

Methods of Numerical Simulation in Fluids and Plasmas

Antonius Otto

January 28, 2011

Contents

1	Introduction	6
1.1	Preliminaries	6
1.2	Why Numerical Simulation	7
1.3	The Numerical Experiment: Limitations, Accuracy, Stability, Computer Speed . . .	9
1.3.1	Limitations	9
1.3.2	Accuracy	10
1.3.3	Stability	11
1.4	Vector and parallel computer performance	11
1.4.1	Vector processing concept:	11
1.4.2	Parallel processing concept	12
1.4.3	Computer performance through the years	16
2	Origin of Partial Differential Equations	20
2.1	Individual Particle Motion	20
2.2	Kinetic Equations	21
2.3	Fluid Equations	23
2.3.1	Definitions and derivation	23
2.3.2	Approximations	26
3	Classification of PDE's and Related Properties	29
3.1	Linear Second Order PDE's in two Independent Variables	29
3.2	Well Posed Problems:	30
3.3	Boundary and Initial Conditions	31
3.4	Classification Through Characteristics	31
3.4.1	First order equation	31

3.4.2	Second order equations	32
3.4.3	Coordinate transformations	34
3.4.4	Multidimensional equations	35
3.5	Classification Through Fourier Analysis	39
3.6	Hyperbolic Partial Differential Equations	40
3.6.1	Examples and general properties	40
3.6.2	Role of Characteristics and Boundary/Initial Conditions:	42
3.7	Parabolic Partial Differential Equations	44
3.8	Elliptic Partial Differential Equations	44
4	Preliminary Computational Techniques	46
4.1	Discretization	46
4.1.1	Spatial derivatives	47
4.1.2	Time derivatives	48
4.2	Approximation to derivatives	49
4.2.1	Taylor series expansion	49
4.2.2	General technique	50
4.2.3	Asymmetric formula	52
4.3	Accuracy	52
4.4	Wave representation	57
4.5	First example for a finite difference simulation	59
5	Theory	64
5.1	Convergence	65
5.1.1	Numerical convergence	65
5.2	Consistency	66
5.3	Stability	68
5.3.1	Matrix method	70
5.3.2	Von Neumann method	73
5.4	Solution accuracy	77
5.5	Efficiency	79

6	Weighted Residual Methods	82
6.1	General Formulation	82
6.2	Finite Volume Method	86
6.2.1	First order derivatives	86
6.2.2	Second order derivatives	88
6.2.3	Program Fivol	92
6.3	Finite Element Method	93
6.3.1	Basic formulation	93
6.3.2	Finite element method applied to the Sturm-Liouville equation	98
6.3.3	Further applications of the finite element method	104
6.4	Spectral method	112
6.4.1	Diffusion equation	112
6.4.2	Neumann boundary conditions	114
6.4.3	Pseudospectral method	116
6.5	Summary on different weighted residual methods:	117
7	Elliptic Equations and Steady State Problems	118
7.1	Newtons Method	118
7.1.1	Example for Newton's method: Burgers equation	120
7.2	Direct Methods to Solve Linear Systems of Equations	123
7.2.1	Notes on the routines "fact" ad "sol":	123
7.2.2	Tridiagonal systems: Thomas algorithm and programs Banfac and Bansol	125
7.2.3	Pentadiagonal systems:	127
7.2.4	Block Tridiagonal systems	128
7.3	Iterative methods	129
7.3.1	Basic approach and simple iteration methods	129
7.4	Duct flow with iterative methods	132
7.5	Multigrid Method	135
7.6	Pseudotransient method	138
7.7	Summary of properties of elliptic solution methods	140

8	Diffusion Equation	143
8.1	Explicit methods	143
8.1.1	Forward time centered space scheme	143
8.1.2	Richardson and DuFort-Frankel schemes	144
8.1.3	Three-level scheme	145
8.1.4	Hopscotch method	146
8.2	Implicit methods	147
8.2.1	Fully implicit scheme	147
8.2.2	Crank-Nicholson scheme	148
8.2.3	Generalized three level schemes	150
8.2.4	Boundary conditions	151
8.2.5	Summary on methods for the one-dimensional diffusion equation	153
8.3	Splitting schemes	154
8.3.1	ADI method	154
8.3.2	Generalized two level scheme	155
8.3.3	Finite element methods	157
9	Convection Equations	160
9.1	Linear convection equations	160
9.1.1	Simple explicit methods	161
9.1.2	Crank-Nicholson scheme	164
9.1.3	Summary of schemes for the one-dimensional convection equation	165
9.2	Numerical dispersion and dissipation	167
9.2.1	Fourier analysis	168
9.3	One- and two-dimensional transport equations	171
9.3.1	Explicit schemes for the transport equation	172
9.3.2	Crank-Nicholson schemes	176
9.3.3	Implementation of the different methods	177
9.3.4	Two-dimensional transport	180
9.4	Nonlinear transport	182
9.4.1	Explicit schemes	183
9.4.2	Implicit Methods	185
9.4.3	Implementation of Burgers equation	187
9.5	Systems of Equations	187

10 Grid Generation	192
10.1 Motivation	192
10.1.1 Basic properties of nonuniform grids	192
10.2 Transformations and transformation parameters	195
10.3 Generalized coordinate structure of typical equations	195
10.4 Grid generation	195
11 Fluid and Plasma Simulation	196
11.1 Explicit and implicit methods	196
11.2 Supersonic flow, shocks, flux corrected transport	196
11.3 Particle simulation	196
11.4 Hybrid simulation	196
11.5 Vlasov simulation	196
12 Applications and Projects	197
12.1 Two-dimensional flow past an obstacle	197
12.2 Three-dimensional diffusion equation	197
12.3 Interchange instabilities	197
12.4 Magnetohydrodynamic waves	197
12.5 Magnetohydrodynamic shocks	197
12.6 Particle simulation: Two stream instability	197
12.7 Vlasov simulation: Two stream instability	197