MESH ENHANCEMENT

This page is intentionally left blank

MESH ENHANCEMENT

Selected Elliptic Methods,
Foundations and Applications

Glen A Hansen
Rod W Douglass
Andrew Zardecki

Los Alamos National Laboratory, USA

Imperial College Press

Published by

Imperial College Press
57 Shelton Street
Covent Garden
London WC2H 9HE

Distributed by

World Scientific Publishing Co. Pte. Ltd.

5 Toh Tuck Link, Singapore 596224

USA office: 27 Warren Street, Suite 401-402, Hackensack, NJ 07601

UK office: 57 Shelton Street, Covent Garden, London WC2H 9HE

British Library Cataloguing-in-Publication Data

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

MESH ENHANCEMENT

Selected Elliptic Methods, Foundations and Applications

Copyright © 2005 by Imperial College Press

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the Publisher.

For photocopying of material in this volume, please pay a copying fee through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. In this case permission to photocopy is not required from the publisher.

ISBN 1-86094-487-6

Printed in Singapore.

We dedicate this book to
Our Families and Colleagues

This page is intentionally left blank

Preface

Simply stated, the purpose for preparing this book was to document the experience within the fields of *grid generation* and *enhancement* accrued over the past years by members of the U. S. Department of Energy's Advanced Simulation and Computing (ASC) Setup Project at the Los Alamos National Laboratory.¹

This work was motivated by the desire to achieve better results when modeling fluid dynamics and heat transfer problems, high-speed fluid flows, along with other applications. Generally, these problems were discretized by multi-dimensional structured and/or unstructured meshes, usually possessing highly-curved external and internal boundary definitions. Furthermore, the vast majority of these two- and three-dimensional meshes were required by the final simulation application to contain predominantly quadrilateral or hexahedral elements. It has been our challenge to meet these, seemingly increasingly complex, requirements. While unstructured mesh generation and enhancement methods present the most difficult challenges, structured meshes continue to have challenges of their own.

Note that we use the terms *mesh* and *grid* interchangeably to mean the set of cells, faces, and/or nodes that represent the discretization of physical space contained and defined by geometrical surfaces, *etc.* to be used by an approximate numerical algorithm for the purpose of simulating a physical process. The reader will also note that we have drawn a distinction between *grid generation* and *grid enhancement*. Historically, the term *grid generation* has been used to designate both operations. It is our view that *grid generation* refers to the process of creating an initial grid based directly

¹ **Acknowledgment:** This work was performed under the auspices of the U. S. Department of Energy by Los Alamos National Laboratory under Contract W-7405-ENG-36 (LA-UR-04-2476).

on domain geometry information. Grid enhancement refers to the operations involved in modifying the initial mesh to improve its computability or ability to meet the requirements of the ultimate simulation application.

It is our goal in writing this monograph that anyone wishing to understand the basics of grid smoothing and enhancement using elliptic methods may find this book useful. Our intent is not to present an exhaustive survey of the field by looking at all elliptic methods; we limit this presentation to those approaches that we are most familiar with or have used successfully. To this end, the book:

- Presents basic background information on grids and terminology as well as on approximation methods for differential equations.
- Includes a discussion of solving the resulting non-linear algebraic equation systems.
- Because the emphasis is upon elliptic enhancement methods which rely on spatial metrics, several chapters (and an appendix) are presented that focus on differential geometry of surfaces.
- These topics are followed by a discussion of existing elliptic enhancement methods, placing them in context of the general Laplace-Beltrami elliptic system (LBES) for grid enhancement.
- The last two chapters detail how the LBES is implemented for structured and unstructured grids and provide motivation for our use of this approach by comparing results with other selected elliptic methods.

This book, therefore, presents information on the computational geometry and mesh enhancement aspects of the Numerical Simulation Process.

Specifically, the introductory chapter on basic concepts places grid generation and enhancement within the numerical simulation process, describes an elliptic enhancement methodology, and presents a primer on meshes and associated terminology. It also briefly summarizes several grid generation methods and introduces the concept of grid quality.

In order to define an initial mesh and to properly enhance it, a detailed description must exist of the geometric objects that define the computational domain. This includes the external boundaries of the mesh as well as the internal geometries defining specific material interfaces. Chapter 2 presents information about curves and surfaces and operations that may be performed upon them. The focus is on parametric curves and surface descriptions, but some information is also provided on constructive solid

geometry. An overview of geometric data structures is also given.

The chapter on numerical approximation methods for differential equations (Chapter 3) is rather extensive, covering finite difference methods and methods of weighted residuals, also called weak solution methods. Weighted residual methods include finite volume and finite element methods as special cases. These approximation methods are central to the mesh topology definition and are used to solve the LBES as well as within the final physics application. Consequently, we have given a thorough introduction to these methods so that the reader can obtain sufficient information to support our stated goals in preparing this book.

As a result of applying the numerical approximations to the LBES, systems of, generally, non-linear algebraic equations for the unknown coordinates of each mesh node are formed. These must then be solved in a reliable and accurate manner. The next chapter (Chapter 4) presents a discussion of the methods we have found effective for obtaining such solutions.

The next two chapters, Chapters 5 and 6, revisit surface geometry by focusing upon the two fundamental differential geometric forms required to understand the metric tensor used in the LBES. A discussion of isothermal coordinates and their generalization, harmonic coordinates, is also presented. An appendix (Appendix A) provides a summary of the mathematical concepts used in discussions on differential geometry and special coordinates.

Before we present the LBES for structured and unstructured meshes, a discussion of selected existing elliptic mesh enhancement methods is given in Chapter 7. They are shown to be derivable from our general perspective. This places the LBES in historical perspective.

Chapter 8 presents the implementation and results for applying the LBES to structured meshes, while Chapter 9 does so for unstructured mesh enhancement. For structured meshes, the LBES results are compared with several existing elliptic results. For unstructured meshes, the finite element method is used to solve the LBES. Results are presented for two- and three-dimensional meshes.

Topics omitted as falling beyond the goals of the monograph include

- parallel processing
- parallel mesh decomposition algorithms
- data structures for unstructured meshes
- application-specific criteria defining “mesh quality”
- solution-adaptive mesh enhancement methods

- embedding solution features into the mesh

The authors are indebted to many who made the development of this material possible. First, we wish to thank the ASC Program at Los Alamos National Laboratory for supporting this work and motivating the development of more effective approaches at mesh enhancement. We wish to acknowledge the Setup Team and its customer base for their roles in the development of this material, which ranged from providing customer requirements to contributing technical and application details, algorithms, assorted codes, and often detailed insight into various problems that were encountered. We specifically thank Alan Stagg, William Hachfeld, and Ahmed Khamayseh for their many contributions, including the *Altair* grid generation capability, the Modified Interpolated Control Function grid enhancement method, impedance matching, element Jacobian development, and countless other approaches and algorithms that they contributed to the Setup Project. We also thank Doran Greening and Randy Bos who motivated the development of several approaches considered here; contributing ideas, algorithms, and theoretical development to this effort, and who spent many hours in the advancement of these approaches. We finally wish to thank Will Dearholt who read early drafts of the manuscript and provided valuable feedback on its improvement.

Ultimately, it is our desire that this monograph will be a useful addition to the mesh generation and enhancement literature and its methods used to enhance meshes of broad application.

G.A. Hansen
R.W. Douglass
A. Zardecki

Contents

<i>Preface</i>	vii
1. Basic Concepts	1
1.1 The Physics Simulation Process	3
1.2 Mesh Enhancement using Elliptic Methods.	9
1.3 A Brief Primer on Meshes	11
1.3.1 Mesh Topology	11
1.3.2 Structured Meshes	12
1.3.3 Unstructured Meshes	15
1.3.4 Basic Grid Generation Algorithms	16
1.3.4.1 Transfinite Interpolation Method (TFI) . . .	17
1.3.4.2 Solution-Based Methods	18
1.3.4.3 Multiblock Method	19
1.3.4.4 Advancing Front Method	19
1.3.4.5 Delaunay Triangulation Method	20
1.3.4.6 Quadtree-Octree Methods	21
1.3.5 Mesh Quality Issues	23
2. Computational Geometry and Geometric Data Structures	25
2.1 Geometric Modeling	28
2.1.1 Curves	28
2.1.2 Properties of Parametric Curves	31
2.1.2.1 Arc-length	31
2.1.2.2 Curvature	31
2.1.2.3 Tangent Vectors	32
2.1.2.4 Principal Unit Normal	34

2.1.2.5	The Binormal Unit Vector	35
2.1.3	Constructing Parametric Curves	35
2.1.3.1	Wilson-Fowler Splines	39
2.1.3.2	Wilson-Fowler Splines for Closed Curves	49
2.1.3.3	The Parametric Cubic (PC) Curve	50
2.1.3.4	Operations on Curves	54
2.1.4	Parametric Surfaces	60
2.1.4.1	Ruled Surfaces	60
2.1.4.2	Translational Surfaces	61
2.1.4.3	Tensor Product Surfaces	63
2.1.4.4	The Parametric Bi-Cubic Patch: The 16-Point Surface	65
2.1.4.5	The Parametric Bi-Cubic Patch: The 4-Curve Surface	66
2.1.4.6	Parametric Surface Properties	69
2.1.4.7	Blending Patches at a Common Border	72
2.1.4.8	Blending Between Non-Adjacent Patches	74
2.1.5	CSG Geometry	74
2.2	Mesh Operations On Geometry	77
2.2.1	Boundary Discretization	78
2.2.1.1	Equal Parameter-Increment Distribution	78
2.2.1.2	Equal Euclidean-Length Distribution	79
2.2.1.3	Equal Angle-Increment Distribution	81
2.2.2	Boundary Node Redistribution	84
2.3	Geometric Data Structures	89
2.3.1	IGES Data	89
2.3.2	Stereo Lithography	90
3.	Discretization Methods for Differential Equations	95
3.1	Finite Difference Methods	96
3.1.1	Finite Difference Operators	99
3.1.2	Non-uniform Difference Approximation	100
3.1.3	Finite Differences Applied to Differential Equations	101
3.1.4	Consistency of Finite Difference Approximations	104
3.1.5	Stability of Finite Difference Approximations	105
3.1.6	Implicit Finite Difference Approximations	109
3.2	Weak Solutions	113
3.2.1	Hilbert Spaces	114
3.2.1.1	Functionals In Hilbert Spaces	118

3.2.1.2	Operators in Hilbert Spaces	120
3.2.2	Sobolev Spaces	124
3.2.3	Boundary Value Problem for Elliptic Operators . . .	126
3.2.3.1	The Dirichlet Boundary Value Problem . . .	130
3.2.3.2	The Neumann Boundary Value Problem . . .	131
3.2.4	Weak Solution Methods	135
3.2.4.1	The Rayleigh-Ritz Method	135
3.2.4.2	The Galerkin Method	136
3.3	Applications of Weighted Residual Methods	138
3.3.1	The Subdomain Method	139
3.3.2	Finite Volume Methods	141
3.3.3	The Galerkin Method	150
3.4	The Finite Element Method	152
3.4.1	One-Dimensional Finite Element Methods	157
3.4.1.1	One-Dimensional Simplex Element Basis Functions	161
3.4.1.2	One-Dimensional Quadratic Element Inter- polation.	163
3.4.1.3	One-Dimensional Cubic Element Interpolation	171
3.4.2	Two-Dimensional Finite Element Methods.	178
3.4.2.1	A Note On Interpolation Error.	181
3.4.2.2	Two-Dimensional Bilinear Element Interpo- lation Using Quadrilateral Elements	181
3.4.2.3	Element Integrals: The Master Element . .	184
3.4.2.4	Two-Dimensional Linear Element Interpola- tion: Triangular Elements	195
3.4.3	Three-Dimensional Elements	199
3.4.3.1	Tetrahedral Elements	199
3.4.3.2	Hexahedral or Rectangular Prism Elements	201
3.4.4	Computation of Element Matrices Using Gaussian Quadrature	202
3.4.5	A Brief Introduction to Errors in the Finite Element Method	204
4.	Solving the Mesh Enhancement Algebraic Equation System	209
4.1	Introduction	209
4.2	Selected Matrix Solution Methods	211
4.2.1	Jacobi Iterative Relaxation	213
4.2.2	Gauss-Seidel Relaxation	216

4.2.3	Other Iterative Approaches	216
4.3	Solution of Nonlinear Problems	221
4.3.1	Picard Linearization	222
4.3.2	Newton Linearization	223
4.4	Nonlinear Solution Methods for Finite Element Applications	226
4.4.1	Picard Linearization	227
4.4.2	Newton Linearization	228
4.4.2.1	Assembling the Tangent Stiffness Matrix (TSM)	230
4.4.2.2	Alternative Schemes of Addressing Nonlinear Terms	231
5.	The Geometry of Surfaces in Euclidean Space	235
5.1	The First Fundamental Form	236
5.2	The Second Fundamental Form	238
5.3	Intrinsic Equations of a Surface	244
5.3.1	The Gauss-Weingarten Equations	245
5.3.2	The Theorem of Gauss and the Codazzi Equations .	247
5.4	Covariant Differentiation	250
5.5	Geodesics in a Riemann Space	254
5.6	Curvature of Space	257
6.	Special Coordinate Systems	261
6.1	Isothermal Coordinates	262
6.1.1	Beltrami Equation	263
6.1.2	Complex Form	266
6.1.3	Solution of the Beltrami Equation	268
6.1.4	Teichmüller Spaces	270
6.2	Harmonic Coordinates	274
6.2.1	Sign Convention and Basic Formulas	277
6.2.2	The Ricci Tensor in Harmonic Coordinates	279
6.3	Conclusions	280
7.	Elliptic Mesh Enhancement Equation Systems	283
7.1	Khamayseh-Mastin Mesh Enhancement	284
7.2	Special Cases	287
7.2.1	Thompson-Thames-Mastin Generator	287
7.2.2	Winslow Grid Generator	290
7.3	Connection with Harmonic Coordinates	290

7.4	Variational Methods	291
7.5	Surface Meshes and Adaptive Methods	295
7.5.1	Numerical Examples	296
7.5.2	Adaptive Grid Methods	299
8.	Structured Mesh Smoothing and Enhancement	305
8.1	Introduction	305
8.1.1	Boundary Curve Discretization, Boundary Condi- tions, and Structured Terminology	309
8.1.2	Development of a Mesh Quality Metric	316
8.1.3	Introduction to Two-Dimensional Structured Mesh Methods	323
8.1.3.1	Transfinite Interpolation	326
8.1.3.2	Node Point Averaging Approaches	327
8.1.3.3	Winslow-Crowley Smoothing	335
8.2	Prescriptive Methods	345
8.2.1	Thompson-Thames-Mastin Generator	345
8.2.2	Specification of Control Functions <i>via</i> an Algebraic Transformation to a Parameter Space.	353
8.3	Laplace-Beltrami Mesh Enhancement Using a Target Metric	363
8.3.1	The Discrete Laplace-Beltrami System	368
8.3.2	Geometric Interpretation of the Metric Terms	372
8.3.3	The Target Metric Tensor	386
8.4	Using a Target Metric Surface to Implement Solution Adap- tivity	394
8.5	Rudimentary Methods for Unstructured Meshes	402
8.5.1	Laplace Smoothing	404
8.5.2	Ad hoc Laplace-Beltrami Methods	406
8.5.3	Winslow-based Unstructured Methods	408
8.6	Three-Dimensional Structured Laplace-Beltrami Methods	410
8.7	Conclusions	413
9.	Mesh Enhancement Methods for Unstructured Meshes	415
9.1	Laplace-Beltrami Enhancement Equations in Two and Three Dimensions	419
9.2	Approximation of the Laplace-Beltrami Equation System	422
9.2.1	Two-Dimensional Finite Element Implementation	424
9.2.2	Three-Dimensional Finite Element Implementation	428

9.2.3	Target Metric Tensor Estimation: Metric Equidistribution	430
9.2.4	Target Metric Tensor Estimation: Coarse Graining	433
9.2.5	Implementation Details and Summary	436
9.2.6	Two-Dimensional Examples	443
9.2.7	Three-Dimensional Examples	453
9.3	Quantitative Mesh Comparisons	465
9.4	Conclusions	469
Appendix A Differential Manifolds and Fiber Bundles		471
A.1	Scalar Field	472
A.2	Vectors and Tensors	473
A.3	Infinitesimal Transformations	475
A.4	Other Transformation Laws	477
A.5	Fiber Bundles	479
A.5.1	Differentiable Manifolds	480
A.5.2	Principal Fiber Bundles	486
A.5.3	Associated Fiber Bundles	487
A.6	Connections in Vector Bundles	489
A.7	Riemannian Manifolds	493
<i>Bibliography</i>		501
<i>Index</i>		511