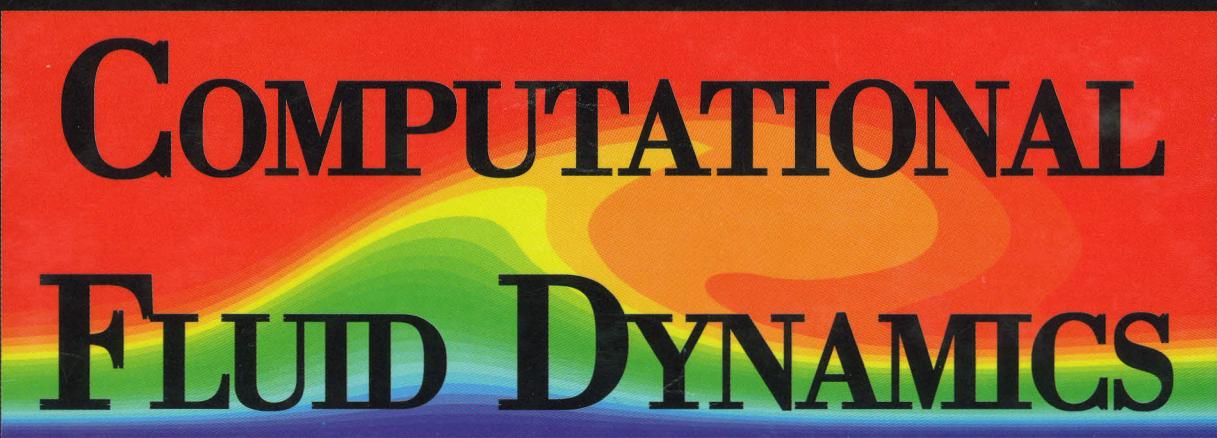


**FUNDAMENTALS OF**

**COMPUTATIONAL**

**FLUID DYNAMICS**



**PATRICK J. ROACHE**

# **FUNDAMENTALS OF COMPUTATIONAL FLUID DYNAMICS**

**BY**

**PATRICK J. ROACHE**

*4416/376*

**Leibniz Universität Hannover**  
Institut für  
**Meteorologie und Klimatologie**  
Herrenhäuser Str. 2 · 30419 Hannover



PO Box 9110  
Albuquerque, New Mexico 87119-9110  
USA  
<http://www.hermosa-pub.com/hermosa>

# Table of Contents

## Part I

<b>Chapter 1 Introduction .....</b>	<b>1</b>
1-A. <i>The Realm of Computational Fluid Dynamics</i> .....	1
1-B. <i>Historical Outline of Computational Fluid Dynamics</i> .....	2
1-C. <i>Existence and Uniqueness of Solutions</i> .....	8
1-D. <i>Preliminary Remarks on Consistency, Convergence, and Stability of Solutions</i> .....	9
1-E. <i>Key Concepts of CFD</i> .....	10
<b>Chapter 2 Incompressible Flow Equations In Rectangular Coordinates .....</b>	<b>13</b>
2-A. <i>Pressure-Velocity Equations</i> .....	13
2-B. <i>Stream Function and Vorticity Transport Equations for Planar Flows</i> .....	14
2-C. <i>Conservation Form</i> .....	15
2-D. <i>Normalizing Systems</i> .....	16
2-E. <i>One-Dimensional Model Transport Equations</i> .....	17
<b>Chapter 3 Basic Computational Methods for Incompressible Flow.....</b>	<b>19</b>
3-A. <i>Methods for Solving the Transport Equation</i> .....	20
3-A-1. Some Basic Forms of Discretized Equations.....	21
3-A-2. Control Volume Approach; Finite Volume Methods; MMOC .....	29
3-A-3. The Conservative Property .....	32
3-A-4. A Description of Instability .....	38
3-A-5. Stability Analyses .....	40
3-A-5-a. Discrete Perturbation Stability Analysis .....	41
3-A-5-b. Von Neumann Stability Analysis.....	46
3-A-5-c. Hirt's Heuristic Stability Analysis and the Modified Equation Approach.....	50
3-A-5-d. Summary and Evaluation of Stability Criteria.....	53
3-A-5-e. The von Neumann Analysis in Multidimensional Problems .....	57
3-A-6. One Step Explicit Methods: The Midpoint Leapfrog Method: Filtering.....	59
3-A-7. The DuFort-Frankel Leapfrog Method .....	66
3-A-8. The First Upwind Differencing Method; Artificial Viscosity Errors .....	69
3-A-9. The Transportive Property .....	74
3-A-10. Transportive and Conservative Differencing.....	76
3-A-11. The Second Upwind Differencing Method.....	79
3-A-12. Adams-Basforth and Crocco Methods.....	81
3-A-13. Leith/Lax-Wendroff Method; Phase Errors, Aliasing Errors and Time-Splitting .....	83
3-A-14. Implicit Methods.....	91
3-A-15. Multi-Step Explicit Methods: Runge-Kutta Methods.....	96
3-A-16. ADI Methods .....	101
3-A-17. ADE Methods .....	105
3-A-18. The Hopscotch Method.....	110
3-A-19. The Fourth-Order Methods of Roberts and Weiss and of Crowley.....	112
3-A-20. Fromm's Method of Zero Average Phase Error; Leonard's QUICK Method.....	114
3-A-21. Arakawa's Method .....	116
3-A-22. Remarks on Steady Flow Methods; Local Time Stepping .....	117
3-A-23. Remarks on Evaluating Methods; Behavioral Errors and Mimetic Properties; Compact Differencing.....	122

## xii Table of Contents

---

<b>3-B. Methods for Solving the Stream Function Equations .....</b>	<b>126</b>
3-B-1. Direct Methods.....	127
3-B-2. Richardson's Method and Lieberman's Method.....	128
3-B-3. Southwell's Residual Relaxation Method.....	130
3-B-4. Successive Over-Relaxation (SOR) Method .....	131
3-B-5. Tactics and Strategy.....	134
3-B-6. ADI and Line SOR Methods .....	135
3-B-7. Other Iterative Methods, Coloring Schemes; Multigrid .....	137
3-B-8. EVP Method; Elliptic Marching Methods .....	139
3-B-9. Fourier-Series Methods.....	146
3-B-10. Higher Order Approximations.....	149
3-B-11. Remarks on Evaluating Methods .....	152
<b>3-C. Boundary Conditions for the Vorticity and Stream Function Equations .....</b>	<b>152</b>
3-C-1. Remarks on the Dominant Importance of Computational Boundary Conditions.....	153
3-C-2. Walls in the First Mesh System .....	154
3-C-3. Walls in Alternate Mesh Systems .....	161
3-C-4. Symmetry Boundaries.....	164
3-C-5. Upper Boundary.....	165
3-C-6. Upstream Boundary .....	168
3-C-7. Outflow Boundary .....	170
3-C-8. "Wiggles" or "Ripples".....	177
3-C-9. The Downstream Paradox.....	181
3-C-10. Computational versus Analytic versus "Fuzzy" Boundary Conditions .....	182
3-C-11. Conditions at "Infinity" .....	184
3-C-12. The Sharp Corners .....	185
3-C-12-A Boundary Conditions at the Sharp Convex Corner .....	185
3-C-12-B Convergence and Accuracy at the Sharp Convex Corner .....	188
3-C-13. Concluding Remarks on Vorticity–Stream Function Boundary Conditions and Coupling .....	189
<b>3-D. Convergence Criteria and Initial Conditions .....</b>	<b>190</b>
<b>3-E. Pressure Solution .....</b>	<b>196</b>
3-E-1. Numerical Cubature .....	196
3-E-2. Poisson Equation for Pressure.....	197
3-E-3. Boundary Conditions of the Second Kind on Pressure .....	199
3-E-4. Iterative Solution Methods with "Condensation" .....	200
3-E-5. Pressure Level .....	201
<b>3-F. Temperature Solutions and Concentration Solutions .....</b>	<b>202</b>
3-F-1. Basic Equations .....	203
3-F-2. Retention of Dissipation.....	204
3-F-3. Finite-Difference Representation of Dissipation.....	205
3-F-4. Boundary Conditions for Temperature and Concentration .....	206
3-F-5. Source Terms and Stiff Equations .....	208
<b>3-G. Methods for Solving the Pressure–Velocity Equations .....</b>	<b>210</b>
3-G-1. General Considerations.....	210
3-G-2. Basic Equations .....	211
3-G-3. Boundary Conditions in Primitive Variables.....	212
3-G-4. The MAC Method; Staggered Grids and Finite Volume Methods.....	213
3-G-5. Other Methods Using Primitive Variables .....	219
3-G-6. Relative Merits of the $(\psi, \zeta)$ and $(u, v, P)$ Systems .....	220
<b>3-H. Three-Dimensional Flows .....</b>	<b>221</b>
<b>3-I. Other Discretization Methodologies .....</b>	<b>226</b>
<b>Chapter 4 Compressible Flow Equations in Rectangular Coordinates .....</b>	<b>227</b>
<b>4-A. Fundamental Difficulties.....</b>	<b>227</b>
<b>4-B. Customary Equations.....</b>	<b>227</b>
<b>4-C. Conservation Form .....</b>	<b>228</b>
<b>4-D. Supplemental Relations.....</b>	<b>232</b>

<i>4-E. Normalized Conservation Equations .....</i>	235
<i>4-F. Short-Form Equations.....</i>	239
<i>4-G. Existence of Shocks Physical and Mathematical .....</i>	240
<i>4-H. Non-Uniqueness of Nonlinear Solutions.....</i>	243
 <b>Chapter 5 Basic Computational Methods for Compressible Flow .....</b> <b>245</b>	
<i>5-A. Preliminary Considerations .....</i>	245
<i>5-A-1. Shock-Free Methods and Shock-Patching Methods .....</i>	245
<i>5-A-2. Stability Considerations.....</i>	247
<i>5-A-3. Early Attempts at Implicit Methods .....</i>	250
<i>5-B. Methods for the Numerical Treatment of Shocks.....</i>	250
<i>5-C. Shock Smearing by Artificial Dissipation .....</i>	252
<i>5-D. Methods Using Explicit Artificial Viscosities .....</i>	252
<i>5-D-1. Von Neumann-Richtmyer Method .....</i>	252
<i>5-D-2. Landshoff's Method and Longley's Method .....</i>	255
<i>5-D-3. Rusanov's Method .....</i>	255
<i>5-D-4. Errors Arising from Artificial Viscosities .....</i>	257
<i>5-E. Methods Using Intrinsic Artificial Damping .....</i>	257
<i>5-E-1. Upwind Differencing .....</i>	258
<i>5-E-2. The Domain of Influence and Truncation Error .....</i>	259
<i>5-E-3. PIC and FLIC .....</i>	261
<i>5-E-4. Lax's Method .....</i>	263
<i>5-E-5. Lax-Wendroff Method .....</i>	266
<i>5-E-6. Two-Step Lax-Wendroff and Second-Order Upwind Methods.....</i>	272
<i>5-E-7. The Method of Abarbanel and Zwas.....</i>	277
<i>5-E-8. Other Methods; Riemann Solvers; FCT.....</i>	278
<i>5-F. Viscous Terms in the Compressible Flow Equations.....</i>	279
<i>5-F-1. Spatial Difference Forms.....</i>	279
<i>5-F-2. General Considerations .....</i>	280
<i>5-F-3. Methods for the Viscous Terms .....</i>	281
<i>5-G. Boundary Conditions for Compressible Flow .....</i>	285
<i>5-G-1. Slip Walls.....</i>	285
<i>5-G-1-a. Slip Walls in the First Mesh System .....</i>	286
<i>5-G-1-b. Slip Walls in the Second Mesh System: FVM.....</i>	288
<i>5-G-2. No-Slip Walls .....</i>	290
<i>5-G-2-a. No-Slip Walls in the First Mesh System.....</i>	291
<i>5-G-2-b. No-Slip Walls in the Second Mesh System .....</i>	294
<i>5-G-2-c. Staggered Mesh Evaluation of Density .....</i>	297
<i>5-G-3. Sharp Corners .....</i>	300
<i>5-G-4. Symmetry Surfaces .....</i>	301
<i>5-G-5. Upstream Boundary .....</i>	302
<i>5-G-6. Downstream Boundary .....</i>	303
<i>5-G-7. Upper Boundary: The Simple Wave Condition.....</i>	305
<i>5-H. Convergence Criteria and Initial Conditions .....</i>	307
<i>5-I. Remarks on Subsonic and Supersonic Solutions .....</i>	308
<i>5-J. Higher Order Systems for Compressible Flows .....</i>	310
<i>5-K. Implicit Methods for Compressible Flow .....</i>	311
<i>5-L. Incompressible Solutions with Implicit Compressible Flow Codes .....</i>	313
<i>5-M. Nonlinear Flux Limiters and Related Methods.....</i>	314
 <b>Chapter 6 Other Mesh Systems, Coordinate Systems, and Equation Systems.....</b> <b>319</b>	
<i>6-A. Special Mesh Systems.....</i>	319
<i>6-B. Coordinate Transformations.....</i>	323
<i>6-C. Other Orthogonal Coordinate Systems.....</i>	333
<i>6-D. Other Systems of Equations .....</i>	336

## **xiv Table of Contents**

---

6-D-1. Gross Simplifications to Navier-Stokes Equations.....	336
6-D-2. Minor Simplifications of Navier-Stokes Equations.....	344
6-D-3. Complications to Navier-Stokes Equations.....	347
6-D-4. Alternate Mathematical Formulations .....	351
6-E. Future Developments .....	353
 <b>Chapter 7 Recommendations on Programming, Testing, and Information Processing .....</b> <span style="float: right;"><b>355</b></span>	
7-A. Computer Programming .....	355
7-B. Debugging and Testing .....	360
7-C. Information Processing.....	368
7-C-1. Numbers.....	368
7-C-2. Plots and Motion Pictures.....	368
7-C-3. Diagnostic Functionals.....	377
7-D. Closure .....	379
 <b>Introduction to Part II .....</b> <span style="float: right;"><b>381</b></span>	
 <b>Chapter 8 Finite Element vs. Finite Difference Methods .....</b> <span style="float: right;"><b>383</b></span>	
References for Chapter 8 .....	385
 <b>Chapter 9 Operation Count for Direct Gaussian Elimination.....</b> <span style="float: right;"><b>387</b></span>	
9-A. Introduction.....	387
9-B. Round-Off Error.....	387
9-C. Speed and Storage Penalty .....	387
9-D. Operation Count as an Index of Merit.....	388
9-E. Operation Count and Storage Penalty for GE in 2D.....	389
9-F. Operation Count and Storage Penalty for GE in 3D.....	391
9-G. Conclusions .....	392
References for Chapter 9 .....	393
 <b>Chapter 10 Multigrid Solvers .....</b> <span style="float: right;"><b>395</b></span>	
10-A. Overview of Multigrid Methods .....	395
10-B. The Basic Multigrid Method .....	396
10-B-1. Motivation for the Cycling.....	396
10-B-2. Transferring the Solutions.....	397
10-C. Other Multigrid Methods .....	399
10-D. Subgrid Coefficient Generation for Black Box Multigrid.....	401
10-D-1. Background and Motivation .....	401
10-D-2. Subgrid Generation.....	402
10-D-3. Upwinding in Subgrid Generation.....	404
10-D-4. Supergrid Generation.....	406
10-D-5. Performance .....	407
References for Chapter 10 .....	408
 <b>Chapter 11 A Sixth-Order Accurate Direct Solver for Poisson and Helmholtz Equations in Polar Coordinates .....</b> <span style="float: right;"><b>411</b></span>	
11-A. Introduction .....	411
11-B. The Method.....	411
11-C. Numerical Verification.....	414
11-D. Discussion .....	415
Acknowledgments.....	417
References for Chapter 11 .....	417

---

<b>Chapter 12 The Legitimacy of the Poisson Pressure Equation .....</b>	<b>419</b>
12-A. Summary.....	419
12-B. Introduction.....	419
12-C. Discussion of Derived Boundary Conditions.....	420
12-D. The Homogeneous Gradient Boundary Condition.....	420
12-E. Equivalence of the Poisson Pressure Approach and Continuity .....	421
12-F. Additional Comments.....	422
12-G. Acknowledgements and Publication Note.....	422
12-H. Additional Discussion .....	423
References for Chapter 12 .....	423
<b>Chapter 13 A Flux-Based Modified Method of Characteristics .....</b>	<b>425</b>
13-A. Summary.....	425
13-B. Introduction.....	425
13-C. Non-Flux-Based MMOC Derivations of Difference Methods .....	426
13-D. Two Problems with Non-Flux-Based MMOC .....	428
13-E. Flux-Based MMOC Derivations of Difference Methods .....	428
13-F. Erroneous Flux-Based MMOC Methodology for $CFL > 1$ .....	429
13-G. Correct Flux-Based MMOC Methodology for $CFL > 1$ .....	430
13-G-1. The Fluxing Velocities at the Interfaces .....	431
13-G-2. The Characteristic-Tracking Velocities.....	431
13-G-3. The Flux Contribution from the Core Cell .....	432
13-G-4. Flux Limiters .....	433
13-H. Recommended Method .....	433
13-I. Velocity Reversals .....	439
13-J. Multidimensions and Additional Terms .....	440
Acknowledgements .....	440
References for Chapter 13 .....	441
<b>Chapter 14 Solution Adaptive Grids and Time Steps .....</b>	<b>445</b>
14-A. A Perfect Coordinate Transformation for the 1-D Advection-Diffusion Equation .....	445
14-B. Transformation of Governing Equations .....	446
14-C. Multidimensional Transformed Equations .....	447
14-D. Solution Adaptive Strategies .....	448
14-E. Time Accuracy Estimation and Adaptive Time Steps .....	450
14-F. Time Resolution of Source Terms .....	452
14-G. Domain Decomposition.....	453
References for Chapter 14 .....	454
<b>Chapter 15 Elliptic Grid Generation and Hybrid Grid Adaptation.....</b>	<b>457</b>
15-A. Summary.....	457
15-B. Introduction.....	457
15-C. Adaptive Poisson Grid Generation .....	457
15-D. Anderson's Adaptive Poisson Grid Generator .....	458
15-E. Details of the Hybrid Adaptive Poisson Grid Generator.....	459
15-F. Example Calculations .....	460
15-G. Comparisons, Costs and Extensions of the Hybrid Technique .....	464
15-H. Grid Smoothness .....	465
15-I. Conclusions .....	465
Acknowledgements .....	466
References for Chapter 15 .....	466

<b>Chapter 16 Semidirect High Order Accuracy Solutions in Non-Orthogonal Grids by Richardson Extrapolation .....</b>	<b>467</b>
16-A. Introduction.....	467
16-B. Basic Numerical Method.....	468
16-C. Coordinate Transformation .....	468
16-D. Boundary Conditions at Outflow .....	470
16-E. Boundary Conditions at Inflow and Upper Boundary.....	471
16-F. Boundary Conditions on the No Slip Wall.....	471
16-G. Initial Conditions and Channel Shape .....	472
16-H. Iterative Convergence Criterion and Performance .....	472
16-I. Richardson Extrapolation .....	473
16-J. Discretization Error Convergence .....	474
16-K. Reynolds Number Scaling Behavior .....	474
16-L. Limit Analysis.....	474
16-M. Effect of Other Boundary Conditions.....	476
16-N. Conclusion.....	476
Acknowledgements .....	477
References for Chapter 16 .....	477
<b>Chapter 17 Nonlinear Flux Limiters Applied to Groundwater Contaminant Transport.....</b>	<b>479</b>
17-A. Summary.....	479
17-B. Introduction.....	480
17-C. Algorithm.....	480
17-D. Results .....	483
17-E. Conclusions .....	485
Acknowledgement.....	485
References for Chapter 17 .....	486
<b>Chapter 18 Verification of Codes and Calculations .....</b>	<b>487</b>
18-A. Summary.....	488
18-B. Introduction.....	488
18-C. Semantics.....	488
18-D. Code Verification and Validation: Numerical vs. Conceptual Modeling.....	488
18-E. Verification of Calculations .....	490
18-F. Code Confirmation and Certification .....	490
18-G. Grid Convergence vs. Iterative Convergence .....	491
18-H. Error Taxonomies .....	491
18-I. Truncation Error vs. Discretization Error.....	492
18-J. Calibration and Tuning .....	493
18-K. Customer Illusions vs. Customer Care .....	493
18-L. Other Distinctions .....	494
18-M. Code Verification via Systematic Grid Convergence Testing .....	494
18-N. Grid Convergence Index .....	495
18-O. Sensitivity of Grid Convergence Testing .....	496
18-P. Esoteric Coding Errors .....	497
18-Q. Special Considerations for Turbulence Modeling .....	497
18-R. Extraction of Observed Order from Grid Convergence Tests .....	497
18-S. Cafe Curves .....	499
18-T. Surrogate Single-Grid Indexes .....	499
18-U. Conclusion.....	500
Acknowledgement.....	500
References for Chapter 18 .....	500

---

<b>Chapter 19 The Grid Convergence Index.....</b>	<b>505</b>
19.1 <i>Introduction.....</i>	505
19.2 <i>Background on Grid Convergence Reporting .....</i>	506
19.3 <i>Richardson Extrapolation .....</i>	506
19.4 <i>Generalization of Richardson Extrapolation.....</i>	509
19.5 <i>Richardson's Extrapolation for <math>\pi</math> .....</i>	510
19.6 <i>Grid Convergence Index for the Fine Grid Solution .....</i>	511
19.7 <i>Grid Convergence Index for the Coarse Grid Solution .....</i>	513
19.8 <i>Example GCI Calculation .....</i>	514
19.9 <i>Should The Coefficient be "1" Or "3" Or "1.25" ? .....</i>	515
19.10 <i>Additional Features of Grid Convergence Studies         for Verification of Codes and Calculations .....</i>	517
19.10.1 <i>Non-Integer Grid Refinement .....</i>	518
19.10.2 <i>Independent Coordinate Refinement and Mixed Order Methods .....</i>	519
19.10.3 <i>Non-Cartesian Grids, Boundary Fitted Grids, Unstructured Grids, Adaptive Grids .....</i>	520
19.10.4 <i>Shocks, Discontinuities, Singularities.....</i>	522
19.10.5 <i>Achieving the Asymptotic Range .....</i>	522
19.10.6 <i>Extraction of the Observed Order of Convergence from Grid Convergence Tests .....</i>	524
19.10.7 <i>Method of Characteristics and Spectral Methods .....</i>	525
19.10.8 <i>Non-Smooth Property Variation and the GCI.....</i>	525
19.10.9 <i>Non-Smooth Property Variation and Geostatistical Realizations .....</i>	526
19.10.10 <i>Stopping Criteria for Iterative Convergence .....</i>	526
19.11 <i>Conclusion.....</i>	527
References for Chapter 19 .....	528
<b>Appendix A Tridiagonal Algorithm.....</b>	<b>533</b>
<b>Appendix B On Artificial Viscosity .....</b>	<b>539</b>
<b>Problems .....</b>	<b>549</b>
<b>References &amp; Bibliography for Part I .....</b>	<b>561</b>
<b>Suggestions for a Course Using This Text.....</b>	<b>629</b>
<b>Subject Index.....</b>	<b>631</b>
<b>Order Forms .....</b>	<b>649</b>