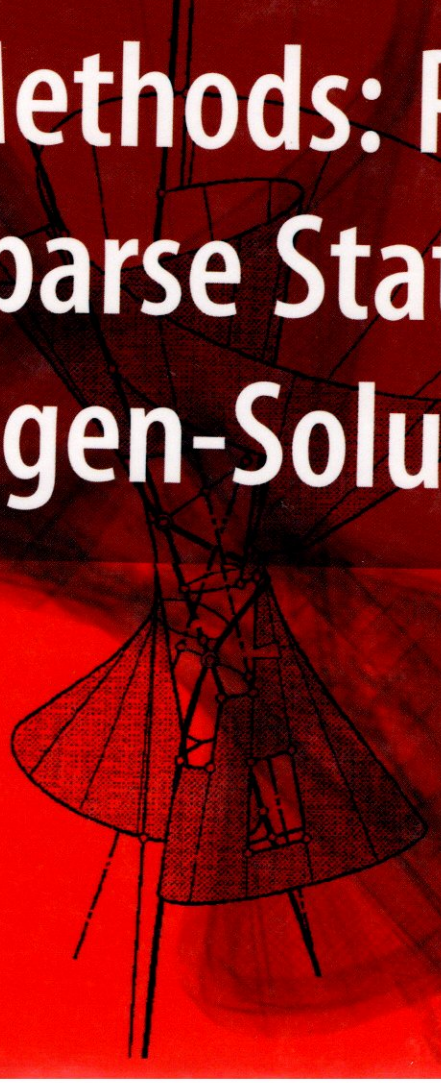
Duc Thai Nguyen

Finite Element Methods: Parallel-Sparse Statics and Eigen-Solutions



Springer

Contents

1. A Review of Basic Finite Element Procedures 1

1.1 Introduction 1
1.2 Numerical Techniques for Solving Ordinary Differential Equations (ODE) 1
1.3 Identifying the "Geometric" versus "Natural" Boundary Conditions 6
1.4 The Weak Formulations 6
1.5 Flowcharts for Statics Finite Element Analysis 9
1.6 Flowcharts for Dynamics Finite Element Analysis 13
1.7 Uncoupling the Dynamical Equilibrium Equations 14
1.8 One-Dimensional Rod Finite Element Procedures 17
1.8.1 One-Dimensional Rod Element Stiffness Matrix 18
1.8.2 Distributed Loads and Equivalent Joint Loads 21
1.8.3 Finite Element Assembly Procedures 22
1.8.4 Imposing the Boundary Conditions 24
1.8.5 Alternative Derivations of System of Equations from Finite Element Equations 25
1.9 Truss Finite Element Equations 27
1.10 Beam (or Frame) Finite Element Equations 29
1.11 Tetrahedral Finite Element Shape Functions 31
1.12 Finite Element Weak Formulations for General 2-D Field Equations 35
1.13 The Isoparametric Formulation 44
1.14 Gauss Quadrature 51
1.15 Summary 59
1.16 Exercises 59

2. Simple MPI/FORTRAN Applications 63

2.1 Introduction 63
2.2 Computing Value of "π" by Integration 63
2.3 Matrix-Matrix Multiplication 68
2.4 MPI Parallel I/O 72
2.5 Unrolling Techniques 75
2.6 Parallel Dense Equation Solvers 77
2.6.1 Basic Symmetrical Equation Solver 77
2.6.2 Parallel Data Storage Scheme 78
2.6.3 Data Generating Subroutine 80
2.6.4 Parallel Choleski Factorization 80
2.6.5 A Blocked and Cache-Based Optimized Matrix-Matrix Multiplication 81
2.6.5.1 Loop Indexes and Temporary Array Usage 81
2.6.5.2 Blocking and Strip Mining 82
2.6.5.3 Unrolling of Loops 82

2.6.6 Parallel "Block" Factorization....83
2.6.7 "Block" Forward Elimination Subroutine....85
2.6.8 "Block" Backward Elimination Subroutine....86
2.6.9 "Block" Error Checking Subroutine....88
2.6.10 Numerical Evaluation....91
2.6.11 Conclusions....95
2.7 Developing/Debugging Parallel MPI Application Code on Your Own Laptop....95
2.8 Summary....103
2.9 Exercises....103

3. Direct Sparse Equation Solvers....105

3.1 Introduction....105
3.2 Sparse Storage Schemes....105
3.3 Three Basic Steps and Re-Ordering Algorithms....110
3.4 Symbolic Factorization with Re-Ordering Column Numbers....118
3.5 Sparse Numerical Factorization....132
3.6 Super (Master) Nodes (Degrees-of-Freedom)....134
3.7 Numerical Factorization with Unrolling Strategies....137
3.8 Forward/Backward Solutions with Unrolling Strategies....137
3.9 Alternative Approach for Handling an Indefinite Matrix....154
3.10 Unsymmetrical Matrix Equation Solver....165
3.11 Summary....180
3.12 Exercises....181

4. Sparse Assembly Process....183

4.1 Introduction....183
4.2 A Simple Finite Element Model (Symmetrical Matrices)....183
4.3 Finite Element Sparse Assembly Algorithms for Symmetrical Matrices....188
4.4 Symbolic Sparse Assembly of Symmetrical Matrices....189
4.5 Numerical Sparse Assembly of Symmetrical Matrices....192
4.6 Step-by-Step Algorithms for Symmetrical Sparse Assembly....200
4.7 A Simple Finite Element Model (Unsymmetrical Matrices)....219
4.8 Re-Ordering Algorithms....224
4.9 Imposing Dirichlet Boundary Conditions....229
4.10 Unsymmetrical Sparse Equations Data Formats....254
4.11 Symbolic Sparse Assembly of Unsymmetrical Matrices....259
4.12 Numerical Sparse Assembly of Unsymmetrical Matrices....260
4.13 Step-by-Step Algorithms for Unsymmetrical Sparse Assembly and Unsymmetrical Sparse Equation Solver....260
4.14 A Numerical Example....265
4.15 Summary....265
4.16 Exercises....266

5. Generalized Eigen-Solvers....269

5.1 Introduction....269
5.2 A Simple Generalized Eigen-Example....269
5.3 Inverse and Forward Iteration Procedures....271
5.4 Shifted Eigen-Problems....274
5.5 Transformation Methods....276
5.6 Sub-Space Iteration Method....286
5.7 Lanczos Eigen-Solution Algorithms....290
5.7.1 Derivation of Lanczos Algorithms....290
5.7.2 Lanczos Eigen-Solution Error Analysis....295
5.7.3 Sturm Sequence Check....302
5.7.4 Proving the Lanczos Vectors Are M-Orthogonal....306
5.7.5 "Classical" Gram-Schmidt Re-Orthogonalization....308
5.7.6 Detailed Step-by-Step Lanczos Algorithms....314
5.7.7 Educational Software for Lanczos Algorithms....316
5.7.8 Efficient Software for Lanczos Eigen-Solver....336
5.8 Unsymmetrical Eigen-Solvers....339
5.9 Balanced Matrix....339
5.10 Reduction to Hessenberg Form....340
5.11 QR Factorization....341
5.12 Householder QR Transformation....341
5.13 "Modified" Gram-Schmidt Re-Orthogonalization....348
5.14 QR Iteration for Unsymmetrical Eigen-Solutions....350
5.15 QR Iteration with Shifts for Unsymmetrical Eigen-Solutions....353
5.16 Panel Flutter Analysis....355
5.17 Block Lanczos Algorithms....365
5.17.1 Details of "Block Lanczos" Algorithms....366
5.17.2 A Numerical Example for "Block Lanczos" Algorithms....371
5.18 Summary....377
5.19 Exercises....378

6. Finite Element Domain Decomposition Procedures....379

6.1 Introduction....379
6.2 A Simple Numerical Example Using Domain Decomposition (DD) Procedures....382
6.3 Imposing Boundary Conditions on "Rectangular" Matrices $K_{BI}^{(r)}$....390
6.4 How to Construct Sparse Assembly of "Rectangular" Matrix $K_{BI}^{(r)}$....392
6.5 Mixed Direct-Iterative Solvers for Domain Decomposition....393
6.6 Preconditioned Matrix for PCG Algorithm with DD Formulation....397
6.7 Generalized Inverse....404
6.8 FETI Domain Decomposition Formulation [6.4 - 6.7]....409
6.9 Preconditioned Conjugate Projected Gradient (PCPG) of

the Dual Interface Problem [6.4] 417
6.10 Automated Procedures for Computing Generalized Inverse and Rigid Body Motions 422
6.11 Numerical Examples of a 2-D Truss by FETI Formulation 433
6.12 A Preconditioning Technique for Indefinite Linear System [6.12] 459
6.13 FETI-DP Domain Decomposition Formulation [6.6, 6.7] 463
6.14 Multi-Level Sub-Domains and Multi-Frontal Solver [6.13 - 6.20] 488
6.15 Iterative Solution with Successive Right-Hand Sides [6.23,6.24] 490
6.16 Summary 510
6.17 Exercises 510

Appendix A Singular Value Decomposition (SVD) 515
References 521
Index 527