

Scientific Computing and Differential Equations

An Introduction to Numerical Methods

Gene H. Golub ■ James M. Ortega

UNIVERSITÄT
DUISBURG
ESSEN

4140, boul. Décarie, bureau 400

Montréal, Québec H3A 2K4

912 289

Scientific Computing and Differential Equations

An Introduction to Numerical Methods

Scientific Computing and Differential Equations

An Introduction to Numerical Methods

Gene H. Golub

Computer Science Department
Stanford University
Stanford, California



James M. Ortega

Institute for Parallel Computation
School of Engineering and
Applied Science
University of Virginia
Charlottesville, Virginia



Academic Press
San Diego New York Boston
London Sydney Tokyo Toronto

This book is printed on acid-free paper. ∞

Copyright ∞ 1992, 1981 by Academic Press

All rights reserved.

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the publisher.

Academic Press

A Division of Harcourt Brace & Company

525 B Street, Suite 1900, San Diego, California 92101-4495

United Kingdom Edition published by

ACADEMIC PRESS LIMITED

24-28 Oval Road, London NW1 7DX

Library of Congress Cataloging-in-Publication Data

Golub, Gene H. (Gene Howard), 1932-

Scientific computing and differential equations : an introduction to numerical methods / Gene H. Golub, James M. Ortega.

p. cm.

Rev. ed. of : Introduction to numerical methods for differential equations / James M. Ortega, 1981.

Includes bibliographical references and index.

ISBN 0-12-289255-0

I. Differential equations — Numerical solutions — Data processing.

II. Ortega, James M., 1932- . III. Ortega, James M., 1932-

Introduction to numerical methods for differential equations.

III. Title.

QA371.G62 1992

515'.35—dc20

91-20106

CIP

Dedicated to the Memory of

George Forsythe

who taught us to try to light the fire,

not fill the bucket

Table of Contents

Preface	ix
Chapter 1. The World of Scientific Computing	1
1.1 What is Scientific Computing?	1
1.2 Mathematical Modeling	3
1.3 The Process of Numerical Solution	6
1.4 The Computational Environment	11
Chapter 2. Letting It Fly: Initial Value Problems	15
2.1 Examples of Initial Value Problems	15
2.2 One-Step Methods	20
2.3 Polynomial Interpolation	37
2.4 Multistep Methods	45
2.5 Stability, Instability, and Stiff Equations	55
Chapter 3. Pinning It Down: Boundary Value Problems	67
3.1 The Finite Difference Method for Linear Problems	67
3.2 Solution of the Discretized Problem	80
Chapter 4. More on Linear Systems of Equations	89
4.1 Introduction and Least Squares Problems	89
4.2 Gaussian Elimination	101
4.3 Interchanges	112
4.4 Ill-conditioning and Error Analysis	122
4.5 Other Factorizations	133

Chapter 5. Life Is Really Nonlinear	145
5.1 Nonlinear Problems and Shooting	145
5.2 Solution of a Single Nonlinear Equation	149
5.3 Systems of Nonlinear Equations	166
Chapter 6. Is There More Than Finite Differences?	179
6.1 Introduction to Projection Methods	179
6.2 Spline Approximation	187
6.3 Numerical Integration	193
6.4 The Discrete Problem Using Splines	202
Chapter 7. N Important Numbers	211
7.1 Eigenvalue Problems	211
7.2 The QR Method	224
7.3 Other Iterative Methods	234
Chapter 8. Space and Time	247
8.1 Partial Differential Equations	247
8.2 Explicit Methods and Stability	253
8.3 Implicit Methods	262
8.4 Semidiscrete Methods	267
Chapter 9. The Curse of Dimensionality	273
9.1 Two and Three Space Dimensions	273
9.2 Direct Methods	283
9.3 Iterative Methods	292
Appendix 1. Analysis and Differential Equations	309
Appendix 2. Linear Algebra	315
Bibliography	321
Author Index	329
Subject Index	333

Preface

This book is a revision of *Introduction to Numerical Methods for Differential Equations* by J. M. Ortega and W. G. Poole, Jr., published by Pitman Publishing, Inc., in 1981.

As discussed in Chapter 1, a large part of scientific computing is concerned with the solution of differential equations and, thus, differential equations is an appropriate focus for an introduction to scientific computing. The need to solve differential equations was one of the original and primary motivations for the development of both analog and digital computers, and the numerical solution of such problems still requires a substantial fraction of all available computing time. It is our goal in this book to introduce numerical methods for both ordinary and partial differential equations with concentration on ordinary differential equations, especially boundary-value problems. Although there are many existing packages for such problems, or at least for the main subproblems such as the solution of linear systems of equations, we believe that it is important for users of such packages to understand the underlying principles of the numerical methods. Moreover, it is even more important to understand the limitation of numerical methods: "Black Boxes" can't solve all problems. Indeed, it may be that one has several excellent black boxes for solving classes of problems, but the combination of such boxes may yield less than optimal results.

We treat initial-value problems for ordinary differential equations in Chapter 2 and introduce finite difference methods for linear boundary value problems in Chapter 3. The latter problems lead to the solution of systems of linear algebraic equations; Chapter 4 is devoted to the general treatment of direct methods for this problem, independently of any connection to differential equations. This chapter also considers the important problem of least-squares approximation. In Chapter 5 we return to boundary value problems, but now they are nonlinear. This motivates the treatment of the solution of nonlinear algebraic equations in the remainder of the chapter. The tool for discretizing differential equations to this point has been finite difference methods; in Chapter 6 we introduce Galerkin and collocation methods as alternatives. These methods lead to the important subtopics of numerical integration and spline approx-

imation. Chapter 7 treats eigenvalue problems, motivated only partially by differential equations. Finally, in Chapters 8 and 9, we introduce some of the simplest methods for partial differential equations, first initial-boundary-value problems and then boundary-value problems.

As the previous paragraph indicates, the solution of differential equations requires techniques from a variety of other areas of numerical analysis: solution of linear and nonlinear algebraic equations, interpolation and approximation, integration, and so on. Thus, most of the usual topics of a first course in numerical methods are covered and the book can serve as text for such a course. Indeed, we view the book to be basically for this purpose but oriented toward students primarily interested in differential equations. We have found the organization of the book, which may seem rather unorthodox for a first course, to be more satisfactory and motivating than the usual one for a rather large number of students. Thus, the book can be used for a variety of different audiences, depending on the background of the students and the purposes of the course.

As a minimum background, the reader is assumed to have had calculus, first courses in computer programming and differential equations and at least some linear algebra. Some basic facts from calculus, differential equations and linear algebra are collected in two appendices and further background material appears in the text itself. Students with a minimum background and no prior numerical methods course will require a full year to cover the book completely; one semester or two quarter courses can easily be taught by eliminating some topics. On the other hand, the entire book is covered in a first-semester graduate course at the University of Virginia; in this case, much of the more elementary material is review and is covered quickly.

The style of the book is on the theoretical side, although rather few theorems are stated as such and many proofs are either omitted or partially sketched. On the other hand, enough mathematical argumentation is usually given to clarify what the mathematical properties of the methods are. In many cases, details of the proofs are left to exercises or to a supplementary discussion section, which also contains references to the literature. We have found this style quite satisfactory for most students, especially those outside of mathematics.

The development of numerical methods for solving differential equations has evolved to a state where accurate, efficient, and easy-to-use mathematical software exists for solving many of the basic problems. For example, excellent subroutine libraries are available for the initial-value problems of Chapter 2, linear equations of Chapter 4, and eigenvalue problems of Chapter 7. The supplementary discussions and references at the ends of sections give information on available software. On the other hand, some of the exercises require the reader to write programs to implement some of the basic algorithms for these same problems. The purpose of these exercises is not to develop high-grade

software but, rather, to have the reader experience what is involved in coding the algorithms, thus leading to a deeper understanding of them.

We owe thanks to many colleagues and students for useful comments on the original version of this book as well as drafts of the current one. We are also indebted to Ms. Susanne Freund and Ms. Brenda Lynch for their expert LaTeXing of the manuscript.

Stanford, California
Charlottesville, Virginia