

Computational Science, Engineering and Technology Series: 24

**Substructuring Techniques
and
Domain Decomposition Methods**

Computational Science, Engineering and Technology Series:

Parallel, Distributed and Grid Computing for Engineering

Edited by: B.H.V. Topping and P. Iványi

Trends in Engineering Computational Technology

Edited by: M. Papadrakakis and B.H.V. Topping

Trends in Computational Structures Technology

Edited by: B.H.V. Topping and M. Papadrakakis

Computational Methods for Acoustics Problems

Edited by: F. Magoulès

Mesh Partitioning Techniques and Domain Decomposition Methods

Edited by: F. Magoulès

Computational Mechanics using High Performance Computing

Edited by: B.H.V. Topping

High Performance Computing for Computational Mechanics

Edited by: B.H.V. Topping, L. Lämmer

Parallel and Distributed Processing for Computational Mechanics:

Systems and Tools

Edited by: B.H.V. Topping

Saxe-Coburg Publications:

Programming Distributed Finite Element Analysis:

An Object Oriented Approach

R.I. Mackie

Object Oriented Methods and Finite Element Analysis

R.I. Mackie

Domain Decomposition Methods for Distributed Computing

J. Kruis

Computer Aided Design of Cable-Membrane Structures

B.H.V. Topping and P. Iványi

Substructuring Techniques and Domain Decomposition Methods

Edited by
F. Magoulès



© Saxe-Coburg Publications, Kippen, Stirling, Scotland

published 2010 by

Saxe-Coburg Publications

Civil-Comp Ltd, Dun Eaglais, Station Brae
Kippen, Stirlingshire, FK8 3DY, Scotland

Saxe-Coburg Publications is an imprint of Civil-Comp Ltd

Computational Science, Engineering and Technology Series: 24

ISSN 1759-3158

ISBN: 978-1-874672-33-3

British Library Cataloguing in Publication Data

A catalogue record for this book is available from the British Library

Front cover: Domain Decomposition for 50 subdomains by T. Miyamura. For more information see Chapter 7.

Printed in Great Britain by Bell & Bain Ltd, Glasgow

Contents

Preface	ix
1 Substructuring and Domain Decomposition Methods: An Overview	1
F. Magoulès and D. Rixen	
1.1 Domain Decomposition and Substructuring: Where do we go?	1
1.1.1 “divide et impera!”	2
1.1.2 Substructuring or Domain Decomposition?	2
1.1.3 Key Issues for the Computational Mechanics Community	3
1.1.3.1 Mathematical Properties	4
1.1.3.2 Heterogeneous Problems	4
1.1.3.3 Multi-Physics and Multi-Models	4
1.1.3.4 Multi-Point Constraints	5
1.1.3.5 Non-Linearities and Contact	5
1.2 The Contributions in this Book	5
2 The ‘Parareal in Time’ Algorithm	19
Y. Maday	
2.1 Introduction	19
2.2 Presentation of the ‘Parareal in Time’ Algorithm	21
2.2.1 Basics on solution for ODE’s	21
2.2.2 The ‘Parareal in Time’ Algorithm	22
2.2.3 Numerical Simulation	23
2.2.4 Complexity and Parallelism Efficiency: Part 1	24
2.2.5 An Algebraic Interpretation	26
2.3 Various Ways to Reduce the Coarse Simulation	27
2.3.1 Convergence Analysis	27
2.3.2 Model Reduction	29
2.3.3 Coarse Spacial Grid	30
2.4 More on Iterative Solvers	32
2.4.1 Coupling with Domain Decomposition: The Overlapping Case	33
2.4.1.1 The Problem and the Decomposition of the Domain	33

2.4.1.2	The Iterative Procedure	33
2.4.1.3	The Coarse Propagator	34
2.4.1.4	The Fine Propagator	34
2.4.1.5	The Numerical Results	35
2.4.2	Coupling with Control	35
2.4.2.1	The Virtual Control Paradigm	35
2.4.2.2	The Parareal Algorithm for Control Problem	37
2.4.2.3	Another Route to Couple the Parareal Algorithm with a Control Strategy	39
2.4.3	Complexity and Parallelism Efficiency: Part 2	39
2.5	Stability Issues	40
2.5.1	Basic Results	40
2.5.2	A Possible Strategy for Convection Dominated Problems	40
2.6	Conclusions	42
3	On Transformation Methods and the Induced Parallel Properties for the Temporal Domain	45
C.-H. Lai		
3.1	Introduction	46
3.2	Temporal Integration Methods	47
3.3	Transformation Methods	48
3.3.1	Similarity Transforms	49
3.3.2	Laplace Transforms	50
3.4	Decoupled Parametric Systems	51
3.4.1	Similarity Transformation Methods	51
3.4.2	Laplace Transformation Methods	53
3.5	Some Numerical Tests	54
3.5.1	A Nonlinear Parabolic Problem	54
3.5.2	An European Option Example	57
3.5.3	Testing a Two-Level Time-Domain Algorithm	65
3.6	Conclusion	68
4	Asynchronous Substructuring Methods	71
C. Venet and F. Magoulès		
4.1	Introduction	71
4.2	Synchronous Iterative Methods	73
4.2.1	Iterative Methods	73
4.2.2	Implementation	75
4.3	Asynchronous Iterative Methods	76
4.3.1	Asynchronous Iteration	76
4.3.2	Mathematical Model	78

4.3.3	Convergence Analysis	79
4.3.4	Implementation	81
4.4	Substructuring Methods	81
4.4.1	Principles	81
4.4.2	Asynchronous Substructuring	84
4.5	Programming Environment	92
4.5.1	Presentation of the JACK Architecture	93
4.5.2	Implementation	94
4.5.3	Convergence Detection	96
4.6	Numerical Results	96
4.7	Conclusion	102
5	Asynchronous Multi-Splitting Methods	105
J.M. Bahi, R. Couturier and D. Laiymani		
5.1	Introduction	106
5.2	Parallel Numerical Iterative Algorithms	107
5.2.1	Generalities	107
5.2.2	Parallel Architectures	108
5.2.3	A Classification of Parallel Iterative Algorithms	109
5.3	Multisplitting Algorithms	113
5.3.1	Generalities	114
5.3.2	Linear Case	114
5.3.2.1	Implementation	116
5.3.3	Non-Linear Case	119
5.3.3.1	Multisplitting-Newton method	121
5.3.3.2	Implementation	121
5.4	The Jace Environment	122
5.4.1	The Daemon	123
5.4.2	The Spawner	124
5.4.3	The Worker	124
5.4.3.1	The Application Layer	125
5.4.3.2	The Communication Layer	125
5.4.4	The User Application	125
5.5	Experiments	126
5.5.1	The Grid'5000 Testbed	126
5.5.2	The linear case	126
5.5.2.1	The Conjugate Gradient NAS Parallel Benchmark	127
5.5.2.2	Experiments Conditions	127
5.5.2.3	Local Context	128
5.5.2.4	Distant Context	129
5.5.3	The Non-Linear Case	131
5.5.3.1	The Application	131

5.5.3.2	Experimental Results	133
5.6	Conclusions and Perspectives	134
6	A Coarse Grid Conjugate Gradient Method and its Application to Realistic Problems: Fully Iterative Method with Coarse Grid	137
H. Akiba		
6.1	Introduction	137
6.2	The Iterative Substructuring Method	139
6.2.1	Basic description	139
6.2.2	Domain Decomposition and the Iterative Substructuring Method	140
6.2.3	Preconditioning the Iterative Substructuring Method and the Schwarz Form	143
6.2.4	Formalization of the Iterative Substructuring Method	144
6.2.4.1	Discrete Harmonic Expansion	144
6.2.4.2	K -Orthogonal Decomposition of Global Space	145
6.2.4.3	Solution of the Stiffness Equations using K -Orthogonal Decomposition	147
6.2.4.4	The Schur Complement and the Conjugate Gradient Method	148
6.3	Preconditioning of the Iterative Substructuring Method	149
6.3.1	Equations of the Substructure	149
6.3.2	Application of the Schwarz Form	152
6.3.3	Separation of the Degrees of Freedom in the Subdomains	152
6.3.4	The Neumann Method	155
6.3.5	The Balancing Domain Decomposition Method	157
6.3.5.1	The Balancing Domain Algorithm	157
6.3.5.2	Construction of the Coarse Grid	158
6.3.5.3	The Procedure of the Balancing Domain Decomposition method	160
6.3.5.4	Preconditioning the Balancing Domain Decomposition Method	161
6.3.6	The Coarse Grid Conjugate Gradient Method	162
6.3.6.1	The Coarse Grid Conjugate Gradient Algorithm	162
6.3.6.2	Construction of the Coarse Grid	162
6.3.6.3	The Procedure for the Coarse Grid Conjugate Gradient Method	163
6.3.6.4	The Preconditioner for the Coarse Grid Conjugate Gradient Method	164
6.4	The Performance of the Coarse Grid Conjugate Gradient Method	164
6.4.1	The ADVC Code	164
6.4.2	Comparison of the BDD and CGCG methods	165

6.4.3	Drop Impact Analysis of a Mobile Phone using the CGCG method	166
6.5	Conclusions	168
7	Incorporation of Multipoint Constraints into Domain Decomposition Methods	171
T. Miyamura		
7.1	Introduction	171
7.2	The Domain Decomposition Method	173
7.2.1	Overview	173
7.2.2	A Domain Decomposition Method based on the Primal Sub-structuring Method	175
7.3	Incorporation of Multipoint Constraints into the Primal Substructuring Method	176
7.3.1	Classification of Multipoint Constraints in a Domain Decomposed Mesh	176
7.3.2	Modification of the Interface Problem	177
7.3.3	The Preconditioned Conjugate Projected Gradient Method	178
7.3.4	Treatment of the Dirichlet Boundary Conditions on the Interface Nodes	179
7.4	Incorporation of Multipoint Constraints into the Balancing Domain Decomposition Method	180
7.4.1	The Balancing Domain Decomposition Method	180
7.4.2	Incorporation of Multipoint Constraints into the Coarse Grid Problem	181
7.4.3	Combination of the Preconditioned Conjugate Projected Gradient Method and the Balancing Domain Decomposition Method	182
7.5	Parallel Implementation	182
7.5.1	Programming Environment	182
7.5.2	Implementation of the Boundary Domain Decomposition Method	182
7.5.3	The I/O format of the Multipoint Constraint Data	183
7.5.4	Parallel Implementation	184
7.6	Illustrative Examples	188
7.6.1	Hexahedron with a Constrained Face	189
7.6.2	Mechanical Parts in Contact	190
7.6.3	Parallel Performance	197
7.6.4	A Large-Scale Problem	197
7.7	Concluding Remarks	198

8 Efficient Approximate Inverse Preconditioning Techniques for Reduced Systems on Parallel Computers	203
K. Moriya, L. Zhang and T. Nodera	
8.1 Introduction	204
8.2 Reduced System with the Schur Complement	205
8.2.1 Greedy Algorithm	205
8.2.2 Making the Schur Complement	207
8.3 Preconditioning Techniques of Approximate Inverse	208
8.3.1 Newton Scheme	208
8.3.2 The Minimum Residual Scheme	210
8.3.3 The Approximate Inverse with the Sherman-Morrison Formulae Scheme	211
8.4 Parallelization	214
8.4.1 Implementation of the Reduced Systems	214
8.4.2 Implementation of the Preconditioner	215
8.5 Numerical Experiments	217
8.5.1 Example 1: A Partial Differential Equation Problem	217
8.5.2 Example 2: Matrix Market Problems	218
8.6 Concluding Remarks	223
9 Finite Element Matrices in Congruent Subdomains and some Techniques for Practical Problems	229
A. Suzuki and M. Tabata	
9.1 Introduction	229
9.2 Finite Element Matrices under Orthogonal Transformations	231
9.2.1 An Affine Transformation with an Orthogonal Matrix	231
9.2.2 Finite Element Bases and Matrices	232
9.2.2.1 Transformation of Scalar-Valued Finite Element Bases and Matrices	233
9.2.2.2 Transformation of Vector-Valued Finite Element Bases and Matrices	234
9.3 Finite Element Matrices Obtained from Decompositions into Congruent Subdomains	236
9.3.1 A Domain Decomposition into a Union of Congruent Subdomains	237
9.3.2 Representation of Total Matrices by Sub-Matrices	238
9.4 Finite Element Matrices under a Class of Orthogonal Transformations	240
9.4.1 Transformation of Vector-Valued Finite Element Bases and Matrices	240
9.4.2 Representation of Total Matrices by Sub-Matrices	241
9.5 Algorithms of Matrix-vector Multiplication for the Iterative Solver	242
9.5.1 General Orthogonal Transformations	242

9.5.2	A Class of Orthogonal Transformations	243
9.6	Treatment of Boundary Conditions	244
9.6.1	Examples from Continuum Mechanics	244
9.6.2	Weak Formulations and Finite Element Equations	246
9.6.3	Orthogonal Projection for Essential Boundary Conditions . .	248
9.6.4	Orthogonal Projection for Periodic Boundary Conditions . .	251
9.6.5	An Algorithm of Matrix-Vector Multiplication for Periodic Boundary Conditions	254
9.7	Reduction of Memory Requirements by Congruent Subdomains . .	255
9.7.1	Congruent Decomposition of a Cylinder	255
9.7.2	Reduction of Memory Requirements with Compressed Row Storage Format	256
9.8	Parallel Computation	259
9.8.1	Parallel Algorithm of Matrix-vector Multiplication	259
9.8.2	Parallel Implementation with OpenMP	262
9.8.3	Numerical Results	263
9.9	Conclusions	264
Index		267

Preface

Substructuring and domain decomposition methods are well suited for parallel computations. Indeed, the division of a problem into smaller subproblems, through artificial subdivisions of the domain, is a means for introducing parallelism. Substructuring and domain decomposition strategies include in one way or another the following ingredients: a decomposer to split a mesh into subdomains using different heuristics; local solvers (direct or iterative, exact or approximate) to find solutions for the subdomains for specific boundary conditions on the interface; interface conditions (weak or strong) enforcing compatibility and equilibrium between overlapping or non-overlapping sub-domains; and a solution strategy for the interface problem. The differences between the methods lie in how those ingredients are actually put to work and how they are combined to form an efficient solution strategy for the problem at hand.

The golden age of domain decomposition probably came with the emergence of parallel computing: in order to efficiently use the computational power of several processors simultaneously first one has attempted to use additive Schwarz iterations or iterative solvers on the entire domain, using domain decomposition to dispatch the cost of matrix multiplications on the processors. Then Schur complement approaches (primal and dual) were developed: combining efficient solution techniques for the local problems with robust iterative algorithms to solve the interface problem one could build strategies to use the full potential of multiprocessor machines. Those methods were further developed to improve their robustness for practical engineering problems. Even today, despite the many reported successful applications of domain decomposition, making the iterative solution of the interface problem robust and efficiently parallel remains a challenge.

This edited book continues the series on Domain Decomposition Methods for engineering problems and follows the two previous volumes respectively entitled:

- *Mesh Partitioning Techniques and Domain Decomposition Methods* (2007), edited by F. Magoulès, published by Saxe-Coburg Publications, Stirling, United Kingdom; and
- *Domain Decomposition Methods: Theory and Applications* (2006), edited by F. Magoulès and T. Kako, published by Gakkotosho, Tokyo, Japan.

The present volume presents in nine chapters a selection of some domain decomposition and substructuring methods including: parareal in time algorithm, transformation methods and induced parallel properties for the temporal domain, asynchronous it-

erative methods, asynchronous sub-structuring methods, asynchronous multi-splitting methods, parallel iterative methods, coarse grid conjugate gradient, multi-point constraints in domain decomposition methods, approximate inverse preconditioning techniques, congruent sub-domains, linear and non-linear problems. The topics covered in this book are wide ranging and demonstrate the extensive use of substructuring and domain decomposition methods in fluid mechanics, structural mechanics, and computational finance.

Frédéric Magoulès
Applied Mathematics and Systems Laboratory
Ecole Centrale Paris, Grande Voie des Vignes
92295 Châtenay-Malabry Cedex, France