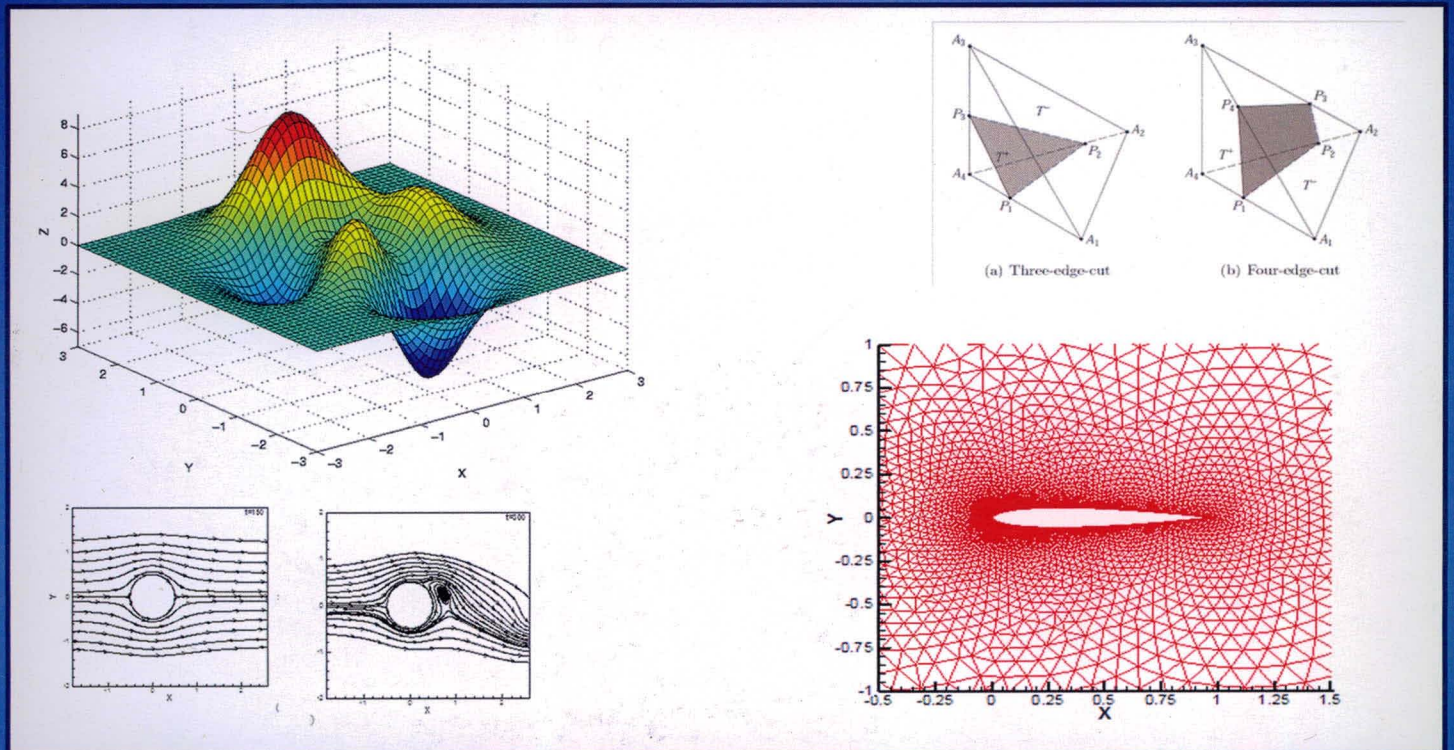


# ADVANCED NUMERICAL TECHNIQUES IN ENGINEERING and SCIENCE



Editors

AHMAD TARIQ JAMEEL

WAQAR ASRAR



IIUM Press

International Islamic University Malaysia

2011

# **ADVANCED NUMERICAL TECHNIQUES IN ENGINEERING AND SCIENCE**

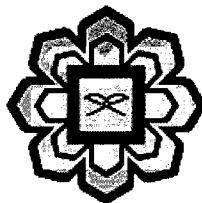
**Editors**

**AHMAD TARIQ JAMEEL**

*Department of Biotechnology Engineering*

**WAQAR ASRAR**

*Department of Mechanical Engineering*



**IIUM Press**  
**International Islamic University Malaysia**  
**2011**

Published by:  
IIUM Press  
International Islamic University Malaysia

First Edition, 2011  
©IIUM Press, IIUM

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without any prior written permission of the publisher.

Perpustakaan Negara Malaysia

Cataloguing-in-Publication Data

Ahmad Tariq Jameel & Waqar Asrar: Advanced Numerical Techniques in Engineering & Science

ISBN: 978-967-418-020-1

Member of Majlis Penerbitan Ilmiah Malaysia – MAPIM  
(Malaysian Scholarly Publishing Council)

Printed by :  
**IIUM PRINTING SDN. BHD.**  
No. 1, Jalan Industri Batu Caves 1/3  
Taman Perindustrian Batu Caves  
Batu Caves Centre Point  
68100 Batu Caves  
Selangor Darul Ehsan

# Contents

	<b>Preface</b>	v
Chapter 1	<b>Numerical Techniques – An Introduction</b> <i>Ahmad Tariq Jameel</i>	1
Chapter 2	<b>Numerical Simulation of a Simple Couette Flow in Matlab Using Explicit And Implicit Finite Difference Schemes</b> <i>Asif Hoda</i>	7
	2.1 Introduction	8
	2.2 The Couette Flow Problem	9
	2.3 Numerical Simulation of Couette Flow	10
	2.3.1 Defining discrete points in the domain of interest	10
	2.3.2 Obtaining numerical approximation for the governing equation	12
	2.3.3 Reducing the differential equation to a set of algebraic equations	13
	2.3.4 Solution of the algebraic equation	15
	2.4 Stability Analysis of Explicit and Implicit Schemes	20
	2.5 Conclusion	21
	Bibliography	22
Chapter 3	<b>Comparison of a Pseudo-Spectral Method and an Implicit Finite Difference Scheme for the Solution of a Nonlinear Dynamic Problem</b> <i>Ahmad Tariq Jameel</i>	23
	3.1 Introduction	24
	3.2 Problem Definition	24
	3.3 Numerical Method	27
	3.3.1 Spectral Methods	27
	3.3.1.1 Fourier Collocation Method	29

	3.3.2 Crank Nicholson Method – Finite Difference Scheme	35
	3.4 Results and Discussion	35
	3.5 Conclusions	41
	References	41
Chapter 4	<b>Unstructured Finite Volume for Two-Dimensional Navier Stokes Equations</b>	43
	<i>Moumen Mohammed Idres and Ahmed Tawfeek El Taweel</i>	
	4.1 Introduction	44
	4.1.1 Finite volume method	44
	4.1.2 Upwind schemes	45
	4.1.3 High resolution schemes	46
	4.2 Roe’s Upwind Scheme	48
	4.2.1 Two-dimensional Navier Stokes equations	48
	4.2.2 Node-Based finite volume method	50
	4.2.3 Definition of control volume	51
	4.2.4 Data structure of Node-Based method	52
	4.2.5 Inviscid residual calculation	53
	4.2.5.1 Roe’s flux difference splitting method	53
	4.2.5.2 Data reconstruction for high-resolution scheme	56
	4.2.5.2.1 TVD schemes	57
	4.2.5.2.2 Barth and Jespersion scheme	60
	4.2.5.2.3 MUSCL differencing approach	62
	4.2.6 Viscous residual calculation	63
	4.2.7 Time integration methods	63
	4.2.7.1 Explicit Euler method	63
	4.2.7.2 Explicit Rungge-Kutta scheme	64
	4.2.8 Boundary conditions	65
	4.2.8.1 Inflow and outflow	65
	4.2.8.2 Wall boundary conditions	65
	4.2.8.2.1 Euler wall boundary conditions	65
	4.2.8.2.2 Navier-Stokes wall boundary conditions	67
	4.2.8.3 Far field boundary conditions	68
	4.2.9 Convergence criterion	69
	4.3 Code Validation	70
	4.3.1 Discretization error estimation	70
	4.3.1.1 Standard Richardson extrapolation	70
	4.3.1.2 Smooth flow test case	71
	4.3.2 Inviscid flow solver	73

	4.3.2.1 Effect of element type on the Inviscid flow solver	73
	4.3.2.2 Flow around NACA-0012 airfoil	78
	4.3.2.2.1 Subsonic case	81
	4.3.2.2.2 Critical case	83
	4.3.2.3 Flow inside a duct with $10^0$ ramp	85
	4.3.3 Viscous flow solver	88
	4.3.3.1 Laminar flow over a flat plate	88
	4.3.3.2 Axisymmetric laminar flow inside JPL nozzle	90
	4.4 Conclusion and Recommendations	94
	References	96
Chapter 5	<b>Higher-Order Compact Finite Difference Schemes</b>	99
	<i>Yap Wen Jiun, Waqar Asra and, Mahmood Khalid Mawlood</i>	
	5.1 Introduction	100
	5.2 Recent Works	102
	5.3 Higher Order Compact Finite Difference Schemes	107
	5.3.1 Classification of Higher-Order compact schemes	108
	5.3.1.1 The Governing-Equation-Based scheme	108
	5.3.1.2 The Hermitian scheme	109
	5.4 Higher Order Time Discretization Method	113
	5.5 Application of HOC Schemes	115
	5.5.1 Viscous Burgers' equation	115
	5.5.1.1 Lax-Wendroff approach	117
	5.5.1.2 Hermitian scheme	119
	5.5.2 HOC solution of Burgers' equation on a clustered grid	122
	5.5.2.1 The Lax-Wendroff approach	124
	5.5.2.2 The Hermitian scheme	128
	5.5.3 Numerical results	129
	5.5.3.1 Numerical studies	134
	5.5.3.2 Numerical boundary conditions	136
	5.5.3.3 Grid clustering	145
	5.6 Conclusion	150
	References	151
Chapter 6	<b>Higher Order Flux-Based Upwind Scheme for Compressible Flows</b>	157
	<i>Nadeem Hasan, S. Mujaheed Khan, and Faisal Shameem</i>	
	6.1 Governing Equations	
	6.2 The PVU Scheme: Origin and Development	158

6.2	The PVU Scheme: Origin and Development	161
6.2.1	The PVU-M+ scheme	162
6.2.1.1	Estimation of inter-cell numerical particle velocity $\mathbf{u}_{i+1/2}$ and convective transport property vector ' $\phi_{i+1/2}$ '	164
6.2.1.2	Estimation of $u_{i+1/2}$ and $\phi_{i+1/2}$ in the vicinity of shocks	168
6.3	Performance Assessment Criteria and 1-D Test Cases	169
6.3.1	One-dimensional Inviscid test cases	171
6.4	Multi-Dimensional Inviscid and viscous test cases	177
6.4.1	Supersonic inviscid flow past a forward facing step in a channel	179
6.4.2	Inviscid Shock-Vortex interaction	184
6.4.3	Two-dimensional inviscid compressible flow past a circular Cylinder	187
6.4.3.1	Low subsonic regime ( $M_\infty = 0.2$ )	188
6.4.3.2	Transonic flow ( $M_\infty = 0.38-0.98$ )	189
6.4.3.3	Supersonic flow at $M_\infty = 3.0$ and $M_\infty = 10.0$	194
6.4.4	Two-dimensional viscous compressible flow past a circular cylinder	196
6.4.4.1	( $M_\infty = 0.1, Re_\infty = 100$ ) flow past a circular cylinder	197
6.4.4.2	( $M_\infty = 0.7, Re_\infty = 2000$ ) flow past an adiabatic circular cylinder	199
6.5	Conclusion	199
	References	201
Chapter 7	<b>Finite Element Modelling of the Powder Compaction Process</b> <i>Meftah Hrair and, Hedi Chtourou</i>	203
7.1	Introduction	204
7.1.1	Powder metallurgy process	204
7.1.2	Powder metallurgy technology	205
7.1.3	Numerical simulation of powder compaction process	208
7.2	Finite Element Method	212
7.2.1	Large displacement formulation	213
7.2.2	Finite element discretization	215
7.2.3	Nonlinear Iterative strategy	216
7.3	Powder Constitutive Model	218
7.3.1	Cap plasticity model	218

7.3.2	Numerical implementation	222
7.3.3	Integration of the Behaviour law	223
7.3.3.1	Elastic prediction	224
7.3.3.2	Plastic correction	225
7.3.3.3	Elastic mode	226
7.3.3.4	Tension mode	226
7.3.3.5	Singular tension mode	226
7.3.3.6	Shear mode	227
7.3.3.7	Singular compression mode	228
7.3.3.8	Cap mode	229
7.3.4	Updating the variables	230
7.3.5	Derivation of Elastoplastic Tangent moduli	231
7.3.5.1	Perfect plasticity	231
7.3.5.2	Hardening plasticity (cap mode)	232
7.4	Application of cap plasticity model	234
7.4.1	Introduction	234
7.4.2	Determination of model parameters	234
7.4.2.1	Elastic parameters	234
7.4.2.2	Hardening law parameters	235
7.4.2.3	Yield surfaces parameters	236
7.4.3	Case studies	239
7.4.3.1	Rotational-Flanged component	239
7.4.3.2	Industrial gear	244
7.5	Conclusion	246
	References	247
Chapter 8	<b>Introduction of Piecewise Virtual Fields Method for Solution of Inverse Problems</b> <i>Syed Muhammad Kashif</i>	253
8.1	Use of Full Field Data for Mechanical Characterization	254
8.1.1	Introduction	254
8.1.2	Solution of inverse problems using full field data	254
8.1.3	Piecewise virtual fields method	257
8.1.4	Conclusion	258
8.2	The Piecewise Virtual Fields Method in Plate Blending Problems	258
8.2.1	Introduction	258
8.2.2	Construction of the virtual fields	263
8.2.2.1	Introduction	263



	Elements	
	8.2.2.3 Computation of virtual curvature fields	266
	8.2.2.4 Computation of integrals	267
	8.2.3 Boundary conditions imposed to virtual deflection field	269
	8.2.4 Constraints imposed due to special virtual fields	269
	8.2.5 Identification of unknown rigidities	270
	8.2.6 Conclusion	270
8.3	Minimization of the Effect of Noisy Data	271
	8.3.1 Introduction	271
	8.3.2 Optimized virtual field: Minimization of noise effect	279
	8.3.3 Conclusion	281
8.4	Numerical Simulations	282
	8.4.1 Introduction	282
	8.4.2 Results without noise	283
	8.4.3 Influence of the virtual elements mesh density	284
	8.4.4 Influence of noisy data	287
	8.4.4.1 Introduction	287
	8.4.4.2 Consistency of the results	287
	8.4.4.3 Comparison with some earlier results	288
	8.4.5 Influence of plate anisotropy	289
8.5	Conclusion	290
	References	291
Chapter 9	<b>Immersed Finite Element Method (IFEM)</b>	295
	<i>Raed Ismail Kafafy</i>	
	9.1 Introduction	296
	9.1.1 Body-Fitting-Grid methods	296
	9.1.2 Cartesian-Grid methods	297
	9.1.3 Cartesian-Grid methods based on finite difference discretization	298
	9.1.3.1 The immersed boundary method (IBM)	298
	9.1.3.2 The level set method (LSM)	298
	9.1.3.3 The smoothing method for discontinuous coefficients	299
	9.1.3.4 The immersed interface method (IIM)	299
	9.1.3.5 The embedded curved boundary method (ECB)	299
	9.1.4 Cartesian-Grid methods based on finite element discretization	299
	9.1.4.1 The partition of unity method (PUM)	299

9.1.4.1	The partition of unity method (PUM)	299
9.1.4.2	The extended finite element method (X-FEM)	300
9.1.4.3	The immersed finite element method (IFE)	300
9.2	Three-Dimensional IFE Method	301
9.2.1	The interface boundary value problem	302
9.2.2	Weak formulation of the field problem	303
9.2.3	A three dimensional IFE space	304
9.2.4	Intersection topology	306
9.2.4.1	Special intersection topology	306
9.2.4.2	Linear local nodal FE basis functions	307
9.2.4.3	Linear local nodal IFE basis functions	308
9.2.4.4	Three-edge cut element	309
9.2.4.5	Four-edge cut element	312
9.2.5	Existence and uniqueness	315
9.2.6	Partition of unity and consistency with classical FEM	316
9.3	Building a 3d IFE field solver	319
9.3.1	Mesh generation	319
9.3.2	Mesh-Object intersection	319
9.3.3	Intersection topology classification	320
9.3.4	Assembly of the IFE system of equations	322
9.3.4.1	Local assembler	322
9.3.4.2	Global assembler	322
9.3.5	Integration rules	323
9.3.5.1	Gaussian Quadratures	323
9.3.5.2	Integration on interface elements	324
9.3.6	Sparse storage of the system matrix	326
9.4	Nonlinear IFE Solver	327
9.4.1	Gauss-Seidel iteration	327
9.4.2	Newton-Raphson iteration	328
9.4.3	Solution of the sparse linear/linearized system	329
9.4.4	Preconditioned-Conjugate Gradient (PCCG) solver	329
9.4.5	Preconditioners	329
9.4.6	Incomplete cholesky decomposition	330
9.4.7	Jacobi diagonal preconditioner	330
9.4.8	Hardwiring the IFE field solver	330
9.4.9	Hardwired local assembler	331
9.5	Numerical Examples	331
9.5.1	Results of Numerical Experiments Using IFE Method	331
9.5.1.1	An interface problem with a spherical interface	332
9.5.1.2	An interface problem with a Hemispherical	335

	interface	
	9.5.2 Error analysis and approximation capability	339
	9.6 Conclusion	340
	References	341
Chapter 10	<b>Lower-Upper Symmetric-Gauss-Seidel (LU-SGS) Algorithm for Pseudo Compressibility Method</b>	347
	<i>Ashraf Ali Omar</i>	
	10.1 Introduction	348
	10.2 Factorization and Relaxation	350
	10.3 Three-Dimensional Incompressible Navier Stoke Equations	351
	10.3.1 Governing equations	351
	10.3.2 Transformation of the Governing equations	352
	10.4 Pseudo-Compressibility Method	355
	10.5 Space Discretization and Implicit Scheme	357
	10.5.1 Space Discretization	357
	10.5.1.1 Introduction	357
	10.5.1.2 Inviscid flux differencing	357
	10.5.1.3 Central differencing method	358
	10.5.1.4 Differencing of viscous flux terms	360
	10.5.2 Implicit scheme	361
	10.5.2.1 Introduction	361
	10.5.2.2 Pseudo-time discretization	362
	10.5.2.3 LU-SGS scheme	363
	10.6 Initial and Boundary Condition	364
	10.7 Pseudo-Time Step	365
	10.8 Applications	366
	10.8.1 Incompressible viscous flow over a multi-element airfoil	366
	10.8.1.1 Studied model	366
	10.8.1.2 Results	368
	10.8.1.2.1 Convergence history	368
	10.8.1.2.2 Surface pressure	369
	10.8.1.2.3 Velocity profiles	371
	10.8.1.2.4 Lift Coefficients	373
	10.8.2 Incompressible vortical flows over a 3-D Tangent-Ogive cylinder	374
	10.8.2.1 Introduction	374
	10.8.2.2 Grid generation and boundary conditions	374
	10.8.2.3 Results and discussion	375

10.9 Conclusion	379
References	380
<b>Subject Index</b>	<b>389</b>

# CHAPTER 1

## **Numerical Techniques – An Introduction**

AHMAD TARIQ JAMEEL

Department of Biotechnology Engineering, Faculty of Engineering, International Islamic University Malaysia, Gombak, 50728 Kuala Lumpur, Malaysia.  
atjameel@yahoo.com; atjameel@iium.edu.my

This chapter provides an overview of the computational methods and its applications presented in later chapters in the book. In the present day, the solution of a design or a research problem in engineering and sciences is almost unthinkable without the aid of numerical methods and digital computers. Broadly speaking, two approaches are generally employed to solve problems using numerical methods. In the first case, the mathematical model is developed and the governing equations are solved using a numerical technique by writing indigenous computer code in a programming language of one's choice. FORTRAN and C languages are currently widely used in engineering applications. The computer code can then be executed to obtain detailed solution for the dependent variable over a wide range of parameters. At times, commercially available mathematical software packages such as MATLAB, POLYMATH, and EXCEL etc. are also used to solve the governing equations directly instead of developing a complete computer code. For more serious computations, often one needs to employ readymade subroutines from commercially available mathematical and statistical software libraries such as IMSL (International Mathematical and Statistical Library) and NAG (Numerical Algorithms Group).

The second approach is where a problem can be solved using more specialized and powerful interactive simulation software packages such as FLUENT, COMSOL, ANSYS, STAR CCM++ etc. FLUENT is widely used for solving CFD (Computational Fluid Dynamics) problems. COMSOL MULTIPHYSICS is suitable for modelling and solving variety of problem in science and engineering involving coupled physics phenomena based on partial differential equations. Applications of these softwares do