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

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

Printed in Beijing

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

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

Chapter 1
Elementary Differential Geometry

In this chapter, we review the basic results of elementary differential geometry for surfaces in Euclidean space and collect some useful materials for the reference of subsequent chapters. Starting from the parametric representation of surfaces, we introduce the curvatures, differential operators, Green's formulas and some global properties of surfaces. Basic knowledge of implicit surfaces (level-set surfaces) is also provided. For a thorough expedition of elementary differential geometry, one is referred to, such as [111, 216, 344]. Some material in this chapter is extracted from [73, 427].

1.1 Parametric Representation of Surfaces

In this book, we denote by $\mathbb{R}$ the one-dimensional real field, $\mathbb{R}^n$ the n-dimensional real Euclidean space, where element $\mathbf{x} = [x_1, \cdots, x_n]^{\mathrm{T}}$ is expressed by a column vector. The set of $m \times n$ real matrices is denoted by $\mathbb{R}^{m\times n}$. We use square brackets $[\cdots]$ to represent a matrix or a vector, parenthesis $(\cdots)$ an ordered array, braces $\{\cdots\}$ a set. An m-dimensional vector is treated as a matrix in $\mathbb{R}^{m\times 1}$. The transpose of matrix $\boldsymbol{A}$ is expressed as $\boldsymbol{A}^{\mathrm{T}}$.

Our starting point is a two-dimensional surface embedded in $\mathbb{R}^3$. Suppose a right-handed Cartesian coordinate system $\{O; x, y, z\}$ has been introduced in $\mathbb{R}^3$.

Definition 1.1 If a one-to-one mapping from a domain $\Omega = \{[u, v]^{\mathrm{T}}\} \subset \mathbb{R}^2$ to $\mathbb{R}^3$

$$\mathbf{x}(u, v) = [x(u, v), y(u, v), z(u, v)]^{\mathrm{T}} \tag{1.1}$$

satisfies

(1) the function $\mathbf{x}(u, v)$ is sufficiently smooth in Ω,

(2) the vectors $\mathbf{x}_u = \dfrac{\partial \mathbf{x}}{\partial u}$ and $\mathbf{x}_v = \dfrac{\partial \mathbf{x}}{\partial v}$ are linearly independent,

then we say that the set $\mathbf{S} = \{\mathbf{x}(u, v) : [u, v]^{\mathrm{T}} \in \Omega\}$ is a *surface* in $\mathbb{R}^3$, and $\mathbf{x}(u, v)$ is the *parametric representation* of $\mathbf{S}$. The variables u and v are called the *parameters* of this representation.

In Definition 1.1, "sufficiently smooth" means that the function considered has the continuous derivatives of the required order. In this book, saying a function is "sufficiently smooth" or "properly smooth" means that it has the required smoothness. For simplifying the notations, we sometimes denote parameter (u,v) by $w=(u^1,u^2)$. Unless otherwise stated, we always assume that Ω is a closed region homeomorphism to a disc in $\mathbb{R}^2$. The second condition can also be expressed as the Jacobian matrix

$$\boldsymbol{J}=\begin{bmatrix} \dfrac{\partial x}{\partial u^1} & \dfrac{\partial x}{\partial u^2} \\ \dfrac{\partial y}{\partial u^1} & \dfrac{\partial y}{\partial u^2} \\ \dfrac{\partial z}{\partial u^1} & \dfrac{\partial z}{\partial u^2} \end{bmatrix}$$

is of rank 2 in Ω.

The second condition in Definition 1.1 enables us to solve locally for u,v from a suitable pair of the three functions $x(u,v), y(u,v)$ and $z(u,v)$. Then we can represent one of the quantities x,y,z as a function of the other two. For instance, if the determinant of the first two rows of $\boldsymbol{J}$ is different from zero in a certain subdomain Ω' of Ω, then u and v can be represented as functions of x and y. By plugging u and v into the parametric representation (1.1), we obtain a *graph representation* $z=F(x,y)$ of the surface $\mathbf{S}$.

Assume that a surface $\mathbf{S}$ has a parametric representation (1.1) and $\mathbf{x}$ is a point on $\mathbf{S}$. The tangent plane $T_{\mathbf{x}}\mathbf{S}$ to the surface $\mathbf{S}$ at the point $\mathbf{x}$ is defined by

$$T_{\mathbf{x}}\mathbf{S}=\operatorname{span}\{\mathbf{x}_u,\mathbf{x}_v\},$$

where $\operatorname{span}\{\mathbf{x}_u,\mathbf{x}_v\}$ is a space spanned by $\mathbf{x}_u$ and $\mathbf{x}_v$. Vectors $\mathbf{x}_u$ and $\mathbf{x}_v$ are called *coordinate tangent vectors*.

The parametric representation (1.1) is not unique. If $\mathbf{x}(\bar{u},\bar{v})$ is another parametric representation of the surface $\mathbf{S}$ in domain $\bar{\Omega}=\{[\bar{u},\bar{v}]^{\mathrm{T}}\}$, then the transformation

$$u^\alpha=u^\alpha(\bar{u}^1,\bar{u}^2),\quad \alpha=1,2, \tag{1.2}$$

is said to be an *allowable coordinate transformation* if the following two conditions hold.

(1) The functions in (1.2) are sufficiently smooth in $\bar{\Omega}$ and the transformation is one-to-one.
(2) The Jacobian matrix

$$\boldsymbol{J}=\begin{bmatrix} \dfrac{\partial u^1}{\partial \bar{u}^1} & \dfrac{\partial u^1}{\partial \bar{u}^2} \\ \dfrac{\partial u^2}{\partial \bar{u}^1} & \dfrac{\partial u^2}{\partial \bar{u}^2} \end{bmatrix}$$

of the transformation is nonsingular everywhere in $\bar{\Omega}$.

The determinant of the Jacobian matrix of the transformation (1.2) is always abbreviated as the Jacobian of the transformation.

Definition 1.2 If a quantity of a surface is independent of the specific parametric representation of the surface, then this quantity is called *geometric*.

For a surface, we are sometimes interested in the invariant properties when we impose a *congruent transformation* on it. A congruent transformation $\mathbf{T}$ in $\mathbb{R}^3$ keeps the surface invariant except for its position and can be expressed by a linear transformation, i.e., $\mathbf{Tx} = \boldsymbol{T}\mathbf{x} + \mathbf{y}$, where $\boldsymbol{T}$ is an orthogonal matrix and $\mathbf{y}$ is a vector. If $\det(\boldsymbol{T}) = 1$, the congruent transformation is called *direct congruent transformation*, which is composed of the rotation and translation. The direct congruent transformation is also called *rigid motion*. Correspondingly, if $\det(\boldsymbol{T}) = -1$, the congruent transformation is called *opposite congruent transformation*, which is composed of the rotation, translation and an odd number of reflections.

The first fundamental form. The differential 2-form

$$\mathrm{I} = \langle \mathrm{d}\mathbf{x}, \mathrm{d}\mathbf{x} \rangle = g_{11}\mathrm{d}u\mathrm{d}u + 2g_{12}\mathrm{d}u\mathrm{d}v + g_{22}\mathrm{d}v\mathrm{d}v = g_{\alpha\beta}\mathrm{d}u^\alpha \mathrm{d}u^\beta$$

is the *first fundamental form of a surface*, where $\mathrm{d}\mathbf{x} = \mathbf{x}_{u^\alpha}\mathrm{d}u^\alpha$ and $g_{\alpha\beta} = \langle \mathbf{x}_{u^\alpha}, \mathbf{x}_{u^\beta} \rangle$ are *the coefficients of the first fundamental form*. The symbol $\langle \cdot, \cdot \rangle$ stands for the Euclidean inner product of two vectors in $\mathbb{R}^3$. We have used the Einstein summation convention in the last equality of the first fundamental form. According to this convention, when an index appears twice in a single term, once in an upper (superscript) position and once in a lower (subscript) position, it implies that we take the summation over all its possible values. This can greatly simplify the usage of notations.

Property 1.1 The first fundamental form of a surface is geometric.

The first fundamental form enables us to measure the length of a curve on a surface and the area of a surface. Let $\mathbf{C}: \mathbf{x}(t) = \mathbf{x}(u^1(t), u^2(t))$ be a curve on a surface $\mathbf{S}: \mathbf{x}(u^1, u^2)$. Then the length of an arc of $\mathbf{C}$ bounded by the points corresponding to the values $t = t_0$ and $t = t_1$ is given by the integral

$$s = \int_{t_0}^{t_1} \sqrt{\langle \mathbf{x}', \mathbf{x}' \rangle}\mathrm{d}t = \int_{t_0}^{t_1} \sqrt{\langle \mathbf{x}_{u^\alpha} u^{\alpha\prime}, \mathbf{x}_{u^\beta} u^{\beta\prime} \rangle}\mathrm{d}t = \int_{t_0}^{t_1} \sqrt{g_{\alpha\beta} u^{\alpha\prime} u^{\beta\prime}}\mathrm{d}t,$$

where primes denote derivatives with respect to t.

The area of the surface $\mathbf{S}$ is defined by $A(\mathbf{S}) = \int_{\mathbf{S}} \mathrm{d}A$ with $\mathrm{d}A$ the area element of the surface $\mathbf{S}$. If the surface $\mathbf{S}$ has a parametric representation (1.1), then $A(\mathbf{S})$ can be expressed by

$$A(\mathbf{S}) = \int_{\mathbf{S}} \mathrm{d}A = \iint_{\Omega} |\mathbf{x}_u \times \mathbf{x}_v| \mathrm{d}u\mathrm{d}v = \iint_{\Omega} \sqrt{g}\mathrm{d}u\mathrm{d}v,$$

where $g = \det[g_{\alpha\beta}] = g_{11}g_{22} - g_{12}^2$ and we have used Lagrange's identity

$$|\mathbf{x}_u \times \mathbf{x}_v|^2 = |\mathbf{x}_u|^2 |\mathbf{x}_v|^2 - \langle \mathbf{x}_u, \mathbf{x}_v \rangle^2$$