Computational Differential Equations

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To Anita, Floris, Ingrid, and Patty.

Contents

Preface

> I admit that each and every thing remains in its state until there is reason for change. (Leibniz)

> I'm sick and tired of this schism between earth and sky.
> Idealism and realism sorely our reason try. (Gustaf Fröding)

This book, together with the companion volumes *Introduction to Computational Differential Equations* and *Advanced Computational Differential Equations*, presents a unified approach to computational mathematical modeling using differential equations based on a principle of a fusion of mathematics and computation. The book is motivated by the rapidly increasing dependence on numerical methods in mathematical modeling driven by the development of powerful computers accessible to everyone. Our goal is to provide a student with the essential theoretical and computational tools that make it possible to use differential equations in mathematical modeling in science and engineering effectively. The backbone of the book is a new unified presentation of numerical methods for differential equations based on Galerkin methods.

Mathematical modeling using differential and integral equations has formed the basis of science and engineering since the creation of calculus by Leibniz and Newton. Mathematical modeling has two basic dual aspects: one symbolic and the other constructive-numerical, which reflect the duality between the infinite and the finite, or the continuum and the discrete. The two aspects have been closely intertwined throughout the development of modern science from the development of calculus in the work of Euler, Lagrange, Laplace and Gauss into the work of von Neumann in our time. For example, Laplace's monumental *Mécanique Céleste* in five volumes presents a symbolic calculus for a mathematical model of gravitation taking the form of Laplace's equation, together with massive numerical computations giving concrete information concerning the motion of the planets in our solar system.

However, beginning with the search for rigor in the foundations of calculus in the 19th century, a split between the symbolic and constructive aspects gradually developed. The split accelerated with the invention of the electronic computer in the 1940s, after which the constructive aspects were pursued in the new fields of numerical analysis and computing sciences, primarily developed outside departments of mathematics. The unfortunate result today is that symbolic mathematics and constructive-numerical mathematics by and large are separate disciplines and are rarely taught together. Typically, a student first meets calculus restricted to its symbolic form and then much later, in a different context, is confronted with the computational side. This state of affairs lacks a sound scientific motivation and causes severe difficulties in courses in physics, mechanics and applied sciences building on mathematical modeling. The difficulties are related to the following two basic questions: (i) How to get applications into mathematics education? (ii) How to use mathematics in applications? Since differential equations are so fundamental in mathematical modeling, these questions may be turned around as follows: (i) How can we teach differential equations in mathematics education? (ii) How can we use differential equations in applications?

Traditionally, the topic of differential equations in basic mathematics education is restricted to separable scalar first order ordinary differential equations and constant coefficient linear scalar n'th order equations for which explicit solution formulas are presented, together with some applications of separation of variables techniques for partial differential equations like the Poisson equation on a square. Even slightly more general problems have to be avoided because the symbolic solution methods quickly become so complex. Unfortunately, the presented tools are not sufficient for applications and as a result the student must be left with the impression that mathematical modeling based on symbolic mathematics is difficult and only seldom really useful. Furthermore, the numerical solution of differential equations, considered with disdain by many pure mathematicians, is often avoided altogether or left until later classes, where it is often taught in a "cookbook" style and not as an integral part of a mathematics education aimed at increasing understanding. The net result is that there seems to be no good answer to the first question in the traditional mathematics education.

The second question is related to the apparent principle of organization of a technical university with departments formed around particular differential equations: mechanics around Lagrange's equation, physics around Schrödinger's equation, electromagnetics around Maxwell's equations, fluid and gas dynamics around the Navier-Stokes equations, solid mechanics around Navier's elasticity equations, nuclear engineering around the transport equation, and so on. Each discipline has largely developed its own set of analytic and numerical tools for attacking its special differential equation independently and this set of tools forms the basic theoretical core of the discipline and its courses. The organization principle reflects both the importance of mathematical modeling using differential equations and the traditional difficulty of obtaining solutions.

Both of these questions would have completely different answers if it were possible to solve differential equations using a unified mathematical methodology simple enough to be introduced in the basic mathematics education and powerful enough to apply to real applications. In a natural way, mathematics education would then be opened to a wealth of applications and applied sciences could start from a more practical mathematical foundation. Moreover, establishing a common methodology opens the possibility of exploring "multiphysics" problems including the interaction of phenomena from solids, fluids, electromagnetics and chemical reactions, for example.

In this book and the companion volumes we seek to develop such a unified mathematical methodology for solving differential equations. Our work is based on the conviction that it is possible to approach this area, which is traditionally considered to be difficult and advanced, in a way that is comparatively easy to understand. However, our goal has not been to write an easy text that can be covered in one term in an independent course. The material in this book takes time to digest, as much as the underlying mathematics itself. It appears to us that the optimal course will involve the gradual integration of the material into the traditional mathematics curriculum from the very beginning.

We emphasize that we are not advocating the study of computational algorithms over the mathematics of calculus and linear algebra; it is always a fusion of analysis and numerical computation that appears to be the most fruitful. The material that we would like to see included in the mathematics curriculum offers a concrete motivation for the development of analytic techniques and mathematical abstraction. Computation does not make analysis obsolete, but gives the analytical mind a focus. Furthermore, the role of symbolic methods changes. Instead of being the workhorse of analytical computations requiring a high degree of technical complexity, symbolic analysis may focus on analytical aspects of model problems in order to increase understanding and develop intuition.

How to use this book

This book begins with a chapter that recalls the close connection between integration and numerical quadrature and then proceeds through introductory material on calculus and linear algebra to linear ordinary and partial differential equations. The companion text *Advanced Computational Differential Equations* widens the scope to nonlinear differential equations modeling a variety of phenomena including reaction-diffusion, fluid flow and many-body dynamics as well as material on implementation, and reaches the frontiers of research. The companion text *Introduction to Computational Differential Equations* goes in the other direction, developing in detail the introductory material on calculus and linear algebra.

We have used the material that serves as the basis for these books in a variety of courses in engineering and science taught at the California Institute of Technology, Chalmers University of Technology, Georgia Institute of Technology, and the University of Michigan. These courses ranged from mathematically oriented courses on numerical methods for differential equations to applications oriented courses in engineering and science based on computation. Students in these kinds of courses tend to have a diverse preparation in mathematics and science and we have tried to handle this by making the material of this book as accessible as possible and including necessary background material from calculus, linear algebra, numerical analysis, mechanics, and physics.

In our experience, beginning a course about solving differential equations by discretizing Poisson's equation presents an overwhelming array of topics to students: approximation theory, linear algebra, numerical solution of systems, differential equations, function spaces, etc. The sheer number of topics introduced at one time in this approach gives rise to an almost insurmountable hurdle to understanding topics which taken one at a time are not so difficult. To overcome these difficulties, we have taken a different approach.

In the first part of this book, we begin by considering the numerical solution of the simplest differential equation by quadrature and we develop the themes of convergence of numerical methods by giving a constructive proof of the Fundamental Theorem of Calculus. We also show the close relationship between convergence and error estimation by studying adaptive quadrature briefly. Next, we present background material on linear algebra and polynomial approximation theory, following a natural line started with the first chapter by applying this material to quadrature. After this, we introduce Galerkin's method for more general differential equations by considering three specific examples. In this chapter, we also raise the important issues that are addressed in the rest of the book. This part concludes with an introduction to the numerical solution of linear systems.

In the second part of the book, we discuss the discretization of time or space dependent ordinary differential equations. The basic theme of this part is to develop an intuitive sense of the classification of differential equations into elliptic, parabolic, and hyperbolic. By discretizing model problems representing these basic types, we can clarify the issues in discretization and convergence. We also develop a sense of the kind of behavior to be expected of approximations and their errors for the different kinds of problems.

Finally in the third part of the book, we study the discretization of the classic linear partial differential equations. The material is centered around specific examples, with generalizations coming as additional material and worked out in exercises. We also introduce the complexities of multi-physics problems with two chapters on convection-diffusion-absorption problems.

While we advocate the arrangement of the material in this book on pedagogical grounds, we have also tried to be flexible. Thus, it is entirely possible to choose a line based on a particular application or type of problem, e.g. stationary problems, and start directly with the pertinent chapters, referring back to background material as needed.

This book is a substantial revision of Johnson ([10]) with changes made in several key ways. First, it includes additional material on the derivation of differential equations as models of physical phenomena and mathematical results on properties of the solutions. Next, the unification of computational methodology using Galerkin discretization begun in the precursor is brought to completion and is applied to a large variety of differential equations. Third, the essential topics of error estimation and adaptive error control are introduced at the start and developed consistently throughout the presentation. We believe that computational error estimation and adaptive error control are fundamentally important in scientific terms and this is where we have spent most of our research energy. Finally, this book starts at a more elementary level than the precursor and proceeds to a more advanced level in the advanced companion volume.

Throughout the book, we discuss both practical issues of implementation and present the error analysis that proves that the methods converge and which provides the means to estimate and control the error. As mathematicians, a careful explanation of this aspect is one of the most important subjects we can offer to students in science and engineering. However, we delay discussing certain technical mathematical issues underlying the Galerkin method for partial differential equations until the last chapter.

We believe that the students' work should involve a combination of mathematical analysis and computation in a problem and project-oriented approach with close connection to applications. The questions may be of mathematical or computational nature, and may concern mathematical modeling and directly relate to topics treated in courses in mechanics, physics and applied sciences. We have provided many problems of this nature that we have assigned in our own courses. Hints and answers for the problems as well as additional problems will be given in the introductory companion volume. The book is complemented by software for solving differential equations using adaptive error control called Femlab that is freely available through the Internet. Femlab implements the computational algorithms presented in the book, and can serve as a laboratory for experiments in mathematical modeling and numerical solution of differential equations. It can serve equally well as a model and toolbox for the development of codes for adaptive finite element methods.

Finally, we mention that we have implemented and tested a reform of the mathematics curriculum based on integrating mathematics and computation during the past year in the engineering physics program at Chalmers University. The new program follows a natural progression from calculus in one variable and ordinary differential equations to calculus in several variables and partial differential equations while developing the mathematical techniques in a natural interplay with applications. For course material, we used this book side-by-side with existing texts in calculus and linear algebra. Our experience has been very positive and gives clear evidence that the goals we have stated may indeed be achieved in practice. With the elementary companion text, we hope to ease the process of fusing the new and classical material at the elementary level and thereby help to promote the reform in a wider context.

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Part I

Introduction

This first part has two main purposes. The first is to review some mathematical prerequisites needed for the numerical solution of differential equations, including material from calculus, linear algebra, numerical linear algebra, and approximation of functions by (piecewise) polynomials. The second purpose is to introduce the basic issues in the numerical solution of differential equations by discussing some concrete examples. We start by proving the Fundamental Theorem of Calculus by proving the convergence of a numerical method for computing an integral. We then introduce Galerkin's method for the numerical solution of differential equations in the context of two basic model problems from population dynamics and stationary heat conduction.

1

The Vision of Leibniz

> Knowing thus the Algorithm of this calculus, which I call Differential Calculus, all differential equations can be solved by a common method. (Leibniz)

> When, several years ago, I saw for the first time an instrument which, when carried, automatically records the number of steps taken by a pedestrian, it occurred to me at once that the entire arithmetic could be subjected to a similar kind of machinery so that not only addition and subtraction, but also multiplication and division could be accomplished by a suitably arranged machine easily, promptly and with sure results.... For it is unworthy of excellent men to lose hours like slaves in the labour of calculations, which could safely be left to anyone else if the machine was used.... And now that we may give final praise to the machine, we may say that it will be desirable to all who are engaged in computations which, as is well known, are the mangers of financial affairs, the administrators of others estates, merchants, surveyors, navigators, astronomers, and those connected with any of the crafts that use mathematics. (Leibniz)

Building on tradition going back to the ancient Greek philosophers, Leibniz and Newton invented calculus in the late 17th century and thereby laid the foundation for the revolutionary development of science and technology that is shaping the world today. Calculus is a method for modeling physical systems mathematically by relating the state of a system to its neighboring states in space-time using differential and integral equations. Because calculus is inherently computational, this revolution began to accelerate tremendously in the 1940s when the electronic computer was created. Today, we are seeing what is essentially a "marriage" of calculus and computation in the creation of the field of *computational mathematical modeling*.

Figure 1.1: Gottfried Wilhelm Leibniz, 1646-1716.

Actually, Leibniz himself sought to realize a unification of calculus and computation, but failed because the mechanical calculator he invented was not sufficiently powerful. The next serious effort was made in the 1830s by Babbage, who designed a steam powered mechanical computer he called the Analytical Engine. Again, technical difficulties and low speed stopped his ambitious plans.

The possibility of realizing Leibniz' and Babbage's visions of a universal computing machine came with the invention of the electronic valve in the 1930s, which enabled the construction of high speed digital computers. The development took a leap during the World War II spurred by the computing demands of the military. Until this time, large scale computations were performed by rooms of people using mechanical adding machines. The war provided an immediate pressure to speed up the process of scientific development by using mathematical modeling to hone a physical problem down to a manageable level, and mathematicians and physicists became interested in the invention of an electronic computing device. The logical design of programmable electronic computers was developed by the mathematician von Neumann, among others. By the late forties, von Neumann was using the first ENIAC (Electronic Numerical Integrator And Calculator) computer to address questions in fluid dynamics and aerodynamics.

The subsequent development of computer power that has resulted in desktop computers of far greater power than the ENIAC, has been paralleled by the rapid introduction of computational mathematical modeling into all areas of science and engineering. Questions routinely addressed computationally using a computer include: What is the weather going to do in three days? Will this airplane fly? Can this bridge carry a load of ten trucks? What happens during a car collision? How do we direct a rocket to pass close by Saturn? How can we create an image of the interior of the human body using very weak X-rays? What is the shape of a tennis racket that has the largest "sweet spot"? What is a design of a bicycle frame that combines low weight with rigidity? How can we create a sharp picture from a blurred picture? What will the deficit be in Sweden in the year 2000? How much would the mean temperature of the earth increase if the amount of carbon dioxide in the atmosphere increased by 20 percent?

The physical situations behind these kinds of questions are modeled by expressing the laws of mechanics and physics (or economics) in terms of equations that relate derivatives and integrals. Common variables in these models are time, position, velocity, acceleration, mass, density, momentum, energy, stress and force, and the basic laws express conservation of mass, momentum and energy, and balance of forces. Information about the physical process being modeled is gained by solving for some of the variables in the equation, i.e. by computing the *solution* of the differential/integral equation in terms of the others, which are assumed to be known data. Calculus is the basic study of differential/integral equations and their solutions.

Sometimes it is possible to find an exact formula for the solution of a differential/integral equation. For example, the solution might be expressed in terms of the data as a combination of elementary functions or as a trigonometric or power series. This is the classical mathematical method of solving a differential equation, which is now partially automated in mathematical software for symbolic computation such as Maple or Mathematica. However, this approach only works on a relatively small class of differential equations. In more realistic models, solutions of differential equations cannot be found explicitly in terms of known functions, and the alternative is to determine an approximate solution for given data through numerical computations on a computer. The basic idea is to *discretize* a given differential/integral equation to obtain a system of equations with a finite number of unknowns, which may be solved using a computer to produce an approximate solution. The finite-dimensional problem is referred to as a *discrete problem* and the corresponding differential/integral equation as a *continuous problem*. A good numerical method has the property that the error decreases as the number of unknowns, and thus the computational work, increases. Discrete problems derived from physical models are usually computationally intensive, and hence the rapid increase of computer power has opened entirely new possibilities for this approach. Using a desktop computer, we can often obtain more information about physical situations by numerically solving differential equations than was obtained over all the previous centuries of study using analytical methods.

Predicting the weather

The progress in weather prediction is a good example for this discussion. Historically, weather forecasting was based on studying previous patterns to predict future behavior. A farmer's almanac gives predictions based on the past behavior, but involves so many variables related to the weather that determining meaningful correlations is an overwhelming task. By modeling the atmosphere with a set of differential equations, the number of variables is reduced to a handful that can be measured closely, albeit at many locations. This was envisioned by the English pioneer of numerical weather prediction Richardson in the 1920s, who proposed the formation of a department of 64,000 employees working in shifts to perform the necessary calculations using mechanical calculators more quickly than the weather changed. After this proposal, the attitude toward numerical weather prediction became pessimistic. Not until the development of the modern computer, could the massive computations required be performed sufficiently rapidly to be useful. The first meaningful numerical forecasts were made by von Neumann and Charney in the late forties using the ENIAC, but of course the reliability was very low due to the extremely coarse discretization of the earth's system they had to use. The most recent model for the global weather uses a discretization grid with roughly 50,000 points horizontally and 31 layers vertically giving a total of five million equations that are solved in a couple of hours on a super-computer.

There are three sources of errors affecting the reliability of a numerical weather forecast: (i) measurement errors in data (or lack of data) (ii) approximation errors in modeling and (iii) approximation errors in computation. The initial data at the start of the computer simulation are always measured with some error; the set of differential equations in the computer model only approximately describes the evolution of the atmosphere; and finally the numerical solution of the differential equations is only an approximation of the true solution. These sources add up to form the total prediction error. It is essential to be able to estimate the total error by estimating individually the contributions from the sources (i)-(iii) and improve the precision where possible. This is a basic issue in all applications in computational mathematical modeling.

Our experience tells that forecasts of the daily weather become very unreliable in predictions for more than say a week. This was discussed in the 1960s by the meteorolgist Lorenz, who coined the phrase "the butterfly effect" to describe situations in which a small cause can have a large effect after some time. Lorenz gave a simple example displaying this phenomenon in the form of the *Lorenz system* of ordinary differential equations with only three unknowns. We plot a typical solution in Fig. 1.2, showing the trajectory of a "particle" being ejected away from the origin to be attracted into a slowly diverging orbit to the left, then making a loop on the right, returning to a few orbits to the left, then back to the right etc. The trajectory is very sensitive to perturbations as to the number of loops to the left or right, and thus is difficult to compute accurately over a longer time interval, just as the evolution of the weather may be difficult to predict for more than a week.

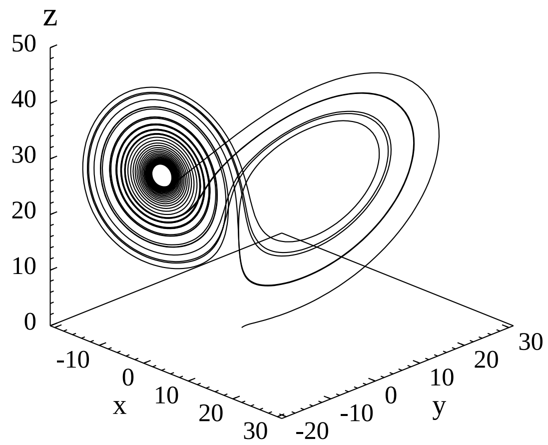


Figure 1.2: A solution of the Lorenz system computed with an error of .1 or less over the time interval $(0, 30)$.

What is this book about?

If we summarize the Leibniz vision as a fusion of mathematical modeling, mathematical analysis and computation, then there are three fundamental issues to be addressed:

- How are physical phenomena modeled using differential equations?
- What are the properties of solutions of differential equations?
- How are approximate solutions of differential equations computed and how can the accuracy of the approximations be controlled?

This book tries to answer these questions for a specific set of problems and to provide a set of tools that can be used to tackle the large variety of problems met in applications.

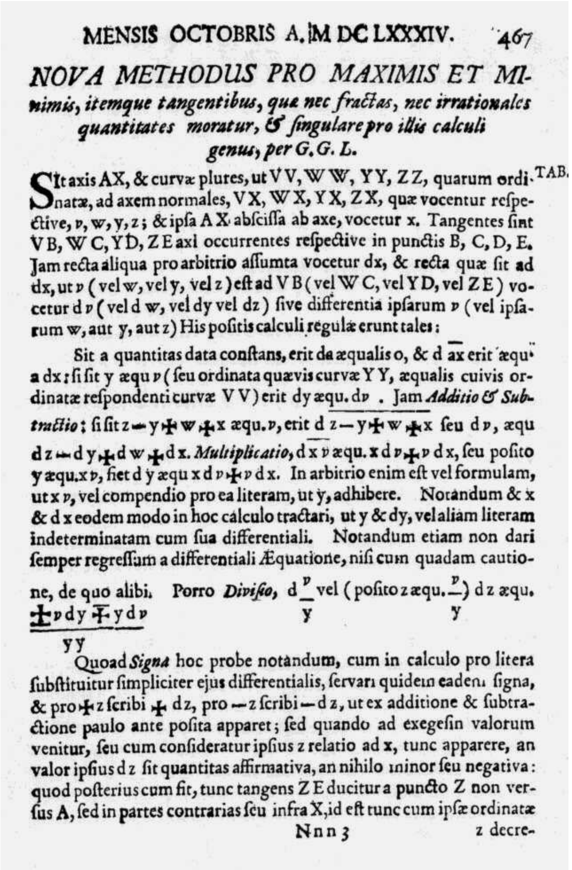
The book begins with some material directly from calculus. Partly this is a review and partly a presentation of elementary material needed to solve differential equations numerically. Next, we study the particular issues that arise in different classes of equations by studying a set of simple model problems from physics, mechanics and biology. The scope is then widened to cover basic linear models for heat conduction, wave propagation, fluid flow and elastic structures. The companion volume extends the scope further to nonlinear differential equations and systems of equations modeling a variety of phenomena including reaction-diffusion, fluid flow and many-body dynamics and reaches the frontiers of research.

Covering most of the material in this book would provide a good preparation and a flexible set of tools for many of the problems that are met in engineering and science undergraduate courses. It is essential to do a good portion of the problems given in the text in order to master the subject. We mark the more difficult and tedious problems (but they must be all the more rewarding, right?) with warnings and often give hints. A companion volume called *Advanced Computational Differential Equations* leads into graduate level, including material on nonlinear differential equations and implementation. Another companion book, *Introduction to Computational Differential Equations*, contains additional material on calculus and linear algebra, hints to problems in this volume and suggestions for project work.

The presentation is unified in the sense that it is always essentially the same set of basic tools that are put to use independently of the level of complexity of the underlying differential equation. The student will discover this gradually going through the material. The methodology is always presented in the simplest possible context to convey an essential idea, which later is applied to successively more complex problems just by "doing the same". This means that a thorough understanding of the simplest case is the best investment; for the student with limited time or energy this minimal preparation allows him or her to computationally address complex problems without necessarily having to go into all the details, because the main ideas have been grasped in a simple case. Thus, we seek to minimize the technical mathematical difficulties while keeping the essence of the ideas.

On the other hand, some ideas cannot be explained in just one application. As a result, the presentation in the simple cases may occasionally seem lengthy, like for instance the careful proof of the Fundamental Theorem of Calculus. But, the reader should feel confident that we have a carefully thought out plan in our minds and some reason for presenting the material in this way.

The book is supplemented by the software Cards and Femlab, where the algorithms presented in the book are implemented. This gives the possibility of a problem/project-oriented approach, where the student may test the performance of the algorithms and his own ideas of application and improvement, and get a direct experience of the possibilities of computational mathematical modeling. Femlab may also be used as a basis for code development in project-oriented work. Femlab is available through the World Wide Web by accessing http://www.math.chalmers.se/femlab. The software is presented in the introductory companion volume.



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NOVA METHODUS PRO MAXIMIS ET MInimis, itemque tangentibus, quæ nec fractas, nec irrationales quantitates moratur, & ſingulare pro illis calculi genus, per G. G. L.

Sit axis AX, & curvæ plures, ut VV, WW, YY, ZZ, quarum ordinatæ, ad axem normales, VX, WX, YX, ZX, quæ vocentur reſpective, v, w, y, z; & ipſa AX abſciſſa ab axe, vocetur x. Tangentes ſint VB, WC, YD, ZE axi occurrentes reſpective in punctis B, C, D, E. Jam recta aliqua pro arbitrio aſſumta vocetur dx, & recta quæ ſit ad dx, ut v (vel w, vel y, vel z) eſt ad VB (vel WC, vel YD, vel ZE) vocetur dv (vel dw, vel dy vel dz) ſive differentia ipſarum v (vel ipſarum w, aut y, aut z) His poſitis calculi regulæ erunt tales: TAB.

Sit a quantitas data conſtans, erit da æqualis 0, & d $\overline{ax}$ erit æqu. a dx; ſi ſit y æqu v (ſeu ordinata quævis curvæ YY, æqualis cuivis ordinatæ reſpondenti curvæ VV) erit dy æqu. dv. Jam *Additio & Subtractio*: ſi ſit z − y + w + x æqu. v, erit d $\overline{z - y + w + x}$ ſeu dv, æqu dz − dy + dw + dx. *Multiplicatio*, d $\overline{xv}$ æqu. x dv + v dx, ſeu poſito y æqu. xv, fiet dy æqu x dv + v dx. In arbitrio enim eſt vel formulam, ut xv, vel compendio pro ea literam, ut y, adhibere. Notandum & x & dx eodem modo in hoc calculo tractari, ut y & dy, vel aliam literam indeterminatam cum ſua differentiali. Notandum etiam non dari ſemper regreſſum a differentiali Æquatione, niſi cum quadam cautione, de quo alibi. Porro *Diviſio*, d $\frac{v}{y}$ vel (poſito z æqu. $\frac{v}{y}$) dz æqu. $\frac{\pm v\,dy \mp y\,dv}{yy}$

Quoad *Signa* hoc probe notandum, cum in calculo pro litera ſubſtituitur ſimpliciter ejus differentialis, ſervari quidem eadem ſigna, & pro + z ſcribi + dz, pro − z ſcribi − dz, ut ex additione & ſubtractione paulo ante poſita apparet; ſed quando ad exegeſin valorum venitur, ſeu cum conſideratur ipſius z relatio ad x, tunc apparere, an valor ipſius dz ſit quantitas affirmativa, an nihilo minor ſeu negativa: quod poſterius cum fit, tunc tangens ZE ducitur a puncto Z non verſus A, ſed in partes contrarias ſeu infra X, id eſt tunc cum ipſæ ordinatæ

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Figure 1.3: Leibniz's first paper on calculus, Acta Eruditorum, 1684.