Chebyshev and Fourier Spectral Methods

Second Edition

John P. Boyd

University of Michigan
Ann Arbor, Michigan 48109-2143
email: jpboyd@engin.umich.edu
http://www-personal.engin.umich.edu/∼jpboyd/

2000

DOVER Publications, Inc.
31 East 2nd Street
Mineola, New York 11501

Dedication

To Marilyn, Ian, and Emma

“A computation is a temptation that should be resisted as long as possible.”

— J. P. Boyd, paraphrasing T. S. Eliot

Contents

PREFACE **x**

Acknowledgments **xiv**

Errata and Extended-Bibliography **xvi**

1 Introduction **1**
1.1 Series expansions 1
1.2 First Example 2
1.3 Comparison with finite element methods 4
1.4 Comparisons with Finite Differences 6
1.5 Parallel Computers 9
1.6 Choice of basis functions 9
1.7 Boundary conditions 10
1.8 Non-Interpolating and Pseudospectral 12
1.9 Nonlinearity 13
1.10 Time-dependent problems 15
1.11 FAQ: Frequently Asked Questions 16
1.12 The Chrysalis 17

2 Chebyshev & Fourier Series **19**
2.1 Introduction 19
2.2 Fourier series 20
2.3 Orders of Convergence 25
2.4 Convergence Order 27
2.5 Assumption of Equal Errors 31
2.6 Darboux's Principle 32
2.7 Why Taylor Series Fail 35
2.8 Location of Singularities 36
2.8.1 Corner Singularities & Compatibility Conditions 37
2.9 FACE: Integration-by-Parts Bound 41
2.10 Asymptotic Calculation of Fourier Coefficients 45
2.11 Convergence Theory: Chebyshev Polynomials 46
2.12 Last Coefficient Rule-of-Thumb 50
2.13 Convergence Theory for Legendre Polynomials 51
2.14 Quasi-Sinusoidal Rule of Thumb 54
2.15 Witch of Agnesi Rule–of–Thumb 56
2.16 Boundary Layer Rule-of-Thumb 57

3 Galerkin & Weighted Residual Methods **61**
3.1 Mean Weighted Residual Methods 61
3.2 Completeness and Boundary Conditions 64
3.3 Inner Product & Orthogonality 65
3.4 Galerkin Method 67
3.5 Integration-by-Parts 68
3.6 Galerkin Method: Case Studies 70
3.7 Separation-of-Variables & the Galerkin Method 76
3.8 Heisenberg Matrix Mechanics 77
3.9 The Galerkin Method Today 80

4 Interpolation, Collocation & All That **81**
4.1 Introduction 81
4.2 Polynomial interpolation 82
4.3 Gaussian Integration & Pseudospectral Grids 86
4.4 Pseudospectral Is Galerkin Method via Quadrature 89
4.5 Pseudospectral Errors 93

5 Cardinal Functions **98**
5.1 Introduction 98
5.2 Whittaker Cardinal or "Sinc" Functions 99
5.3 Trigonometric Interpolation 100
5.4 Cardinal Functions for Orthogonal Polynomials 104
5.5 Transformations and Interpolation 107

6 Pseudospectral Methods for BVPs **109**
6.1 Introduction 109
6.2 Choice of Basis Set 109
6.3 Boundary Conditions: Behavioral & Numerical 109
6.4 "Boundary-Bordering" 111
6.5 "Basis Recombination" 112
6.6 Transfinite Interpolation 114
6.7 The Cardinal Function Basis 115
6.8 The Interpolation Grid 116
6.9 Computing Basis Functions & Derivatives 116
6.10 Higher Dimensions: Indexing 118
6.11 Higher Dimensions 120
6.12 Corner Singularities 120
6.13 Matrix methods 121
6.14 Checking 121
6.15 Summary 123

7 Linear Eigenvalue Problems **127**
7.1 The No-Brain Method 127
7.2 QR/QZ Algorithm 128
7.3 Eigenvalue Rule-of-Thumb 129
7.4 Four Kinds of Sturm-Liouville Problems 134
7.5 Criteria for Rejecting Eigenvalues 137
7.6 "Spurious" Eigenvalues 139
7.7 Reducing the Condition Number 142
7.8 The Power Method 145
7.9 Inverse Power Method 149

7.10 Combining Global & Local Methods 149
7.11 Detouring into the Complex Plane 151
7.12 Common Errors 155

8 Symmetry & Parity **159**
8.1 Introduction 159
8.2 Parity 159
8.3 Modifying the Grid to Exploit Parity 165
8.4 Other Discrete Symmetries 165
8.5 Axisymmetric & Apple-Slicing Models 170

9 Explicit Time-Integration Methods **172**
9.1 Introduction 172
9.2 Spatially-Varying Coefficients 175
9.3 The Shamrock Principle 177
9.4 Linear and Nonlinear 178
9.5 Example: KdV Equation 179
9.6 Implicitly-Implicit: RLW & QG 181

10 Partial Summation, the FFT and MMT **183**
10.1 Introduction 183
10.2 Partial Summation 184
10.3 The Fast Fourier Transform: Theory 187
10.4 Matrix Multiplication Transform 190
10.5 Costs of the Fast Fourier Transform 192
10.6 Generalized FFTs and Multipole Methods 195
10.7 Off-Grid Interpolation 198
10.8 Fast Fourier Transform: Practical Matters 200
10.9 Summary 200

11 Aliasing, Spectral Blocking, & Blow-Up **202**
11.1 Introduction 202
11.2 Aliasing and Equality-on-the-Grid 202
11.3 “2 h-Waves” and Spectral Blocking 205
11.4 Aliasing Instability: History and Remedies 210
11.5 Dealiasing and the Orszag Two-Thirds Rule 211
11.6 Energy-Conserving: Constrained Interpolation 213
11.7 Energy-Conserving Schemes: Discussion 214
11.8 Aliasing Instability: Theory 216
11.9 Summary 218

12 Implicit Schemes & the Slow Manifold **222**
12.1 Introduction 222
12.2 Dispersion and Amplitude Errors 224
12.3 Errors & CFL Limit for Explicit Schemes 226
12.4 Implicit Time-Marching Algorithms 228
12.5 Semi-Implicit Methods 229
12.6 Speed-Reduction Rule-of-Thumb 230
12.7 Slow Manifold: Meteorology 231
12.8 Slow Manifold: Definition & Examples 232
12.9 Numerically-Induced Slow Manifolds 236
12.10Initialization 239

12.11 The Method of Multiple Scales(Baer-Tribbia) 241
12.12 Nonlinear Galerkin Methods 243
12.13 Weaknesses of the Nonlinear Galerkin Method 245
12.14 Tracking the Slow Manifold 248
12.15 Three Parts to Multiple Scale Algorithms 249

13 Splitting & Its Cousins **252**
13.1 Introduction 252
13.2 Fractional Steps for Diffusion 255
13.3 Pitfalls in Splitting, I: Boundary Conditions 256
13.4 Pitfalls in Splitting, II: Consistency 258
13.5 Operator Theory of Time-Stepping 259
13.6 High Order Splitting 261
13.7 Splitting and Fluid Mechanics 262

14 Semi-Lagrangian Advection **265**
14.1 Concept of an Integrating Factor 265
14.2 Misuse of Integrating Factor Methods 267
14.3 Semi-Lagrangian Advection: Introduction 270
14.4 Advection & Method of Characteristics 271
14.5 Three-Level, 2D Order Semi-Implicit 273
14.6 Multiply-Upstream SL 275
14.7 Numerical Illustrations & Superconvergence 277
14.8 Two-Level SL / SI Algorithms 280
14.9 Noninterpolating SL & Numerical Diffusion 281
14.10 Off-Grid Interpolation 283
14.10.1 Off-Grid Interpolation: Generalities 283
14.10.2 Spectral Off-grid 284
14.10.3 Low-order Polynomial Interpolation 284
14.10.4 McGregor's Taylor Series Scheme 286
14.11 Higher Order SL Methods 286
14.12 History and Relationships to Other Methods 286
14.13 Summary 289

15 Matrix-Solving Methods **290**
15.1 Introduction 290
15.2 Stationary One-Step Iterations 291
15.3 Preconditioning: Finite Difference 293
15.4 Computing Iterates: FFT / Matrix Multiplication 297
15.5 Alternative Preconditioners 299
15.6 Raising the Order Through Preconditioning 301
15.7 Multigrid: An Overview 301
15.8 MRR Method 304
15.9 Delves-Freeman Block-and-Diagonal Iteration 307
15.10 Recursions & Formal Integration: Constant Coefficient ODEs 312
15.11 Direct Methods for Separable PDE's 314
15.12 Fast Iterations for Almost Separable PDEs 317
15.13 Positive Definite and Indefinite Matrices 318
15.14 Preconditioned Newton Flow 320
15.15 Summary & Proverbs 322

16 Coordinate Transformations **323**
16.1 Introduction . . . 323
16.2 Programming Chebyshev Methods . . . 323
16.3 Theory of 1-D Transformations . . . 325
16.4 Infinite and Semi-Infinite Intervals . . . 326
16.5 Maps for Endpoint & Corner Singularities . . . 327
16.6 Two-Dimensional Maps & Corner Branch Points . . . 329
16.7 Periodic Problems & the Arctan / Tan Map . . . 330
16.8 Adaptive Methods . . . 332
16.9 Almost-Equispaced Kosloff / Tal-Ezer Grid . . . 334

17 Methods for Unbounded Intervals **338**
17.1 Introduction . . . 338
17.2 Domain Truncation . . . 339
17.2.1 Domain Truncation for Rapidly-decaying Functions . . . 339
17.2.2 Domain Truncation for Slowly-Decaying Functions . . . 340
17.2.3 Domain Truncation for Time-Dependent Wave Propagation: Sponge Layers . . . 340
17.3 Whittaker Cardinal or "Sinc" Functions . . . 341
17.4 Hermite functions . . . 346
17.5 Semi-Infinite Interval: Laguerre Functions . . . 353
17.6 New Basis Sets via Change of Coordinate . . . 355
17.7 Rational Chebyshev Functions: TB_n . . . 356
17.8 Behavioral versus Numerical Boundary Conditions . . . 361
17.9 Strategy for Slowly Decaying Functions . . . 363
17.10 Numerical Examples: Rational Chebyshev Functions . . . 366
17.11 Semi-Infinite Interval: Rational Chebyshev TL_n . . . 369
17.12 Numerical Examples: Chebyshev for Semi-Infinite Interval . . . 370
17.13 Strategy: Oscillatory, Non-Decaying Functions . . . 372
17.14 Weideman-Cloot Sinh Mapping . . . 374
17.15 Summary . . . 377

18 Spherical & Cylindrical Geometry **380**
18.1 Introduction . . . 380
18.2 Polar, Cylindrical, Toroidal, Spherical . . . 381
18.3 Apparent Singularity at the Pole . . . 382
18.4 Polar Coordinates: Parity Theorem . . . 383
18.5 Radial Basis Sets and Radial Grids . . . 385
18.5.1 One-Sided Jacobi Basis for the Radial Coordinate . . . 387
18.5.2 Boundary Value & Eigenvalue Problems on a Disk . . . 389
18.5.3 Unbounded Domains Including the Origin in Cylindrical Coordinates 390
18.6 Annular Domains . . . 390
18.7 Spherical Coordinates: An Overview . . . 391
18.8 The Parity Factor for Scalars: Sphere versus Torus . . . 391
18.9 Parity II: Horizontal Velocities & Other Vector Components . . . 395
18.10 The Pole Problem: Spherical Coordinates . . . 398
18.11 Spherical Harmonics: Introduction . . . 399
18.12 Legendre Transforms and Other Sorrows . . . 402
18.12.1 FFT in Longitude / MMT in Latitude . . . 402
18.12.2 Substitutes and Accelerators for the MMT . . . 403
18.12.3 Parity and Legendre Transforms . . . 404

18.12.4 Hurrah for Matrix/Vector Multiplication 404
18.12.5 Reduced Grid and Other Tricks 405
18.12.6 Schuster-Dilts Triangular Matrix Acceleration 405
18.12.7 Generalized FFT: Multipoles and All That 407
18.12.8 Summary 407
18.13 Equiareal Resolution 408
18.14 Spherical Harmonics: Limited-Area Models 409
18.15 Spherical Harmonics and Physics 410
18.16 Asymptotic Approximations, I 410
18.17 Asymptotic Approximations, II 412
18.18 Software: Spherical Harmonics 414
18.19 Semi-Implicit: Shallow Water 416
18.20 Fronts and Topography: Smoothing/Filters 418
18.20.1 Fronts and Topography 418
18.20.2 Mechanics of Filtering 419
18.20.3 Spherical splines 420
18.20.4 Filter Order 422
18.20.5 Filtering with Spatially-Variable Order 423
18.20.6 Topographic Filtering in Meteorology 423
18.21 Resolution of Spectral Models 425
18.22 Vector Harmonics & Hough Functions 428
18.23 Radial/Vertical Coordinate: Spectral or Non-Spectral? 429
18.23.1 Basis for Axial Coordinate in Cylindrical Coordinates 429
18.23.2 Axial Basis in Toroidal Coordinates 429
18.23.3 Vertical/Radial Basis in Spherical Coordinates 429
18.24 Stellar Convection in a Spherical Annulus: Glatzmaier (1984) 430
18.25 Non-Tensor Grids: Icosahedral, etc. 431
18.26 Robert Basis for the Sphere 433
18.27 Parity-Modified Latitudinal Fourier Series 434
18.28 Projective Filtering for Latitudinal Fourier Series 435
18.29 Spectral Elements on the Sphere 437
18.30 Spherical Harmonics Besieged 438
18.31 Elliptic and Elliptic Cylinder Coordinates 439
18.32 Summary 440

19 Special Tricks **442**
19.1 Introduction 442
19.2 Sideband Truncation 443
19.3 Special Basis Functions, I: Corner Singularities 446
19.4 Special Basis Functions, II: Wave Scattering 448
19.5 Weakly Nonlocal Solitary Waves 450
19.6 Root-Finding by Chebyshev Polynomials 450
19.7 Hilbert Transform 453
19.8 Spectrally-Accurate Quadrature Methods 454
19.8.1 Introduction: Gaussian and Clenshaw-Curtis Quadrature 454
19.8.2 Clenshaw-Curtis Adaptivity 455
19.8.3 Mechanics 456
19.8.4 Integration of Periodic Functions and the Trapezoidal Rule 457
19.8.5 Infinite Intervals and the Trapezoidal Rule 458
19.8.6 Singular Integrands 458
19.8.7 Sets and Solitaries 460

20 Symbolic Calculations **461**
20.1 Introduction . . . 461
20.2 Strategy . . . 462
20.3 Examples . . . 465
20.4 Summary and Open Problems . . . 472

21 The Tau-Method **473**
21.1 Introduction . . . 473
21.2 τ-Approximation for a Rational Function . . . 474
21.3 Differential Equations . . . 476
21.4 Canonical Polynomials . . . 476
21.5 Nomenclature . . . 478

22 Domain Decomposition Methods **479**
22.1 Introduction . . . 479
22.2 Notation . . . 480
22.3 Connecting the Subdomains: Patching . . . 480
22.4 Weak Coupling of Elemental Solutions . . . 481
22.5 Variational Principles . . . 484
22.6 Choice of Basis & Grid . . . 485
22.7 Patching versus Variational Formalism . . . 486
22.8 Matrix Inversion . . . 487
22.9 The Influence Matrix Method . . . 488
22.10 Two-Dimensional Mappings & Sectorial Elements . . . 491
22.11 Prospectus . . . 492

23 Books and Reviews **494**

A A Bestiary of Basis Functions **495**
A.1 Trigonometric Basis Functions: Fourier Series . . . 495
A.2 Chebyshev Polynomials: $T_n(x)$ . . . 497
A.3 Chebyshev Polynomials of the Second Kind: $U_n(x)$ . . . 499
A.4 Legendre Polynomials: $P_n(x)$ . . . 500
A.5 Gegenbauer Polynomials . . . 502
A.6 Hermite Polynomials: $H_n(x)$ . . . 505
A.7 Rational Chebyshev Functions: $TB_n(y)$ . . . 507
A.8 Laguerre Polynomials: $L_n(x)$ . . . 508
A.9 Rational Chebyshev Functions: $TL_n(y)$ . . . 509
A.10 Graphs of Convergence Domains in the Complex Plane . . . 511

B Direct Matrix-Solvers **514**
B.1 Matrix Factorizations . . . 514
B.2 Banded Matrix . . . 518
B.3 Matrix-of-Matrices Theorem . . . 520
B.4 Block-Banded Elimination: the “Lindzen-Kuo” Algorithm . . . 520
B.5 Block and “Bordered” Matrices . . . 522
B.6 Cyclic Banded Matrices (Periodic Boundary Conditions) . . . 524
B.7 Parting shots . . . 524

C Newton Iteration **526**
C.1 Introduction 526
C.2 Examples 529
C.3 Eigenvalue Problems 531
C.4 Summary 534

D The Continuation Method **536**
D.1 Introduction 536
D.2 Examples 537
D.3 Initialization Strategies 538
D.4 Limit Points 542
D.5 Bifurcation points 544
D.6 Pseudoarclength Continuation 546

E Change-of-Coordinate Derivative Transformations **550**

F Cardinal Functions **561**
F.1 Introduction 561
F.2 General Fourier Series: Endpoint Grid 562
F.3 Fourier Cosine Series: Endpoint Grid 563
F.4 Fourier Sine Series: Endpoint Grid 565
F.5 Cosine Cardinal Functions: Interior Grid 567
F.6 Sine Cardinal Functions: Interior Grid 568
F.7 Sinc(x): Whittaker cardinal function 569
F.8 Chebyshev Gauss-Lobatto ("Endpoints") 570
F.9 Chebyshev Polynomials: Interior or "Roots" Grid 571
F.10 Legendre Polynomials: Gauss-Lobatto Grid 572

G Transformation of Derivative Boundary Conditions **575**

Glossary **577**

Index **586**

References **595**