude,
e) oscillating with decreasing amplitude?

Exercise 1.2.3. If a is a complex constant what condition on a is needed if e^{at} is to be bounded for $t \geq 0$?

Exercise 1.2.4. Show that the general solution of $u_t + au_x = 0$ is $u(x, t) = F(x - at)$ by introducing the transformation

$$\xi = x + at, \quad \eta = x - at$$

Transform the original problem to a PDE in the variables ξ and η, and solve this PDE. Sketch the two coordinate systems in the same graph.

Exercise 1.2.5. Show that a solution of (1.4) starting at $t = 0$, $x = x_0$ is constant along the straight line $x - at = x_0$. This means that the initial value $u(x_0, 0) = u_0(x_0)$ is transported unchanged along this line, which is called a *characteristic* of the hyperbolic PDE (1.4).

1.3 NUMERICAL ANALYSIS, A NECESSITY FOR SCIENTIFIC COMPUTING

In scientific computing, the numerical methods used to solve mathematical models should be *robust*, i.e., they should be reliable and give accurate values for a large range of parameter values. Sometimes, however, a method may fail and give unexpected results. Then, it is important to know how to investigate why an erroneous result has occurred and how it can be remedied.

Two basic concepts in numerical analysis are *stability* and *accuracy*. When choosing a method for solving a differential equation problem, it is necessary to have some knowledge about how to analyze the result of the method with respect to these concepts. This necessity has been well expressed by the late Prof. Germund Dahlquist, famous for his fundamental research in the theory of numerical treatment of differential equations: “There is nothing as practical as a little good theory.”

As an example of what may be unexpected results, choose the well-known *vibration equation*, occurring in, e.g., mechanical vibrations, electrical vibrations, and sound vibrations. The form of this equation with initial conditions is

$$m\frac{d^2u}{dt^2} + c\frac{du}{dt} + ku = f(t), \qquad u(0) = u_0, \frac{du}{dt}(0) = v_0 \tag{1.7}$$

In mechanical vibrations, m is the mass of the vibrating particle, c the damping coefficient, k the spring constant, $f(t)$ an external force acting on the particle, u_0 the initial position, and v_0 the initial velocity of the particle. The five quantities m, c, k, u_0, v_0 are referred to as the *parameters* of the problem.

Solving (1.7) numerically for a set of values of the parameters is an example of *simulation* of a mechanical process and it is desirable to choose a robust method, i.e., a method for which the results are reliable for a large range of values of the parameters. The following two examples based on the vibration equation show that unexpected results depending on instability and/or bad accuracy may occur.

Example 1.1. Assume that $f(t) = 0$ (free vibrations) and the following values of the parameters: $m = 1, c = 0.4, k = 4.5, u_0 = 1, v_0 = 0$. Without too much knowledge about mechanics, we would expect the solution to be oscillatory and damped, i.e., the amplitude of the vibrations is decreasing. If we use the simple *Euler method with constant stepsize* $h = 0.1$ (see Chapter 3), we obtain the following numerical solution, visualized together with the exact solution (Figure 1.4).

The graph shows a numerical solution that is oscillatory but unstable with increasing amplitude. Why? The answer is given in Chapter 3. For the moment just accept that insight in *stability* concepts and experience in handling unexpected results are needed for successful simulations.

Example 1.2. When the parameters in equation (1.7) are changed to $m = 1$, $c = 10$, $k = 10^3$, $u_0 = 0$, $v_0 = 0$, and $f(t) = 10^{-4}\sin(40t)$ (forced vibrations) we obtain the following numerical result with a method from a commercial software product for solving differential equations (Figure 1.5).

The graph shows that the numerical result is not correct. Why? In this example there is an *accuracy* problem. The default accuracy used in the method is not sufficient; the corresponding *numerical parameter* must be *tuned* appropriately. Accuracy for ODEs is discussed in Chapter 3.

Numerical solution of PDEs can also give rise to unexpected results. As an example consider the PDE (1.4), which has the property of propagating the initial function along the x-axis. One important application of this equation occurs in gas dynamics where simulation of *shock waves* is essential. A simple 1D model of a

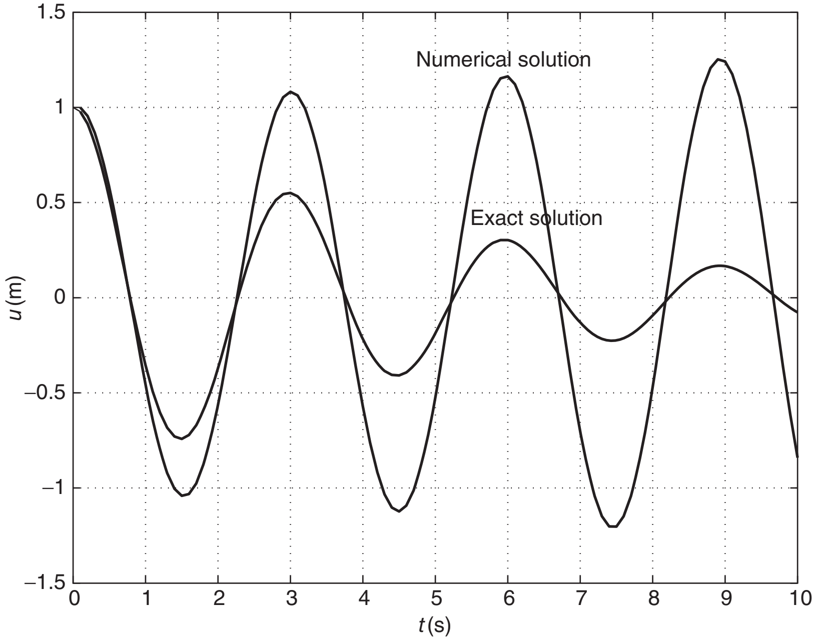

Figure 1.4 An example of numerical instability

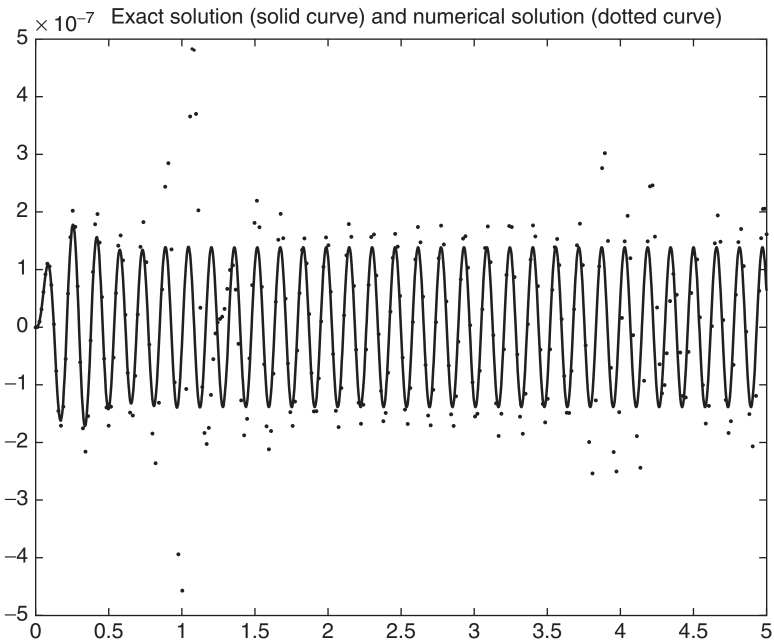

Figure 1.5 An example of insufficient accuracy

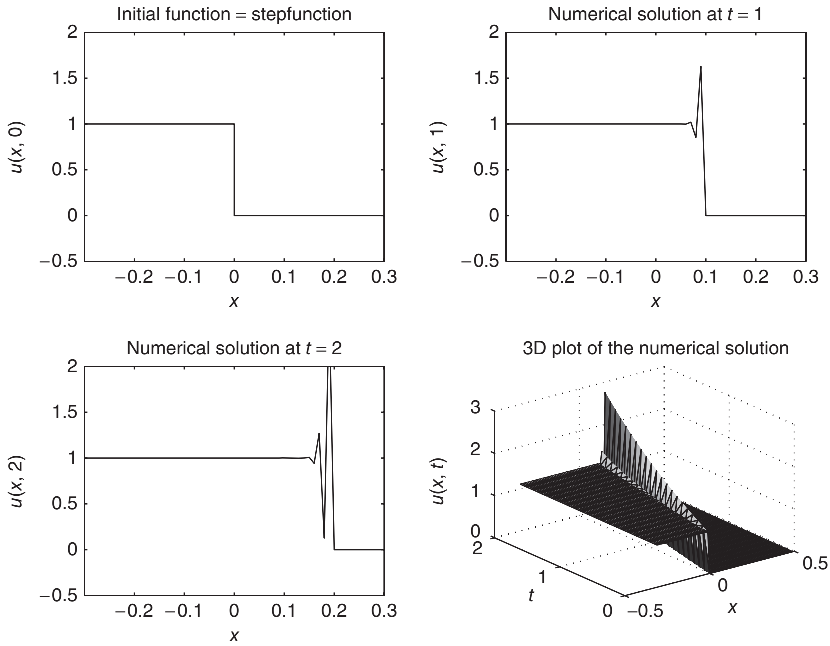

Figure 1.6 Numerical solution of the advection equation

shockwave is a *stepfunction*. Assume the initial function $u_0(x)$ is a stepfunction (Figure 1.6). In the exact solution of (1.4) with a stepfunction as initial condition, the solution propagates along the x-axis *without changing shape*.

However, using a numerical method, where simple difference approximations are used in both the t- and the x-direction, wiggles are generated as the solution propagates (see the graphs in Figure 1.6). The shape of the initial function is distorted. Why? Answers will be given in Chapter 8.

1.4 OUTLINE OF THE CONTENTS OF THIS BOOK

After this introductory chapter, the text is organized so that *ODEs* are treated first, followed by *PDEs*. The aim of this book is to be an introduction to *scientific computing*. Therefore, not only *numerical methods* are presented but also

1. how to set up a *mathematical model* in the form of an ODE or a PDE;
2. an outline of the *mathematical properties* of differential equation problems and explicit analytical solutions (when they exist); and
3. examples of how results are presented with proper *visualization*.

The ODE part starts in Chapter 2 presenting some mathematical properties of ODEs, first the basic and important problem class of ODE systems which are *linear with* *constant coefficients* applied to important models from classical mechanics, electrical networks, and chemical kinetics. This is followed by numerical treatment of ODE problems in general, following the classical subdivision into *IVPs* in Chapter 3, and *boundary value problems*, BVPs, in Chapter 4. For IVPs, the *finite difference method* (FDM) is described starting with the elementary Euler method. Important concepts brought up for ODEs are *accuracy* and *stability* which is followed up also for PDEs in later chapters. For BVPs, both the FDM and the *finite element method* (FEM) are described.

Important application areas where ODEs are used as mathematical model are presented, selected examples are described in the chapters and exercises, sometimes suitable for computer labs, are inserted into the text.

PDEs are introduced in Chapter 5, which deals with some mathematical properties of their solutions. There is also a presentation of several of the important PDEs of science and engineering, such as the equations of Navier–Stokes, Maxwell and Schrödinger.

The three chapters to follow are devoted to the numerical treatment of PDEs following the classical subdivision into *parabolic, elliptic*, and *hyperbolic* problems. Concepts from the ODE chapters such as accuracy and stability are treated for time-dependent, parabolic and hyperbolic PDEs. For stationary problems (elliptic PDEs), sparse linear systems of algebraic equations are essential and hence discussed.

Selected models introduced in Chapters 2, 5, and 9 are used as illustrations of the different methods introduced. Models are taken from mechanics, fluid dynamics, electromagnetics, reaction engineering, biochemistry, control theory, quantum mechanics, solid mechanics, etc. and are suitable for computer labs.

In Chapter 9, an outline of *mathematical modeling* is brought up with the intention of giving a feeling of the principles used when a differential equation (ODE or PDE) is set up from *conservation laws* and *constitutive relations*. It is also shown by examples how a general differential equation model can be simplified by suitable assumptions. This chapter can be studied in parallel with Chapters 3, 4, 6, 7, and 8 if the reader wants to see how the models are constructed.

In a number of Appendices (A.1–A.6), different parts of mathematics and numerical mathematics that are essential for numerical treatment of differential equations are presented as summaries.

Appendix B gives an overview of existing software for scientific computing with emphasis on the use of MATLAB® for programming and COMSOL Multiphysics® for modeling and parameter studies. Many of the exercises in this chapter and in Chapters 2–8 are solved with MATLAB programs in this appendix.

Appendix C contains a number of computer exercises to support the chapters containing numerical solution of ODEs and PDEs.

In Chapter 10, a number of projects are suggested. These projects involve problems where knowledge from several chapters and appendices are needed to compute a solution.

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