

# Contents

*Preface to the second edition* xv

*Nomenclature* xviii

<b>Introduction: An Initial Guide to CFD and to this Volume</b>	<b>1</b>
I.1 The position of CFD in the world of virtual prototyping	1
I.1.1 The Definition Phase	2
I.1.2 The Simulation and Analysis Phase	3
I.1.3 The Manufacturing Cycle Phase	5
I.2 The components of a CFD simulation system	11
I.2.1 Step 1: Defining the Mathematical Model	11
I.2.2 Step 2: Defining the Discretization Process	13
I.2.3 Step 3: Performing the Analysis Phase	15
I.2.4 Step 4: Defining the Resolution Phase	16
I.3 The structure of this volume	18
References	20

## **Part I The Mathematical Models for Fluid Flow Simulations at Various Levels of Approximation** **21**

<b>1 The Basic Equations of Fluid Dynamics</b>	<b>27</b>
Objectives and guidelines	27
1.1 General form of a conservation law	29
1.1.1 Scalar Conservation Law	30
1.1.2 Convection–Diffusion Form of a Conservation Law	33
1.1.3 Vector Conservation Law	38
The Equations of Fluid Mechanics	39
1.2 The mass conservation equation	40
1.3 The momentum conservation law or equation of motion	43
1.4 The energy conservation equation	47
1.4.1 Conservative Formulation of the Energy Equation	49
1.4.2 The Equations for Internal Energy and Entropy	49
1.4.3 Perfect Gas Model	50
1.4.4 Incompressible Fluid Model	53
A1.5 Rotating frame of reference	54
A1.5.1 Equation of Motion in the Relative System	54
A1.5.2 Energy Equation in the Relative System	55
A1.5.3 Crocco's Form of the Equations of Motion	56
A1.6 Advanced applications of control volume formulations	57
A1.6.1 Lift and Drag Estimations from CFD Results	57
A1.6.2 Conservation Law for a Moving Control Volume	58
Summary of the basic flow equations	60

Conclusions and main topics to remember	63
References	63
Problems	63
<b>2 The Dynamical Levels of Approximation</b>	<b>65</b>
Objectives and guidelines	65
2.1 The Navier–Stokes equations	70
2.1.1 Non-uniqueness in Viscous Flows	73
2.1.1.1 Marangoni thermo-capillary flow in a liquid bridge	73
2.1.1.2 Flow around a circular cylinder	77
2.1.2 Direct Numerical Simulation of Turbulent Flows (DNS)	83
2.2 Approximations of turbulent flows	86
2.2.1 Large Eddy Simulation (LES) of Turbulent Flows	87
2.2.2 Reynolds Averaged Navier–Stokes Equations (RANS)	89
2.3 Thin shear layer approximation (TSL)	94
2.4 Parabolized Navier–Stokes equations	94
2.5 Boundary layer approximation	95
2.6 The distributed loss model	96
2.7 Inviscid flow model: Euler equations	97
2.8 Potential flow model	98
2.9 Summary	101
References	101
Problems	103
<b>3 The Mathematical Nature of the Flow Equations and Their Boundary Conditions</b>	<b>105</b>
Objectives and guidelines	105
3.1 Simplified models of a convection–diffusion equation	108
3.1.1 1D Convection–Diffusion Equation	108
3.1.2 Pure Convection	109
3.1.3 Pure Diffusion in Time	110
3.1.4 Pure Diffusion in Space	111
3.2 Definition of the mathematical properties of a system of PDEs	111
3.2.1 System of First Order PDEs	112
3.2.2 Partial Differential Equation of Second Order	116
3.3 Hyperbolic and parabolic equations: characteristic surfaces and domain of dependence	117
3.3.1 Characteristic Surfaces	118
3.3.2 Domain of Dependence: Zone of Influence	120
3.3.2.1 Parabolic problems	120
3.3.2.2 Elliptic problems	122
3.4 Time-dependent and conservation form of the PDEs	122
3.4.1 Plane Wave Solutions with Time Variable	123
3.4.2 Characteristics in a One-Dimensional Space	128
3.4.3 Nonlinear Definitions	129
3.5 Initial and boundary conditions	130
A.3.6 Alternative definition: compatibility relations	132
A3.6.1 Compatibility Relations	133

Conclusions and main topics to remember	136
References	137
Problems	137
<b>Part II Basic Discretization Techniques</b>	<b>141</b>
<b>4 The Finite Difference Method for Structured Grids</b>	<b>145</b>
Objectives and guidelines	145
4.1 The basics of finite difference methods	147
4.1.1 Difference Formulas for First and Second Derivatives	149
4.1.1.1 Difference formula for first derivatives	150
4.1.1.2 FD formulas for second derivatives	153
4.1.2 Difference Schemes for One-Dimensional Model Equations	154
4.1.2.1 Linear one-dimensional convection equation	154
4.1.2.2 Linear diffusion equation	159
4.2 Multidimensional finite difference formulas	160
4.2.1 Difference Schemes for the Laplace Operator	162
4.2.2 Mixed Derivatives	166
4.3 Finite difference formulas on non-uniform grids	169
4.3.1 Difference Formulas for First Derivatives	172
4.3.1.1 Conservative FD formulas	173
4.3.2 A General Formulation	174
4.3.3 Cell-Centered Grids	177
4.3.4 Guidelines for Non-uniform Grids	179
A4.4 General method for finite difference formulas	180
A4.4.1 Generation of Difference Formulas for First Derivatives	181
A4.4.1.1 Forward differences	182
A4.4.1.2 Backward differences	183
A4.4.1.3 Central differences	183
A4.4.2 Higher Order Derivatives	184
A4.4.2.1 Second order derivative	186
A4.4.2.2 Third order derivatives	187
A4.4.2.3 Fourth order derivatives	189
A4.5 Implicit finite difference formulas	189
A4.5.1 General Approach	189
A4.5.2 General Derivation of Implicit Finite Difference Formula's for First and Second Derivatives	191
Conclusions and main topics to remember	195
References	196
Problems	197
<b>5 Finite Volume Method and Conservative Discretization with an Introduction to Finite Element Method</b>	<b>203</b>
Objectives and guidelines	203
5.1 The conservative discretization	204
5.1.1 Formal Expression of a Conservative Discretization	208

5.2	The basis of the finite volume method	209
5.2.1	Conditions on Finite Volume Selections	210
5.2.2	Definition of the Finite Volume Discretization	212
5.2.3	General Formulation of a Numerical Scheme	213
5.3	Practical implementation of finite volume method	216
5.3.1	Two-Dimensional Finite Volume Method	216
5.3.2	Finite Volume Estimation of Gradients	221
A.5.4	The finite element method	225
A5.4.1	Finite Element Definition of Interpolation Functions	226
A5.4.1.1	One-dimensional linear elements	228
A5.4.1.2	Two-dimensional linear elements	231
A5.4.2	Finite Element Definition of the Equation	
	Discretization: Integral Formulation	232
A5.4.3	The Method of Weighted Residuals or Weak Formulation	232
A5.4.4	The Galerkin Method	234
A5.4.5	Finite Element Galerkin Method for a	
	Conservation Law	237
A5.4.6	Subdomain Collocation: Finite Volume Method	238
	Conclusions and main topics to remember	241
	References	242
	Problems	243
<b>6</b>	<b>Structured and Unstructured Grid Properties</b>	<b>249</b>
	Objectives and guidelines	249
6.1	Structured Grids	250
6.1.1	Cartesian Grids	252
6.1.2	Non-uniform Cartesian Grids	252
6.1.3	Body-Fitted Structured Grids	254
6.1.4	Multi-block Grids	256
6.2	Unstructured grids	261
6.2.1	Triangle/Tetrahedra Cells	262
6.2.2	Hybrid Grids	264
6.2.3	Quadrilateral/Hexahedra Cells	264
6.2.4	Arbitrary Shaped Elements	265
6.3	Surface and volume estimations	267
6.3.1	Evaluation of Cell Face Areas	269
6.3.2	Evaluation of Control Cell Volumes	270
6.4	Grid quality and best practice guidelines	274
6.4.1	Error Analysis of 2D Finite Volume Schemes	274
6.4.2	Recommendations and Best Practice Advice on Grid	
	Quality	276
	Conclusions and main topics to remember	276
	References	277
<b>Part III</b>	<b>The Analysis of Numerical Schemes</b>	<b>279</b>
<b>7</b>	<b>Consistency, Stability and Error Analysis of Numerical Schemes</b>	<b>283</b>
	Objectives and guidelines	283

7.1	Basic concepts and definitions	285
7.1.1	Consistency Condition, Truncation Error and Equivalent Differential Equation of a Numerical Scheme	287
7.1.1.1	Methodology	287
7.2	The Von Neumann method for stability analysis	292
7.2.1	Fourier Decomposition of the Solution	293
7.2.2	Amplification factor	296
7.2.2.1	Methodology	296
7.2.3	Comments on the CFL Condition	300
7.3	New schemes for the linear convection equation	303
7.3.1	The Leapfrog Scheme for the Convection Equation	304
7.3.2	Lax–Friedrichs Scheme for the Convection Equation	305
7.3.3	The Lax–Wendroff Scheme for the Convection Equation	306
7.4	The spectral analysis of numerical errors	313
7.4.1	Error Analysis for Hyperbolic Problems	316
7.4.1.1	Error analysis of the explicit First Order Upwind scheme (FOU)	317
7.4.1.2	Error analysis of the Lax–Friedrichs scheme for the convection equation	320
7.4.1.3	Error analysis of the Lax–Wendroff scheme for the convection equation	320
7.4.1.4	Error analysis of the leapfrog scheme for the convection equation	323
7.4.2	The Issue of Numerical Oscillations	324
7.4.3	The Numerical Group Velocity	326
7.4.4	Error Analysis for Parabolic Problems	330
7.4.5	Lessons Learned and Recommendations	330
	Conclusions and main topics to remember	332
	References	332
	Problems	333
<b>8</b>	<b>General Properties and High-Resolution Numerical Schemes</b>	<b>337</b>
	Objectives and guidelines	337
8.1	General formulation of numerical schemes	339
8.1.1	Two-Level Explicit Schemes	340
8.1.2	Two-Level Schemes for the Linear Convection Equation	343
8.1.3	Amplification Factor, Error Estimation and Equivalent Differential Equation	346
8.1.4	Accuracy Barrier for Stable Scalar Convection Schemes	349
A8.1.5	An Addition to the Stability Analysis	351
A8.1.6	An Advanced Addition to the Accuracy Barrier	352
8.2	The generation of new schemes with prescribed order of accuracy	354
8.2.1	One-Parameter Family of Schemes on the Support ( $i - 1, i, i + 1$ )	355
8.2.2	The Convection–Diffusion Equation	357
8.2.3	One-Parameter Family of Schemes on the Support ( $i - 2, i - 1, i, i + 1$ )	361

8.3	Monotonicity of numerical schemes	365
8.3.1	Monotonicity Conditions	366
8.3.2	Semi-Discretized Schemes or Method of Lines	370
8.3.3	Godunov's Theorem	372
8.3.4	High-Resolution Schemes and the Concept of Limiters	373
8.4	Finite volume formulation of schemes and limiters	389
8.4.1	Numerical flux	390
8.4.2	The Normalized Variable Representation	397
	Conclusions and main topics to remember	400
	References	403
	Problems	406
<b>Part IV</b>	<b>The Resolution of Numerical Schemes</b>	<b>411</b>
<b>9</b>	<b>Time Integration Methods for Space-discretized Equations</b>	<b>413</b>
	Objectives and guidelines	413
9.1	Analysis of the space-discretized systems	414
9.1.1	The Matrix Representation of the Diffusion Space Operator	416
9.1.2	The Matrix Representation of the Convection Space Operator	418
9.1.3	The Eigenvalue Spectrum of Space-discretized Systems	421
9.1.4	Matrix Method and Fourier Modes	425
9.1.5	Amplification Factor of the Semi-discretized System	428
9.1.6	Spectrum of Second Order Upwind Discretizations of the Convection Operator	429
9.2	Analysis of time integration schemes	429
9.2.1	Stability Regions in the Complex $\Omega$ Plane and Fourier Modes	431
9.2.2	Error Analysis of Space and Time Discretized Systems	434
	9.2.2.1 Diffusion and dispersion errors of the time integration	434
	9.2.2.2 Diffusion and dispersion errors of space and time discretization	435
	9.2.2.3 Relation with the equivalent differential equation	436
9.2.3	Forward Euler Method	436
9.2.4	Central Time Differencing or Leapfrog Method	438
9.2.5	Backward Euler Method	439
9.3	A selection of time integration methods	441
9.3.1	Nonlinear System of ODEs and their Linearization	443
9.3.2	General Multistep Method	445
	9.3.2.1 Beam and Warming schemes for the convection equation	449
	9.3.2.2 Nonlinear systems and approximate Jacobian linearizations	450
9.3.3	Predictor–Corrector Methods	453
9.3.4	The Runge–Kutta Methods	458
	9.3.4.1 Stability analysis for the Runge–Kutta method	460

9.3.5	Application of the Methodology and Implicit Methods	465
9.3.6	The Importance of Artificial Dissipation with Central Schemes	469
A9.4	Implicit schemes for multidimensional problems: approximate factorization methods	475
A9.4.1	Two-Dimensional Diffusion Equation	478
A9.4.2	ADI Method for the Convection Equation	480
	Conclusions and main topics to remember	482
	References	483
	Problems	485
<b>10</b>	<b>Iterative Methods for the Resolution of Algebraic Systems</b>	<b>491</b>
	Objectives and guidelines	491
10.1	Basic iterative methods	493
10.1.1	Poisson's Equation on a Cartesian, Two-Dimensional Mesh	493
10.1.2	Point Jacobi Method/Point Gauss-Seidel Method	495
10.1.3	Convergence Analysis of Iterative Schemes	498
10.1.4	Eigenvalue Analysis of an Iterative Method	501
10.1.5	Fourier Analysis of an Iterative Method	504
10.2	Overrelaxation methods	505
10.2.1	Jacobi Overrelaxation	506
10.2.2	Gauss-Seidel Overrelaxation: Successive Overrelaxation (SOR)	507
10.2.3	Symmetric Successive Overrelaxation (SSOR)	509
10.2.4	Successive Line Overrelaxation Methods (SLOR)	510
10.3	Preconditioning techniques	512
10.3.1	Richardson Method	513
10.3.2	Alternating Direction Implicit Method (ADI)	515
10.3.3	Other Preconditioning and Relaxation Methods	516
10.4	Nonlinear problems	518
10.5	The multigrid method	520
10.5.1	Smoothing Properties	523
10.5.2	The Coarse Grid Correction Method (CGC) for Linear Problems	525
10.5.3	The Two-Grid Iteration Method for Linear Problems	529
10.5.4	The Multigrid Method for Linear Problems	530
10.5.5	The Multigrid Method for Nonlinear Problems	532
	Conclusions and main topics to remember	533
	References	533
	Problems	535
	Appendix A: Thomas Algorithm for Tridiagonal Systems	536
A.1.	Scalar Tridiagonal Systems	536
A.2.	Periodic Tridiagonal Systems	538
<b>Part V</b>	<b>Applications to Inviscid and Viscous Flows</b>	<b>541</b>
<b>11</b>	<b>Numerical Simulation of Inviscid Flows</b>	<b>545</b>
	Objectives and guidelines	545

11.1	The inviscid Euler equations	548
11.1.1	Steady Compressible Flows	549
11.1.2	The Influence of Compressibility	549
11.1.3	The Properties of Discontinuous Solutions	551
11.1.3.1	Contact Discontinuities	553
11.1.3.2	Vortex sheets or slip lines	553
11.1.3.3	Shock surfaces	553
11.1.4	Lift and Drag on Solid Bodies	554
11.2	The potential flow model	556
11.2.1	The Limitations of the Potential Flow Model for Transonic Flows	557
11.2.2	Incompressible Potential Flows	557
11.3	Numerical solutions for the potential equation	558
11.3.1	Incompressible Flow Around a Circular Cylinder	558
11.3.1.1	Define the grid	561
11.3.1.2	Define the numerical scheme	566
11.3.1.3	Solve the algebraic system	569
11.3.1.4	Analyze the results and evaluate the accuracy	570
11.3.2	Compressible Potential Flow Around the Circular Cylinder	571
11.3.2.1	Numerical estimation of the density and its nonlinearity	571
11.3.2.2	Transonic potential flow	572
11.3.3	Additional Optional Tasks	574
11.4	Finite volume discretization of the Euler equations	574
11.4.1	Finite Volume Method for Euler Equations	575
11.4.1.1	Space discretization	576
11.4.1.2	Time integration	578
11.4.1.3	Boundary conditions for the Euler equations	579
11.5	Numerical solutions for the Euler equations	583
11.5.1	Application to the Flow Around a Cylinder	583
11.5.2	Application to the Internal Flow in a Channel with a Circular Bump	587
11.5.3	Application to the Supersonic Flow on a Wedge at $M = 2.5$	591
11.5.4	Additional Hands-On Suggestions	595
	Conclusions and main topics to remember	596
	References	597
<b>12</b>	<b>Numerical Solutions of Viscous Laminar Flows</b>	<b>599</b>
	Objectives and guidelines	599
12.1	Navier–Stokes equations for laminar flows	601
12.1.1	Boundary Conditions for Viscous Flows	603
12.1.2	Grids for Boundary Layer Flows	604
12.2	Density-based methods for viscous flows	604
12.2.1	Discretization of Viscous and Thermal Fluxes	605
12.2.2	Boundary Conditions	607
12.2.2.1	Physical boundary conditions	607



12.2.2.2	Numerical boundary conditions	609
12.2.2.3	Periodic boundary conditions	609
12.2.3	Estimation of Viscous Time Step and CFL Conditions	610
12.3	Numerical solutions with the density-based method	610
12.3.1	Couette Thermal Flow	611
12.3.1.1	Numerical simulation conditions	613
12.3.1.2	Grid definition	614
12.3.1.3	Results	614
12.3.1.4	Other options for solving the Couette flow	616
12.3.2	Flat Plate	618
12.3.2.1	Exact solution	618
12.3.2.2	Grid definition	619
12.3.2.3	Results	622
12.4	Pressure correction method	625
12.4.1	Basic Approach of Pressure Correction Methods	627
12.4.2	The Issue of Staggered Versus Collocated Grids	629
12.4.3	Implementation of a Pressure Correction Method	632
12.4.3.1	Numerical discretization	634
12.4.3.2	Algorithm for the pressure Poisson equation	636
12.5	Numerical solutions with the pressure correction method	638
12.5.1	Lid Driven Cavity	638
12.5.2	Additional Suggestions	639
12.6	Best practice advice	640
12.6.1	List of Possible Error Sources	642
12.6.2	Best Practice Recommendations	642
	Conclusions and main topics to remember	644
	References	645