

国家出版基金项目
NATIONAL PUBLICATION FOUNDATION



Series in Information and Computational Science

54

Geometric Partial Differential Equation Methods in Computational Geometry

Guoliang Xu Qin Zhang

(计算几何中的几何偏微分方程方法)



SCIENCE PRESS
Beijing



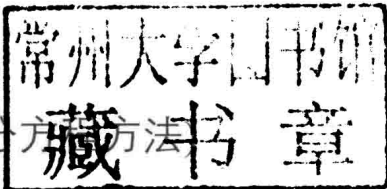
国家出版基金项目
NATIONAL PUBLICATION FOUNDATION


Series in Information and Computational Science 54

Guoliang Xu, Qin Zhang

Geometric Partial Differential Equation Methods in Computational Geometry

(计算几何中的几何偏微分方程方法)



 Science Press
Beijing

Responsible Editors: Liping Wang and Baojun Tang

Copyright© 2013 by Science Press
Published by Science Press
16 Donghuangchenggen North Street
Beijing 100717, China

Printed in Beijing

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 the prior written permission of the copyright owner.

ISBN 978-7-03-036764-8 (Beijing)

Editorial Board

Editor-in-Chief: Shi Zhongci

Vice Editor-in-Chief: Wang Xinghua Yu Dehao

Members:	Bai Fengshan	Bai Zhongzhi	Chen Falai
	Chen Zhiming	Chen Zhongying	Cheng Jin
	E Weinan	Guo Benyu	He Bingsheng
	Hou Yizhao	Shu C.-W.	Song Yongzhong
	Tang Tao	Wu Wei	Xu Jinchao
	Xu Zongben	Yang Danping	Zhang Pingwen

Preface to the Series in Information and Computational Science

Since the 1970s, Science Press has published more than thirty volumes in its series Monographs in Computational Methods. This series was established and led by the late academician, Feng Kang, the founding director of the Computing Center of the Chinese Academy of Sciences. The monograph series has provided timely information of the frontier directions and latest research results in computational mathematics. It has had great impact on young scientists and the entire research community, and has played a very important role in the development of computational mathematics in China.

To cope with these new scientific developments, the Ministry of Education of the People's Republic of China in 1998 combined several subjects, such as computational mathematics, numerical algorithms, information science, and operations research and optimal control, into a new discipline called Information and Computational Science. As a result, Science Press also reorganized the editorial board of the monograph series and changed its name to Series in Information and Computational Science. The first editorial board meeting was held in Beijing in September 2004, and it discussed the new objectives, and the directions and contents of the new monograph series.

The aim of the new series is to present the state of the art in Information and Computational Science to senior undergraduate and graduate students, as well as to scientists working in these fields. Hence, the series will provide concrete and systematic expositions of the advances in information and computational science, encompassing also related interdisciplinary developments.

I would like to thank the previous editorial board members and assistants, and all the mathematicians who have contributed significantly to the monograph series on Computational Methods. As a result of their contributions the monograph series achieved an outstanding reputation in the community. I sincerely wish that we will extend this support to the new Series in Information and Computational Science, so that the new series can equally enhance the scientific development in information and computational science in this century.

Shi Zhongci
2005.7

Preface

Computational geometry is an interdisciplinary subject composed of approximation theory, differential geometry, computational mathematics, and computer graphics, etc. This subject studies the structure, representation, analysis and synthesis of geometric shapes using computers. It is the mathematical foundation of computer aided geometric design (CAGD).

In the 1960s, computer aided design (CAD) and computer aided manufacturing (CAM) entered the shipbuilding, aviation and the automobile industries helping to shape, design and manufacture. Stimulated by the development of computer technology and wide applications of industrial design, the subject of computational geometry has been developing rapidly. Heretofore, many effective methods, such as Bézier, B-spline, non-uniform rational B-spline (NURBS), subdivision, and partial differential equations have been established, based on the parametric, implicit and discrete presentations of surfaces and the theory of interpolation and approximation. At present, CAGD is still an attractive field with large number of the researchers engaged with classical approximation theory, differential geometry, computational mathematics and computer graphics, devoting themselves to this area, helping to promote its comprehensive development. Under such a background, an emerging field of research, geometric partial differential equation methods in computational geometry, is generated.

It is generally known that partial differential equations (PDEs) are equations describing the relationship among independent variables, unknown functions, and their partial derivatives. However, geometric partial differential equations, which are used to control the motion of surfaces and manifolds, are partial differential equations which include only geometric quantities, except the time variable. Geometric partial differential equations are geometric, which means that they do not depend on specific parametrization. More importantly, surfaces satisfying the geometric partial differential equations usually have some global optimal properties. For instance, the mean curvature flow, the Willmore flow, and the minimal mean curvature variation flow minimize the area, the total squared mean curvature and the total squared variation of the mean curvature of the surfaces, respectively. These optimal properties make the generated surfaces possess a perfect fairing effect and even an aesthetic feeling of art.

The method of solving various geometric design problems using geometric partial differential equations is named as the geometric partial differential equation method. In recent

years, with the development of computer technology, the geometric partial differential equation method has exhibited obvious superiority in many fields, such as CAD, CAGD, surface processing and image processing. The method has many advantages, such as solid theoretical basis, high efficiency, ease of programming, possessing a generic and wide applicability, and so forth. It can be used in the domains of image processing, surface processing, quality meshing, free-form surface design, surface blending, surface reconstruction, surface recovery, shape deformation, and so on.

Geometric partial differential equations also involve many other theoretical and application areas. In the areas of physics, chemistry, biology, fluid mechanics, material science, combustion theory, seismology and computer vision, there exists many interface motion problems. Many of these problems can be abstracted as geometric problems and described by geometric partial differential equations. In theory, geometric partial differential equations are closely related to geometrical analysis, manifold theory, topology, complex analysis, variational method, geometric measurement theory, and critical point theory. For example, the mean curvature flow and the Ricci flow relate to the positive mass conjecture and Poincaré conjecture, respectively.

Earlier research on using PDEs to handle surface modeling problems can be traced back to the work of Bloor et al. at the end of the 1980s. The basic idea in their work is to use biharmonic equation on a rectangular domain to solve the blending and hole filling problems. However, the biharmonic equation is not intrinsic. The solution of the equation depends on specific parametrization. Therefore, the biharmonic equation is not a geometric partial differential equation we considered in this book. There are many successful examples of solving geometry design problems by geometric partial differential equations. In the early days, the mean curvature flow was used to smooth noise surfaces and very desirable results are obtained. However, since the second-order flow, such as the mean curvature flow, cannot achieve a smooth blending of different surface patches, the fourth- and sixth-order geometric flows are used afterward in the surface blending, free-form surface design, surface recovery, and so on, yielding perfect results.

In conclusion, the geometric partial differential equation method used in computational geometry is still a fresh field with wide development potential and is currently at its newborn stage. The content of this book is mainly about the authors' research results and work experience in this field. Our wish is to promote the development of the geometric partial differential equation method so as to make it a systemic, integrated and effective method in the area of computational geometry. In Chapter 1, elementary differential geometry is reviewed, including surface representations, curvatures and differential geometric operators, and Green's formulas for differential operators. In Chapter 2, geometric partial differential equations for parametric surfaces are constructed for several general energy functionals by complete variational calculus and normal variational calculus. Parallel to Chapter 2, in Chapter 3, geometric partial differential equations are constructed for implicit surfaces by several approaches and their relationship is discussed. Chapter 4 is devoted to the discretization of differential operators and curvatures and their convergence analysis. In Chapter 5, discrete surface design by quasi finite difference method is discussed. Chapter 6 deals with the spline surface design problem by quasi finite difference method and finite element method. Subdivision surface design by finite element methods is presented in Chapter 7. In Chapter 8, we discuss the level-set method for surface designs and its applications, such

as surface reconstruction from scattered data set, and surface metamorphosis. In Chapter 9, we discuss quality meshing by geometric flows, such as triangular, quadrilateral, tetrahedral and hexahedral meshing with single domain or multiple domains.

The content of the book covers the main research work of the computational geometry research group in the Institute of Computational Mathematics and Scientific Engineering Computing in Chinese Academy of Sciences in the past decade. Postdoctoral fellows Huanxi Zhao and Hongqing Zhao, PhD students Qing Pan, Qin Zhang, Dan Liu, Ming Li, Yanmei Zheng, Zhucui Jing, Chong Chen, Xia Wang and Juelin Leng, successively, participated in this research work, and for their contributions to this book the authors are sincerely grateful. My graduate students, Ming Li and Yanmei Zheng, carefully read the first draft of the book, and made a comprehensive discussion in our seminar and put forward many suggestions for revision. Professor Chadrajit Bajaj of the University of Texas at Austin, Dr. Zhiqiang Xu in the Institute of Computing Mathematics and Scientific Engineering Computing, Professor Yongjie Zhang of Carnegie Mellon University and Dr. Wenqi Zhao of the University of Texas at Austin cooperated with me and also contributed to the content of the book. The authors give their earnest thanks to them.

The project was successively supported by Chinese Academy of Sciences Innovation Fund (1770900), National Natural Science Foundation of China (10241004, 10371130, 60773165), National Key Basic Research Program (2004CB318000), NSFC key project under grant (10990013) and NSFC Funds for Creative Research Groups of China (grant No. 11021101). The State Key Laboratory of Scientific and Engineering Computing also constantly supports the project with its various software tools, hardware facilities, as well as research fund. Obviously, without these funds and supports, the project would not have been completed smoothly. On the occasion of the forthcoming book, the authors give their heartfelt thanks to these supports.

Lastly, the authors would like to thank their families for their continuous support.

Guoliang Xu

State Key Laboratory of Scientific and Engineering Computing
The Institute of Computational Mathematics and
Scientific/Engineering Computing
Chinese Academy of Sciences

Beijing, July, 2012

Acronyms

1D	One-Dimensional
2D	Two-Dimensional
3D	Three-Dimensional
AMCF	Averaged Mean Curvature Flow
CAD	Computer Aided Design
CAGD	Computer Aided Geometric Design
CAM	Computer Aided Manufacture
CT	Computed Tomography
EMDB	Electron Microscopy Data Bank
ENO	Essentially Non-Oscillatory
FEM	Finite Element Method
GHO	Giaquinta-Hildebrandt Operator
GMRES	Generalized Minimal RESidual method
GPDE	Geometric Partial Differential Equation
IOS	International Organization for Standardization
LBO	Laplace-Beltrami Operator
MCF	Mean Curvature Flow
MFEM	Mixed Finite Element Method
MMCVF	Minimal Mean Curvature Variation Flow
MRI	Magnetic Resonance Imaging
NURBS	Non-Uniform Rational B-Spline
PDB	Protein Data Bank
PDE	Partial Differential Equation
QFDM	Quasi Finite Difference Method
QSDF	Quasi Surface Diffusion Flow
rRNA	ribosomal RNA
SAS	Solvent-Accessible Surface
SDF	Surface Diffusion Flow
SES	Solvent-Excluded Surface
STEP	STandard for the Exchange of Product model data
SVD	Singular Value Decomposition
TVD	Total Variation Diminishing
VWS	Van der Waals Surface
WENO	Weighted Essentially Non-Oscillatory
WF	Willmore Flow

Contents

Preface

Acronyms

Chapter 1 Elementary Differential Geometry	1
1.1 Parametric Representation of Surfaces	1
1.2 Curvatures of Surfaces	5
1.3 The Fundamental Equations and the Fundamental Theorem of Surfaces	7
1.4 Gauss-Bonnet Theorem	10
1.5 Differential Operators on Surfaces	11
1.6 Basic Properties of Differential Operators	17
1.7 Differential Operators Acting on Surface and Normal Vector	20
1.8 Some Global Properties of Surfaces	25
1.8.1 Green's Formulas	26
1.8.2 Integral Formulas of Surfaces	28
1.9 Differential Geometry of Implicit Surfaces	31
Chapter 2 Construction of Geometric Partial Differential Equations for	
Parametric Surfaces	34
2.1 Variation of Functionals for Parametric Surfaces	35
2.2 The Second-order Euler-Lagrange Operator	37
2.3 The Fourth-order Euler-Lagrange Operator	41
2.4 The Sixth-order Euler-Lagrange Operator	46
2.5 Other Euler-Lagrange Operators	51
2.5.1 Additivity of Euler-Lagrange Operators	52
2.5.2 Euler-Lagrange Operator for Surfaces with Graph Representation	53
2.6 Gradient Flow	54
2.6.1 L^2 -Gradient Flow for Parametric Surfaces	54
2.6.2 H^{-1} -Gradient Flow for Parametric Surfaces	59
2.7 Other Geometric Flows	62
2.7.1 Area-Preserving or Volume-Preserving Second-order Geometric Flows	62
2.7.2 Other Sixth-order Geometric Flows	65

2.7.3	Geometric Flow for Surfaces with Graph Representation	65
2.8	Notes	66
2.9	Related Works	67
2.9.1	The Choice of Energy Functionals	67
2.9.2	About Geometric Flows	68
Chapter 3 Construction of Geometric Partial Differential Equations for Level-Set Surfaces		
	Level-Set Surfaces	71
3.1	Variation of Functionals on Level-Set Surfaces	71
3.2	The Second-order Euler-Lagrange Operator	74
3.3	The Fourth-order Euler-Lagrange Operator	75
3.4	The Sixth-order Euler-Lagrange Operator	77
3.5	L^2 -Gradient Flows for Level Sets	79
3.6	H^{-1} -Gradient Flow for Level Sets	82
3.7	Construction of Geometric Flows from Operator Conversion	83
3.8	Relationship Among Three Construction Methods of the Geometric Flows	85
Chapter 4 Discretization of Differential Geometric Operators and Curvatures		
4.1	Discretization of the Laplace-Beltrami Operator over Triangular Meshes	88
4.1.1	Discretization of the Laplace-Beltrami Operator over Triangular Meshes	89
4.1.2	Convergence Test of Different Discretization Schemes of the LB Operator	92
4.1.3	Convergence of the Discrete LB Operator over Triangular Meshes	95
4.1.4	Proof of the Convergence Results	96
4.2	Discretization of the Laplace-Beltrami Operator over Quadrilateral Meshes and Its Convergence Analysis	104
4.2.1	Discretization of LB Operator over Quadrilateral Meshes	104
4.2.2	Convergence Property of the Discrete LB Operator	106
4.2.3	Simplified Integration Rule	107
4.2.4	Numerical Experiments	108
4.3	Discretization of the Gaussian Curvature over Triangular Meshes	111
4.3.1	Discretization of the Gaussian Curvature over Triangular Meshes	111
4.3.2	Numerical Experiments	111
4.3.3	Convergence Properties of the Discrete Gaussian Curvatures	113
4.3.4	Modified Gauss-Bonnet Schemes and Their Convergence	118
4.3.5	A Counterexample for the Regular Vertex with Valence 4	121
4.4	Discretization of the Gaussian Curvature over Quadrilateral Meshes and Its Convergence Analysis	121
4.4.1	Discretization of the Gaussian Curvature over Quadrilateral Meshes	122
4.4.2	Convergence Property of the Discrete Gaussian Curvature	124
4.5	Consistent Approximations of Some Geometric Differential Operators	127
4.5.1	Consistent Discretizations of Differential Geometric Operators and Curvatures Based on the Quadratic Fitting of Surfaces	127
4.5.2	Convergence Property of Discrete Differential Operators	131
4.5.3	Consistent Discretization of Differential Operators Based on Biquadratic Interpolation	138

4.6	Related Work on the Discretization of the Gaussian Curvature	140
Chapter 5 Discrete Surface Design by Quasi Finite Difference Method		142
5.1	Introduction	142
5.2	$2k$ -th Order Geometric Partial Differential Equations of Special Forms	144
5.2.1	Numerical Solving Methods	144
5.2.2	Comparative Results and Application Examples	150
5.3	Fourth-order Geometric Partial Differential Equations of General Forms	156
5.3.1	Numerical Solving of Fourth-order Geometric Partial Differential Equation of General Forms	157
5.3.2	Comparative Results and Application Examples	159
5.4	Minimal Mean Curvature Variation Flow	164
5.4.1	Numerical Solving of the Minimal Mean Curvature Variation Flow	164
5.4.2	Application Examples	166
5.5	A Note About the Convergence	170
5.5.1	Fully Discrete Scheme of the Boundary Conditions	170
5.5.2	Semi-Discretization of Boundary Conditions	178
Chapter 6 Spline Surface Design by Quasi Finite Difference Method and Finite Element Method		182
6.1	Spline Surface Construction by Quasi Finite Difference Method	182
6.1.1	B-spline Surface	182
6.1.2	Construction of Geometric Partial Differential Equation B-spline Surface	187
6.1.3	Minimal B-spline Surface	194
6.1.4	Numerical Experiments of Convergence	194
6.2	Spline Surface Construction by Finite Element Methods	195
6.2.1	GPDEs and Their Mixed Variational Forms	196
6.2.2	Construction Steps of GPDE Spline Surfaces	197
6.2.3	Numerical Examples of Convergence	201
6.3	Regularization of Spline Surfaces	203
6.3.1	L^2 -Gradient Flows	204
6.3.2	Numerical Solutions of the L^2 -Gradient Flows	207
6.3.3	Regularization of B-Spline Curves	208
6.4	About Finite Difference Method and Finite Element Method	209
6.5	Numerical Integration	210
6.6	Related Work	212
6.6.1	Bézier and B-spline Curves and Surfaces	212
6.6.2	Differential Equation Surfaces	213
6.6.3	Geometric Differential Equation Surfaces	214
Chapter 7 Subdivision Surface Design by Finite Element Methods		215
7.1	Sobolev Spaces on Surfaces	215
7.2	Finite Element Spaces	216
7.2.1	Loop's Subdivision Scheme	217
7.2.2	The Limit Surface Corresponding to Vertices	219
7.2.3	Evaluation of Regular Surface Patches	219
7.2.4	Evaluation of Irregular Surface Patches	220

- 7.2.5 Basis Functions and Classifications of Surface Patches 222
- 7.2.6 Parametric Representation and Isoparametric Elements 224
- 7.3 Mean Curvature Flow and Surface Modeling 224
 - 7.3.1 The Background of Surface Modeling 225
 - 7.3.2 A Variant of the Mean Curvature Flow 228
 - 7.3.3 Numerical Solutions 230
- 7.4 Fourth-order Geometric Partial Differential Equations 234
 - 7.4.1 Variational Form of the Fourth-order Equation 234
 - 7.4.2 Discretization of Fourth-order Equations 238
 - 7.4.3 Applications and Examples of Fourth-order Equations 247
- 7.5 Sixth-order Geometric Partial Differential Equations 252
 - 7.5.1 Weak Forms 253
 - 7.5.2 Discretization of the Sixth-order Equations 255
- 7.6 Subdivision Surfaces with Boundaries 260
 - 7.6.1 Extended Loop’s Subdivision Surfaces 262
 - 7.6.2 Minimal Surface Construction 266
 - 7.6.3 G^1 Surface Construction 268
- 7.7 Related Work on Subdivision Surfaces 272
- Chapter 8 Level-Set Method for Surface Design and Its Applications 274**
 - 8.1 Introduction 274
 - 8.2 Preliminaries 276
 - 8.2.1 Cubic B-spline Interpolation 276
 - 8.2.2 Runge-Kutta Method with Variable Time Step-Size 283
 - 8.2.3 ENO Interpolation 284
 - 8.2.4 Upwind Scheme 285
 - 8.3 Local Level-Set Method 286
 - 8.3.1 Algorithm Outline 287
 - 8.3.2 Calculation of the Global Distance Function 288
 - 8.3.3 Thin Shell of a Level Set of a Cubic Spline Function 290
 - 8.3.4 Initialization 290
 - 8.3.5 Evolution 293
 - 8.3.6 Re-initialization 294
 - 8.4 Applications of the Level-Set Method in Geometric Design 295
 - 8.4.1 3D Surface Reconstruction from Scattered Data Set 296
 - 8.4.2 Biomolecular Surface Construction 299
 - 8.4.3 Surface Metamorphosis 303
 - 8.4.4 Surface Restoration 306
- Chapter 9 Quality Meshing with Geometric Flows 311**
 - 9.1 Introduction 311
 - 9.2 Single-domain Triangular and Tetrahedral Quality Meshing 313
 - 9.3 Single-domain Quadrilateral and Hexahedral Quality Meshing 316
 - 9.4 Multi-domain Tetrahedral Quality Meshing 319
 - 9.4.1 Quality Improvement Algorithm and Implementation 321
 - 9.4.2 Application Examples 328

- 9.5 Multi-domain Hexahedral Quality Meshing 331
 - 9.5.1 Quality Improvement Algorithm and Implementation 332
 - 9.5.2 Application Examples and Discussion 338
- 9.6 Multi-domain Triangular Quality Meshing with Gaps 341
 - 9.6.1 Problem Background 341
 - 9.6.2 Sketch of Multi-domain Meshing Algorithm 342
 - 9.6.3 Algorithm Details 343
 - 9.6.4 Results 347
- References** 349
- Index** 368

