MACHINE METHODS FOR SOLVING PROBLEMS OF APPLIED MATHEMATICS. ALGEBRA, APPROXIMATION OF FUNCTIONS, ORDINARY DIFFERENTIAL EQUATIONS
PREFACE

The penetration of the computing machinery and information technologies into all spheres of human’s activity is a characteristic feature of the information society. A triad: computers, mathematical models and methods for solving equations describing mathematical models on computers is a tool for the cognition of the contemporary world as well as for the creation of the new machinery specimens that contributes to progress in science and technology.

In our opinion, it is the creation and theoretical investigation of both various-level models as to the fields of application and computer methods for solving equations describing mathematical models with approximately given initial data that represents the subject matter of the applied mathematics.

A distinctive characteristic of applied mathematics' problems is the fact that along with mathematical equations describing models, the initial data error should be considered and taken into account and, in the long run, the reliability of the obtained computer results should be guaranteed.

A problem of the reliability of computer solutions to scientific and engineering problems involves two natural aspects: the reliability of mathematical models describing a real-life problem and the reliability of computer solution to equations describing mathematical model of either object or phenomenon under investigation.

An objective of the monography is to describe both a research procedure and algorithms for solving mathematical problems with approximately given initial data on computers, as well as the reliability analysis of machine solutions to scientific and engineering problems that can be reduced to problems of computational mathematics.

The monography being proposed is the reflection of computational procedure created by the numerical software and problems solving department of V.M. Glushkov Institute of cybernetics of the National Academy of Sciences of Ukraine.

During a long period of time the author jointly with his colleagues from the department of the numerical software and solving problems were engaged in the solving of real-life problems in the interest of industry, as well as in the creation of the numerical software for various-architecture computers and had an opportunity to correlate numerical results with results of natural experiments carried out by industrial enterprises. The real-life problems have been solved on the following computers: ES EVM (a Soviet counterpart of IBM/360), ES 1766 MIMD-computer, transputer systems, Parsytect Explorer MIMD-computer. By means of the finite-element method [156] a number of real-life problems have been reduced to the solving of either linear algebraic systems with dense matrices whose order had attained ten thousand or linear algebraic systems with band matrices whose order had attained several tens of thousands, to the solving of
generalized or standard matrix problems with either band or dense matrices, as well as to the solving of non-linear systems with Jacoby matrices, both band and dense, whose order had attained ten thousand. Besides, initial-value problems for systems of ordinary differential equations, the number of equations being equal to five hundred, as well as systems of equations non-solvable with respect to the first derivative. Those problems arising in the solving of real-life problems reducible to problems of the computational mathematics were selected [108] and they were illustrated by simplest examples given in the monography. The surmounting of difficulties so as to the data of numerical experiments correlate with data of natural experiments resulted in the development of a methodology for solving real-life problems presented in the monography being proposed to the reader.

This methodology served as a basis for the creation of intelligent numerical software and, finally, for the development of the Inparcom MIMD-computers whose structure and architecture support an intelligent software.

Intelligent Inparcom MIMD-computers are the knowledge-oriented computers and intended for the investigating and solving of problems with approximately given initial data occurring in science and engineering.

Inparcom enables to formulate a problem in computer in terms of the subject area language and automatically investigate characteristics of machine model of the problem with approximately given initial data; according to the revealed characteristics and with taking into account mathematical and engineering characteristics of the computer to determine the number of processors required for the solving of problem and construct both an algorithm and computational scheme; to form a topology on the basis of the MIMD-computer’s microprocessors so as to solve the problem with minimal consumption of the machine time; according to this configuration to synthesize a parallel program; to solve the problem and estimate both the reliability of the obtained computer solution(i.e. estimate the proximity between machine and mathematical solutions) and inherited error in the mathematical solution of the problem: to visualize the obtained results in terms of the subject area language.

As a rule, each chapter of the monography contains the following: a statement of the problem; some relevant reference information from other branches of mathematics; basic concepts and ideas inherent in every class of problems; numerical solution methods; investigation methodology for the numerical methods which can be used for solving non-standard (non-classic) problems (its utilization is shown on the simplest problems); a description of difficulties and pitfalls arising in the implementation of algorithms on a computer; analysis procedure for the reliability of the solution being obtained; concluding remarks analyzing up-to-data state of arts and perspectives for solution methods in every class of problems.

I am indebted to T.V. Chistyakova, A.N. Khimich, A.V. Popov, Ye.F. Galba and M.F. Yakovlev for their numerous helpful suggestions. I also would like to
thank T.V. Chistyakova, Ye.G. Geez, T.A. Gerasimova and Yu.M. Orishchak for their assistance in preparation of the book. I am very grateful to everybody who assisted me in seeing the book through press.

The book is addressed to specialists engaged in posing and solving scientific and engineering problems with approximately given initial data on computers, to senior and post-graduate students mastering engineering, physics and mathematics.
CONTENTS

1. INTRODUCTION

1.1. STATEMENT OF THE APPLIED MATHEMATICS PROBLEMS

1.2. SOME INFORMATION FROM A THEORY OF ERRORS

1.3. CAUSES GIVING RISE TO ERRORS

2. DIRECT METHODS FOR SOLVING LINEAR ALGEBRAIC SYSTEMS

2.1. STATEMENT OF THE PROBLEM, DEFINITIONS, GENERAL PROPERTIES

2.2. CLASSIFICATION OF LINEAR ALGEBRAIC SYSTEMS DESCRIBING REAL–LIFE PROBLEMS

2.3. PROBLEMS ARISING IN SOLVING LINEAR ALGEBRAIC SYSTEMS ON COMPUTERS

2.4. SOME DIRECT METHODS FOR SOLVING LINEAR ALGEBRAIC
1. The Gauss-Seidel method .................................................. 105
2. The upper relaxation method ............................................. 107

3.4. SOME QUESTIONS RELATED TO THE MACHINE IMPLEMENTATION OF ONE-STEP ITERATIVE PROCESSES .............. 109
   1. Examples of theoretically convergent processes non-implementable on computers ............................................. 109
   2. Some questions related to reliability of solutions obtained by iterative methods ............................................... 110

CONCLUDING REMARKS .................................................. 112

4. METHODS FOR THE EVALUATING OF EIGENVALUES AND EIGENVECTORS OF MATRICES ............................................. 118

4.1. RELEVANT INFORMATION FROM THE LINEAR ALGEBRA .... 118
   1. Statement of the problem ............................................... 118
   2. Some properties of eigenvalues of a symmetric tridiagonal matrix ................................................................. 119
   3. Orthogonal matrices ................................................... 121
   4. Elementary rotation matrices ........................................ 122
   5. The reflection matrices ............................................... 123
   6. The Jordan’s canonical form ......................................... 124
   7. Elementary divisors ................................................... 126

4.2. THE CONDITIONING OF MATRICES IN EIGENVALUE PROBLEMS ................................................................. 127
   1. Statement of computational eigenvalue problems ............... 127
   2. The conditioning of matrices when finding the eigenvalues ... 128
   3. The conditioning of matrices when finding eigenvectors ...... 129
   4. The conditioning of matrices when evaluating eigenvalues and eigenvectors of normal matrices ......................... 130
   5. The machine implementation error of algorithms ............... 130

4.3. SOME METHODS FOR SOLVING A FULL EIGENVALUE PROBLEM ................................................................. 132
   1. Preliminary information ............................................... 132
   2. The Jacobi method .................................................... 132
   3. The Householder’s method for reducing a symmetric matrix to the tridiagonal form ........................................ 138
   4. The Givens’s and Schwarz’s methods for reducing a symmetric matrix to the tridiagonal form .............................. 140
   5. The QR- and QL-methods ............................................. 143
   6. The QL-method for finding eigenvalues of a symmetric tridiagonal
7. Estimates for the reliability of solutions to systems with rectangular and square singular matrices ............................................................. 196

5.3. ITERATIVE METHODS FOR SOLVING SYSTEMS POSSESSING NON-UNIQUE SOLUTIONS AND NON-CONSISTENT SYSTEMS WITH SYMMETRIC POSITIVE SEMI-DEFINITE MATRICES ........................................... 198

1. Methods for solving systems with non-unique solution ................... 198
2. Iterative methods for the obtaining of a generalized solution for one class of non-consistent linear algebraic systems .......................... 200
CONCLUDING REMARKS ................................................................. 205

6. METHODS FOR SOLVING NON-LINEAR ALGEBRAIC AND TRANSCENDENTAL EQUATIONS ................................................................. 209

6.1. STATEMENT OF THE PROBLEM, DEFINITIONS, SOME GENERAL INFORMATION .......................................................... 209

1. Problem on the reflection of a sonic wave on the division boundary of two environments .............................................................. 209
2. Non-linear systems ..................................................................... 211
3. Non-linear equations in one unknown ......................................... 213

6.2. NUMERICAL SOLVING OF NON-LINEAR EQUATIONS IN ONE UNKNOWN ............................................................ 215

1. Non-linear algebraic equations describing physical models ............ 215
2. Location of roots ...................................................................... 217
3. Theorem on the stationary point ................................................... 219
4. The construction principle for one-step iterative processes .......... 220
5. Evaluation of all real roots in the interval ..................................... 225
6. Secants' method ........................................................................ 227
7. Evaluation of complex roots of transcendental equations .............. 229
8. Numerical solution of polynomial equations ................................. 232
9. Machine implementation error ..................................................... 235

6.3. THE SOLVING OF NON-LINEAR SYSTEMS .............................................. 236

1. Preliminary remarks .................................................................... 236
2. The simple iteration method ........................................................ 238
3. The Newton’s method .................................................................. 241
4. The quasi-Newton-type methods .................................................. 242
CONCLUDING REMARKS ................................................................. 246
8.2 ONE-STEP METHODS

1. Basic concepts in the numerical integration of initial-value problems 319
2. Euler-Cauchy method with iterations 331
3. The Runge-Kutta methods 338
4. Methods based on the Darbu-Obreshkov decomposition 351
5. Construction of explicit methods for investigating and integrating systems of ordinary differential equations with an a priori given accuracy 353
6. Construction of implicit methods for investigating and integrating systems of ordinary differential equations with an a priori given accuracy 357

8.3 MULTISTEP METHODS 362

1. Adams methods 362
2. Implicit Curtiss – Hirschfelder’s methods 368
3. Convergence and numerical stability of multi-step methods 369
4. Gear’s method 371

CONCLUDING REMARKS 372

LITERATURE 375

INDEX 388