TABLE OF CONTENTS

Preface xi

1. Observations on the Mathematical Software Effort
   — *W. J. Cody* 1

   Introduction 1
   The Past 2
   The Present 7
   The Future 12
   References 14

2. LINPACK — A Package for Solving Linear Systems
   — *J. J. Dongarra and G. W. Stewart* 20

   Introduction 20
   History 21
   LINPACK and Matrix Decomposition 22
   Nomenclature and Conventions 25
   The Square Part of LINPACK 27
   The Least Squares Part of LINPACK 31
   Numerical Properties 34
   Efficiency 37
   Design and Implementation 39
   Testing 43
   Conclusions 45
   References 47

3. FUNPACK — A Package of Special Function Routines
   — *W. J. Cody* 49

   Introduction 49
   History 50
   Design 53
   Implementation 57
   Tuning and Testing 61
   Retrospect 63
   Acknowledgments 64
   References 65

4. EISPACK — A Package for Solving Matrix Eigenvalue Problems
— *J. J. Dongarra and C. B. Moler* 68

Introduction 68
History 69
Organization 72
Algorithms 76
Numerical Properties 82
EISPACK-3 85
References 87

5. The MINPACK Project
— *J. Moré, D. Sorensen, B. Garbow, and K. Hillstrom* 88

Introduction 88
History 89
Algorithms 91
Scale Invariant Algorithms 95
Robust Software 98
Convergence Testing 100
User Interface 103
Documentation 104
Transportability 106
Concluding Remarks 109
References 109

6. Software for Ordinary Differential Equations
— *L. F. Shampine and H. A. Watts* 112

Introduction 112
Mathematical Problem 113
Numerical Methods and Codes 114
Software Matters for Solutions Output 115
Error Control 117
Choice of Step Size 121
Accuracy Considerations 122
Specifying the Differential Equations 124
Storage Management and Levels of Codes 126
Providing User Assistance 127
Choosing a Code 128
DEPAC Software 129
Summary 130
References 130

7. Sources of Information on Quadrature Software
— *D. Kahaner* 134

Introduction 134
One-Dimensional Quadrature 135
Quadrature Formulas 135

Gaussian Quadrature 137
Kronrod Quadrature 138

Using Quadrature Formulas 140
Automated Quadrature Programs 141

Program 1: Direct Communication 141
Program 2: Reverse Communication 142
Program 3: An ODE-like Adaptive Quadrature 143
Program 4: Model 1970 Adaptive Quadrature 144
Program 5: Modern Global Adaptive Quadrature 147

Multidimensional Quadrature 148
Iterated Integral 148

Program 6: Evaluation of 2-D Iterated Integrals 149

Pure Multidimensional Methods 150

Korobov Quadrature 151
Monte Carlo Quadrature 152

Software in the Standard Libraries 152
References 161

8. A Survey of Sparse Matrix Software
— *Iain S. Duff* 165

Introduction 165
Direct Solution of Linear Equations 167
Iterative Methods 171
Elliptic Partial Differential Equations 175
Eigensystems 179
Least-Squares Problems 182
Nonlinear Systems 183
Linear Programming 184
Sparse Matrix Packages 185

Acknowledgments 186
References 186

9. Mathematical Software for Elliptic Boundary Value Problems
— *Ronald F. Boisvert and Roland A. Sweet* 200

Mathematical Preliminaries 201

The Operator 201
The Domain 203
The Boundary Conditions 203
Example 1 206
Example 2 206

Algorithmic Issues 207

Approximation Methods 207
Solution Algorithms 210

Software Engineering Issues 214

Basic Software Organization 214
Representation of Input and Output 218
Testing and Evaluation 222
Distribution and Maintenance 224

Case Studies 224

Case Study: FISHPAK 224
Example 3 228
Example 4 229
Example 5 230
Case Study: ELLPACK 231

Sources of Software for Partial Differential Equations 237

Commercial Libraries 237
Software Clearing Houses 237
Journals That Distribute Software 238
Journals That Publish Descriptions of Programs 238

Catalog of Software for Elliptic Problems 238
References 255
Appendix A: Solution of Example 3 Using FISHPAK 261

Appendix B: List of Contributors to ELLPACK 263

10. The IMSL Library
— *Thomas J. Aird* 264

Introduction 264

IMSL Company History 264
Company Organization and Advisory Board 267
Facts about the IMSL Library 268
Library Contents 269
Documentation 276
Support 278
Availability 279
Subscription Fees and Policies 280

Library Development 281

The Research and Development Organization 283
The Development System 284

References 291
Appendix A: Sample Chapter Documentation 292
Appendix B: Sample Subroutine Documentation 297
Appendix C: Fortran Reference Manuals 300

11. The SLATEC Common Mathematical Library
— *Bill L. Buzbee* 302

Introduction 302

Motivations 302

Organization and Administration 304

Goals 304

Library Development 305

Portability 305
Standards 306
Code Selections 306

Documentation 310

Quick Checks 310
Disclaimer 310
Classification System 311
Abstracts 311
Distribution of Library Source 311
Maintenance 311
Unexpected Benefits from SLATEC 312
Future Plans 312
Lessons Learned 313
Acknowledgments 315
References 316
Appendix A: SLATEC Programming Standards 319
Appendix B: Prologue Comment Cards for Documentation Program 320

12. The Boeing Mathematical Software Library
— *A. H. Erisman, K. W. Neves, and I. R. Philips* 321

Introduction 321
The Boeing Library as a Product 321
The Boeing Library as a User Tool 326
The Boeing Library as a Project 330
The Boeing Library: History and Future 332
Summary 335
Acknowledgments 336
References 337
Appendix: BCSLIB Standards 338

13. The PORT Mathematical Subroutine Library
— *Phyllis Fox* 346

Motivation and History of Development 346

Portability 346
PORT's Development in a Research Setting 350

The PORT Framework 351

Error Handling 351
Dynamic Storage Allocation Using a Stack 352
Language Considerations 353
Modularity 353

Testing — An Axiomatic Approach 354

Documentation And Installation 355

User Reference Sheets 355
Installation 356

PORT Sites 356
Current PORT-related Activities 357

Benchmarking 357
Monitoring PORT 358

Summary 358
References 358
Appendix A: Determination of Correct Floating-Point Model Parameters — *N. L. Schryer* 360
Appendix B: Definition of Real Floating-Point Quantities: R1MACH 367
Appendix C: PORT User Reference Sheets: Example 372

14. The Evolving NAG Library Service — *Brian Ford and James C. T. Pool* 375

Introduction 375
History of NAG 376
NAG Library "Machine" 377

Contribution 378
Validation 379
Assembly 379
Implementation 382
Distribution 383
Maintenance/Service 383

Library Contents 384

Hierarchy of Software 384
Organization of the Library and Documentation 385
Algorithmic Content 387

Evolution of the NAG Fortran Library 390

High-Performance Computers 390
Fortran Standards 391
Mark 11 of the NAG Fortran Library 391

The Fortran Programming Environment 393

Interactive Access to Documentation 393
Graphics 394
Software Tools 395
The Future Scientific Workstation

Conclusion 396
References 396

Subject Index 399