

Contents

Part I Foundation

1	Introduction	3
1.1	What Is Computational Fluid Dynamics (CFD)	3
1.2	What Is the Finite Volume Method	4
1.3	This Book	5
	1.3.1 Foundation	5
	1.3.2 Numerics	6
	1.3.3 Algorithms	7
	1.3.4 Applications	8
1.4	Closure	8
2	Review of Vector Calculus	9
2.1	Introduction	9
2.2	Vectors and Vector Operations	10
	2.2.1 The Dot Product of Two Vectors	11
	2.2.2 Vector Magnitude	11
	2.2.3 The Unit Direction Vector	12
	2.2.4 The Cross Product of Two Vectors	12
	2.2.5 The Scalar Triple Product	14
	2.2.6 Gradient of a Scalar and Directional Derivatives	15
	2.2.7 Operations on the Nabla Operator	17
	2.2.8 Additional Vector Operations	19
2.3	Matrices and Matrix Operations	20
	2.3.1 Square Matrices	21
	2.3.2 Using Matrices to Describe Systems of Equations	23
	2.3.3 The Determinant of a Square Matrix	23
	2.3.4 Eigenvectors and Eigenvalues	26
	2.3.5 A Symmetric Positive-Definite Matrix	27

2.3.6	Additional Matrix Operations	28
2.4	Tensors and Tensor Operations	29
2.5	Fundamental Theorems of Vector Calculus	32
2.5.1	Gradient Theorem for Line Integrals	32
2.5.2	Green's Theorem	33
2.5.3	Stokes' Theorem	34
2.5.4	Divergence Theorem	35
2.5.5	Leibniz Integral Rule	37
2.6	Closure	38
2.7	Exercises	39
	References	41
3	Mathematical Description of Physical Phenomena	43
3.1	Introduction	43
3.2	Classification of Fluid Flows	44
3.3	Eulerian and Lagrangian Description of Conservation Laws	45
3.3.1	Substantial Versus Local Derivative	46
3.3.2	Reynolds Transport Theorem	47
3.4	Conservation of Mass (Continuity Equation)	48
3.5	Conservation of Linear Momentum	50
3.5.1	Non-Conservative Form	51
3.5.2	Conservative Form	52
3.5.3	Surface Forces	52
3.5.4	Body Forces	54
3.5.5	Stress Tensor and the Momentum Equation for Newtonian Fluids	55
3.6	Conservation of Energy	57
3.6.1	Conservation of Energy in Terms of Specific Internal Energy	60
3.6.2	Conservation of Energy in Terms of Specific Enthalpy	61
3.6.3	Conservation of Energy in Terms of Specific Total Enthalpy	61
3.6.4	Conservation of Energy in Terms of Temperature	62
3.7	General Conservation Equation	65
3.8	Non-dimensionalization Procedure	67
3.9	Dimensionless Numbers	72
3.9.1	Reynolds Number	72
3.9.2	Grashof Number	73
3.9.3	Prandtl Number	73
3.9.4	Péclet Number	75
3.9.5	Schmidt Number	75

3.9.6	Nusselt Number	77
3.9.7	Mach Number.	77
3.9.8	Eckert Number	78
3.9.9	Froude Number.	79
3.9.10	Weber Number	79
3.10	Closure	80
3.11	Exercises	80
	References.	82
4	The Discretization Process.	85
4.1	The Discretization Process	85
4.1.1	Step I: Geometric and Physical Modeling.	87
4.1.2	Step II: Domain Discretization	88
4.1.3	Mesh Topology.	90
4.1.4	Step III: Equation Discretization	93
4.1.5	Step IV: Solution of the Discretized Equations	98
4.1.6	Other Types of Fields	100
4.2	Closure	101
5	The Finite Volume Method	103
5.1	Introduction	103
5.2	The Semi-Discretized Equation	104
5.2.1	Flux Integration Over Element Faces.	105
5.2.2	Source Term Volume Integration.	107
5.2.3	The Discrete Conservation Equation for One Integration Point	108
5.2.4	Flux Linearization	109
5.3	Boundary Conditions	111
5.3.1	Value Specified (Dirichlet Boundary Condition)	111
5.3.2	Flux Specified (Neumann Boundary Condition).	112
5.4	Order of Accuracy.	113
5.4.1	Spatial Variation Approximation	113
5.4.2	Mean Value Approximation	114
5.5	Transient Semi-Discretized Equation	117
5.6	Properties of the Discretized Equations	118
5.6.1	Conservation.	118
5.6.2	Accuracy	119
5.6.3	Convergence.	119
5.6.4	Consistency	120
5.6.5	Stability	120
5.6.6	Economy	120
5.6.7	Transportiveness	120
5.6.8	Boundedness of the Interpolation Profile	121

5.7	Variable Arrangement	122
5.7.1	Vertex-Centered FVM	123
5.7.2	Cell-Centered FVM	124
5.8	Implicit Versus Explicit Numerical Methods	126
5.9	The Mesh Support	127
5.10	Computational Pointers	128
5.10.1	uFVM	128
5.10.2	OpenFOAM [®]	129
5.11	Closure	133
5.12	Exercises	133
	References.	134
6	The Finite Volume Mesh	137
6.1	Domain Discretization	137
6.2	The Finite Volume Mesh	138
6.2.1	Mesh Support for Gradient Computation	139
6.3	Structured Grids	142
6.3.1	Topological Information	142
6.3.2	Geometric Information	144
6.3.3	Accessing the Element Field	145
6.4	Unstructured Grids	146
6.4.1	Topological Information (Connectivities)	147
6.5	Geometric Quantities	152
6.5.1	Element Types	153
6.5.2	Computing Surface Area and Centroid of Faces	154
6.6	Computational Pointers	162
6.6.1	uFVM	162
6.6.2	OpenFOAM [®]	164
6.7	Closure	170
6.8	Exercises	170
	References.	170
7	The Finite Volume Mesh in OpenFOAM[®] and uFVM	173
7.1	uFVM	173
7.1.1	An OpenFOAM [®] Test Case	173
7.1.2	The polyMesh Folder	175
7.1.3	The uFVM Mesh	178
7.1.4	uFVM Geometric Fields	183
7.1.5	Working with the uFVM Mesh	187
7.1.6	Computing the Gauss Gradient	188
7.2	OpenFOAM [®]	191
7.2.1	Fields and Memory	197
7.2.2	InternalField Data	199

7.2.3	BoundaryField Data	200
7.2.4	lduAddressing	200
7.2.5	Computing the Gradient	202
7.3	Mesh Conversion Tools	204
7.4	Closure	205
7.5	Exercises	205
	References.	207

Part II Discretization

8	Spatial Discretization: The Diffusion Term.	211
8.1	Two-Dimensional Diffusion in a Rectangular Domain	211
8.2	Comments on the Discretized Equation	216
	8.2.1 The Zero Sum Rule	216
	8.2.2 The Opposite Signs Rule	217
8.3	Boundary Conditions	217
	8.3.1 Dirichlet Boundary Condition	218
	8.3.2 Von Neumann Boundary Condition	220
	8.3.3 Mixed Boundary Condition	222
	8.3.4 Symmetry Boundary Condition	223
8.4	The Interface Diffusivity	224
8.5	Non-Cartesian Orthogonal Grids	239
8.6	Non-orthogonal Unstructured Grid.	241
	8.6.1 Non-orthogonality	241
	8.6.2 Minimum Correction Approach	242
	8.6.3 Orthogonal Correction Approach	243
	8.6.4 Over-Relaxed Approach	243
	8.6.5 Treatment of the Cross-Diffusion Term	244
	8.6.6 Gradient Computation	244
	8.6.7 Algebraic Equation for Non-orthogonal Meshes	245
	8.6.8 Boundary Conditions for Non-orthogonal Grids.	252
8.7	Skewness	254
8.8	Anisotropic Diffusion	255
8.9	Under-Relaxation of the Iterative Solution Process	256
8.10	Computational Pointers	258
	8.10.1 uFVM	258
	8.10.2 OpenFOAM®	260
8.11	Closure	265
8.12	Exercises	265
	References.	270

9	Gradient Computation	273
9.1	Computing Gradients in Cartesian Grids	273
9.2	Green-Gauss Gradient	275
9.3	Least-Square Gradient	285
9.4	Interpolating Gradients to Faces	289
9.5	Computational Pointers	290
9.5.1	uFVM	290
9.5.2	OpenFOAM®	295
9.6	Closure	298
9.7	Exercises	298
	References.	302
10	Solving the System of Algebraic Equations.	303
10.1	Introduction	303
10.2	Direct or Gauss Elimination Method	305
10.2.1	Gauss Elimination	305
10.2.2	Forward Elimination	306
10.2.3	Forward Elimination Algorithm.	307
10.2.4	Backward Substitution	307
10.2.5	Back Substitution Algorithm.	308
10.2.6	LU Decomposition	308
10.2.7	The Decomposition Step	310
10.2.8	LU Decomposition Algorithm.	311
10.2.9	The Substitution Step.	312
10.2.10	LU Decomposition and Gauss Elimination	312
10.2.11	LU Decomposition Algorithm by Gauss Elimination.	313
10.2.12	Direct Methods for Banded Sparse Matrices	315
10.2.13	TriDiagonal Matrix Algorithm (TDMA).	316
10.2.14	PentaDiagonal Matrix Algorithm (PDMA)	317
10.3	Iterative Methods	319
10.3.1	Jacobi Method	323
10.3.2	Gauss-Seidel Method	325
10.3.3	Preconditioning and Iterative Methods	327
10.3.4	Matrix Decomposition Techniques.	329
10.3.5	Incomplete LU (ILU) Decomposition.	329
10.3.6	Incomplete LU Factorization with no Fill-in ILU(0)	330
10.3.7	ILU(0) Factorization Algorithm.	331
10.3.8	ILU Factorization Preconditioners	331
10.3.9	Algorithm for the Calculation of \mathbf{D}^* in the DILU Method	332
10.3.10	Forward and Backward Solution Algorithm with the DILU Method	333

10.3.11	Gradient Methods for Solving Algebraic Systems	333
10.3.12	The Method of Steepest Descent	335
10.3.13	The Conjugate Gradient Method	337
10.3.14	The Bi-conjugate Gradient Method (BiCG) and Preconditioned BICG	340
10.4	The Multigrid Approach.	343
10.4.1	Element Agglomeration/Coarsening	345
10.4.2	The Restriction Step and Coarse Level Coefficients	346
10.4.3	The Prolongation Step and Fine Grid Level Corrections	349
10.4.4	Traversal Strategies and Algebraic Multigrid Cycles	349
10.5	Computational Pointers	350
10.5.1	uFVM	350
10.5.2	OpenFOAM [®]	351
10.6	Closure	358
10.7	Exercises	358
	References.	362
11	Discretization of the Convection Term	365
11.1	Introduction	365
11.2	Steady One Dimensional Convection and Diffusion.	366
11.2.1	Analytical Solution	366
11.2.2	Numerical Solution	368
11.2.3	A Preliminary Derivation: The Central Difference (CD) Scheme	369
11.2.4	The Upwind Scheme	375
11.2.5	The Downwind Scheme	379
11.3	Truncation Error: Numerical Diffusion and Anti-Diffusion	380
11.3.1	The Upwind Scheme	381
11.3.2	The Downwind Scheme	382
11.3.3	The Central Difference (CD) Scheme.	383
11.4	Numerical Stability	385
11.5	Higher Order Upwind Schemes.	388
11.5.1	Second Order Upwind Scheme	389
11.5.2	The Interpolation Profile.	390
11.5.3	The Discretized Equation	390
11.5.4	Truncation Error	391
11.5.5	Stability Analysis	392
11.5.6	The QUICK Scheme	392
11.5.7	The Interpolation Profile.	393
11.5.8	Truncation Error	394

11.5.9	Stability Analysis	394
11.5.10	The FROMM Scheme	395
11.5.11	The Interpolation Profile.	395
11.5.12	The Discretized Equation	396
11.5.13	Truncation Error	397
11.5.14	Stability Analysis	397
11.5.15	Comparison of the Various Schemes	398
11.5.16	Functional Relationships for Uniform and Non-uniform Grids	399
11.6	Steady Two Dimensional Advection	400
11.6.1	Error Sources	404
11.7	High Order Schemes on Unstructured Grids	406
11.7.1	Reformulating HO Schemes in Terms of Gradients	407
11.8	The Deferred Correction Approach	409
11.9	Computational Pointers	411
11.9.1	uFVM	411
11.9.2	OpenFOAM [®]	413
11.10	Closure	421
11.11	Exercises	422
	References.	426
12	High Resolution Schemes	429
12.1	The Normalized Variable Formulation (NVF).	429
12.2	The Convection Boundedness Criterion (CBC).	436
12.3	High Resolution (HR) Schemes.	438
12.4	The TVD Framework	443
12.5	The NVF-TVD Relation.	450
12.6	HR Schemes in Unstructured Grid Systems	456
12.7	Deferred Correction for HR Schemes.	456
12.7.1	The Difficulty with the Direct Use of Nodal Values	458
12.8	The DWF and NWF Methods.	459
12.8.1	The Downwind Weighing Factor (DWF) Method	460
12.8.2	The Normalized Weighing Factor (NWF) Method	463
12.9	Boundary Conditions	467
12.9.1	Inlet Boundary Condition	468
12.9.2	Outlet Boundary Condition.	470
12.9.3	Wall Boundary Condition.	471
12.9.4	Symmetry Boundary Condition	472

12.10	Computational Pointers	472
12.10.1	uFVM	472
12.10.2	OpenFOAM®	475
12.11	Closure	483
12.12	Exercises	483
	References.	487
13	Temporal Discretization: The Transient Term	489
13.1	Introduction	489
13.2	The Finite Difference Approach	492
13.2.1	Forward Euler Scheme	492
13.2.2	Stability of the Forward Euler Scheme	494
13.2.3	Backward Euler Scheme.	498
13.2.4	Crank-Nicolson Scheme	500
13.2.5	Implementation Details.	502
13.2.6	Adams-Moulton Scheme	503
13.3	The Finite Volume Approach	507
13.3.1	First Order Transient Schemes	508
13.3.2	First Order Implicit Euler Scheme	508
13.3.3	First Order Explicit Euler Scheme	510
13.3.4	Second Order Transient Euler Schemes	512
13.3.5	Crank-Nicolson (Central Difference Profile)	512
13.3.6	Second Order Upwind Euler (SOUE) Scheme.	514
13.3.7	Initial Condition for the FV Approach	515
13.4	Non-Uniform Time Steps	519
13.4.1	Non-Uniform Time Steps with the Finite Difference Approach	519
13.4.2	Adams-Moulton (or SOUE) Scheme	521
13.4.3	Non-Uniform Time Steps with the Finite Volume Approach	522
13.4.4	Crank-Nicolson Scheme	523
13.4.5	Adams-Moulton (or SOUE) Scheme	524
13.5	Computational Pointers	525
13.5.1	uFVM	525
13.5.2	OpenFOAM®	526
13.6	Closure	529
13.7	Exercises	529
	References.	533
14	Discretization of the Source Term, Relaxation, and Other Details	535
14.1	Source Term Discretization.	535
14.2	Under-Relaxation of the Algebraic Equations	538
14.2.1	Under-Relaxation Methods	539

- 14.2.2 Explicit Under-Relaxation. 540
- 14.2.3 Implicit Under-Relaxation Methods 540
- 14.3 Residual Form of the Equation 544
 - 14.3.1 Residual Form of Patankar’s Under-Relaxation 545
- 14.4 Residuals and Solution Convergence 546
 - 14.4.1 Residuals 546
 - 14.4.2 Absolute Residual 547
 - 14.4.3 Maximum Residual 547
 - 14.4.4 Root-Mean Square Residual 547
 - 14.4.5 Normalization of the Residual 548
- 14.5 Computational Pointers 549
 - 14.5.1 uFVM 549
 - 14.5.2 OpenFOAM® 550
- 14.6 Closure 555
- 14.7 Exercises 555
- References. 557

Part III Algorithms

- 15 Fluid Flow Computation: Incompressible Flows 561**
 - 15.1 The Main Difficulty. 561
 - 15.2 A Preliminary Derivation 563
 - 15.2.1 Discretization of the Momentum Equation 564
 - 15.2.2 Discretization of the Continuity Equation 565
 - 15.2.3 The Checkerboard Problem. 565
 - 15.2.4 The Staggered Grid 567
 - 15.2.5 The Pressure Correction Equation 569
 - 15.2.6 The SIMPLE Algorithm on Staggered Grid 572
 - 15.2.7 Pressure Correction Equation in Two Dimensional Staggered Cartesian Grids 578
 - 15.2.8 Pressure Correction Equation in Three Dimensional Staggered Cartesian Grid 581
 - 15.3 Disadvantages of the Staggered Grid 582
 - 15.4 The Rhie-Chow Interpolation 585
 - 15.5 General Derivation 588
 - 15.5.1 The Discretized Momentum Equation 588
 - 15.5.2 The Collocated Pressure Correction Equation 592
 - 15.5.3 Calculation of the \mathcal{D}_f Term 596
 - 15.5.4 The Collocated SIMPLE Algorithm. 597
 - 15.6 Boundary Conditions 602
 - 15.6.1 Boundary Conditions for the Momentum Equation. 603

15.6.2	Boundary Conditions for the Pressure Correction Equation	617
15.7	The SIMPLE Family of Algorithms	621
15.7.1	The SIMPLER Algorithm	623
15.7.2	The PRIME Algorithm	624
15.7.3	The PISO Algorithm	625
15.8	Optimum Under-Relaxation Factor Values for v and p'	628
15.9	Treatment of Various Terms with the Rhie-Chow Interpolation	630
15.9.1	Treatment of the Under-Relaxation Term	630
15.9.2	Treatment of the Transient Term	631
15.9.3	Treatment of the Body Force Term	632
15.9.4	Combined Treatment of Under-Relaxation, Transient, and Body Force Terms	636
15.10	Computational Pointers	636
15.10.1	uFVM	636
15.10.2	OpenFOAM [®]	638
15.11	Closure	649
15.12	Exercises	649
	References	653
16	Fluid Flow Computation: Compressible Flows	655
16.1	Historical	655
16.2	Introduction	656
16.3	The Conservation Equations	657
16.4	Discretization of the Momentum Equation	658
16.5	The Pressure Correction Equation	659
16.6	Discretization of The Energy Equation	663
16.6.1	Discretization of the Extra Terms	663
16.6.2	The Algebraic Form of the Energy Equation	665
16.7	The Compressible SIMPLE Algorithm	666
16.8	Boundary Conditions	667
16.8.1	Inlet Boundary Conditions	669
16.8.2	Outlet Boundary Conditions	672
16.9	Computational Pointers	673
16.9.1	uFVM	673
16.9.2	OpenFOAM [®]	674
16.10	Closure	687
16.11	Exercises	687
	References	689

Part IV Applications

17 Turbulence Modeling 693

17.1 Turbulence Modeling 693

17.2 Reynolds Averaging 696

17.2.1 Time Averaging 696

17.2.2 Spatial Averaging 696

17.2.3 Ensemble Averaging 697

17.2.4 Averaging Rules 697

17.2.5 Incompressible RANS Equations 697

17.3 Boussinesq Hypothesis 699

17.4 Turbulence Models 700

17.5 Two-Equation Turbulence Models 700

17.5.1 Standard $k - \epsilon$ Model 700

17.5.2 The $k - \omega$ Model 702

17.5.3 The Baseline (BSL) $k - \omega$ Model 704

17.5.4 The Shear Stress Transport (SST) $k - \omega$ Model 705

17.6 Summary of Incompressible Turbulent Flow Equations 707

17.7 Discretization of the Turbulent Flow Equations 707

17.7.1 The Discretized Form of the k Equation 708

17.7.2 The Discretized Form of the ϵ Equation 708

17.7.3 The Discretized Form of the ω Equation 709

17.8 Boundary Conditions 710

17.8.1 Modeling Flow Near the Wall 710

17.8.2 Standard Wall Functions 711

17.8.3 Improved Wall Functions 716

17.8.4 Scalable Wall Functions 718

17.8.5 Wall Boundary Conditions for Low Reynolds Number Models 719

17.8.6 Automatic Near-Wall Treatment 720

17.8.7 Near-Wall Heat Transfer 721

17.8.8 Other Boundary Conditions 722

17.9 Calculating Normal Distance to the Wall 723

17.10 Computational Pointers 725

17.10.1 The $k - \epsilon$ Model 727

17.10.2 The SST $k - \omega$ Model 734

17.10.3 simpleFoamTurbulent 738

17.11 Closure 740

17.12 Exercises 740

References 742

18 Boundary Conditions in OpenFOAM® and uFVM 745

18.1 Boundary Conditions in OpenFOAM® 745

18.2 Boundary Condition Customization 747

- 18.3 Development of a New BC: No Slip Wall Condition 752
- 18.4 The No-Slip Boundary Condition in uFVM 756
- 18.5 Closure 759
- Reference 759

- 19 An OpenFOAM® Turbulent Flow Application 761**
 - 19.1 Introduction 761
 - 19.2 The Ahmed Bluff Body 761
 - 19.3 Domain Discretization 763
 - 19.3.1 Initial and Boundary Conditions 768
 - 19.3.2 Systems Files 770
 - 19.3.3 Running the Solver 773
 - 19.4 Conclusion 776
 - References. 776

- 20 Closing Remarks 777**

- Appendix: uFVM 779**