Geometric Partial Differential Equations Methods in Geometric Design and Modeling

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Outline

1. Introduction
2. The Construction of GPDE
3. Numerical Solutions of GPDEs
   - Generalized Finite Difference Methods
   - Mixed Finite Element Methods
   - Level-Set Methods
4. Conclusion
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1. Introduction

What is a GPDE?

A PDE which controls the motion of curves or surfaces and is merely formulated by the geometric entries is known as Geometric PDE.
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A PDE which controls the motion of curves or surfaces and is merely formulated by the geometric entries is known as Geometric PDE.
Mean Curvature Flow (MCF) (1956, Mullins)

\[
\frac{\partial \mathbf{x}}{\partial t} = 2H
\]

Willmore Flow (WF) (1923, Thomsen)

\[
\frac{\partial \mathbf{x}}{\partial t} = -[\Delta_s H + 2H(H^2 - K)]n
\]

Minimal Mean-Curvature-Variation Flow (MMCVF) (2006, Xu & Zhang)

\[
\frac{\partial \mathbf{x}}{\partial t} = (\Delta_s^2 H + 2(2H^2 - K)\Delta_s H + 2\langle \nabla_s H, H \rangle - 2H\|\nabla_s H\|^2) n
\]
Several Differential Geometric Operators of First Order

Assume

\[ S = \{ \mathbf{x}(u, v) \in \mathbb{R}^3 : (u, v) \in \Omega \subset \mathbb{R}^2 \}, \]

\[ f : S \rightarrow \mathbb{R} \]

- Tangential Gradient Operator of Surface \( S \)

\[ \nabla_s f = [\mathbf{x}_u, \mathbf{x}_v][g^\alpha\beta][f_u, f_v]^T \in \mathbb{R}^3, \]

- The Second Tangential Operator

\[ \diamond f = [\mathbf{x}_u, \mathbf{x}_v][K b^\alpha\beta][f_u, f_v]^T \in \mathbb{R}^3. \]

- Tangential Divergence Operator

\[ \text{div}(\mathbf{v}) = \frac{1}{\sqrt{g}} \left[ \frac{\partial}{\partial u}, \frac{\partial}{\partial v} \right] \left[ \sqrt{g} [g^{\alpha\beta}] [\mathbf{x}_u, \mathbf{x}_v]^T \mathbf{v} \right]. \]
Several Differential Geometric Operators of Second Order

- **Laplace-Beltrami Operator**

  \[ \Delta_s f = \text{div}(\nabla_s f). \]

- **Giaquinta-Hildebrandt Operator**

  \[ \Box f = \text{div}(\diamond f). \]
Why GPDE is important?

**Theory aspect:** Relate intimately to
- geometric analysis
- manifold theory
- topology
- complex analysis
- PDE
- calculus of variation
- geometric measure theory
- critical point theory

**Application aspect:** Relate intimately to
- physics,
- chemistry,
- biology,
- computational geometry,
- computer graphics,
- image processing
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What can GPDE do in geometric design and modeling?

- Surface Processing
- Surface Reconstruction
- Surface Restoration
- Surface Blending
- Free-Form Design
- Biomolecular Design
- Image Processing
- Interface Simulation
- ...........
What’s about the result of GPDE?

- Some optimal property, e.g.,
  - minimize area \( \int_S dA = \min \)
  - minimize the sum of square of principal curvatures \( \int_S (\kappa_1^2 + \kappa_2^2) dA = \min \)
  - minimize the variation of mean curvature \( \int_S \| \nabla_s H \|^2 dA = \min \)
  - etc. \( \int_S f(H, K) dA = \min \)

- The surfaces designed by GPDEs
  - Clear geometric sense
  - Boundary condition with prescribed smoothness
  - Fairness
  - Aesthetic demanding
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Surface Processing

input Mean curvature flow

(From Bajaj, Xu 2004)
Surface Reconstruction

scattered data

reconstructed surface
(Level set method)

(From Bajaj, Xu, Zhang 2006)
Surface Blending

Initial input

MCF (2nd order)

WF (4th order)

MMCVF (6th order)
Free-Form Surface Design I

input

initial surface

surface diffusion flow
Free-Form Surface Design II

input skeleton

PDE surface of 4th order
Surface Restoration I

input head without jaws

MCF (2nd order)

WF (4th order)

MMCVF (6th order)
Surface Restoration II

MCF  
SDF  
6th order flow
Biomolecular Design

van der Waals surface

SES

(from Bajaj, Xu, Zhang 2006)
Image Processing

- initial input
- denoising process with MCF
Comparison Results Among 2,4,6-th Order Flows

- MCF — $G^0$
- WF — $G^1$
- MMCVF — $G^2$

- 2nd order flows usually used
- 4th order flows often used
- 6th order flows occasionally used
The domains of classical PDEs are usually fixed, but GPDE’s are always changeable.

GPDE is geometrically intrinsic, independent of the parameter representation of surface.

GPDE is highly nonlinear, which makes theoretical analysis challenging.

Classical methods can not be used directly and classical theories are not effective.
2. The Construction of GPDE

How to construct GPDE?

- **Manual approach**

\[ \partial, \nabla_s, \text{div}_s, \Delta_s, \Box, \Diamond, \ldots, \]

\[ \Downarrow \]

\[ E(x) = 0, \quad x \in S \]

For example, \( \Delta^2_s x = 0, \quad \Delta^2_s H = 0, \ldots \)

\[ \Downarrow \]

\[ \begin{cases} \frac{\partial x}{\partial t} = \pm E(x)n, & x \in S(t), \\ S(0) = S_0. \end{cases} \]

- **Energy based variational approach**
2. The Construction of GPDE

How to construct GPDE?

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\end{array} \right. \]

- Energy based variational approach
Energy Based Variational Approach to Construct GPDE

Energy $\mathcal{E}(S)$ → Variational Calculus $\mathcal{E}'(S)$ → Construct Flow $\frac{\partial \mathbf{x}}{\partial t} = -\mathcal{E}'$

Energy $\int_S dA$ → $-2H\mathbf{n}$ → $\frac{\partial \mathbf{x}}{\partial t} = 2H\mathbf{n}$
Define inner product space:

\[ S = \{ \mathbf{x}(u, v) \in \mathbb{R}^3 : (u, v) \in \Omega \} \text{ is smooth.} \]

\[ \mathbf{f}, \mathbf{g} \in C^2(S, \mathbb{R}^3) \]

define inner product

\[ (\mathbf{f}, \mathbf{g}) = \int_S \langle \mathbf{f}, \mathbf{g} \rangle dA \]
Three Steps to Construct GPDE

1. Define energy functional

\[ E(S) = \int_S dA \]

2. Compute first order variation

\[ \delta(E(S), \Theta) = \int_S \langle E'(S), \Theta \rangle dA, \]

here, \( E'(S) \) is named as the \( L^2 \) gradient of \( E(S) \).

3. Construct GPDE of weak form and general form.

\[ \int_S \langle \frac{\partial \mathbf{x}}{\partial t}, \Theta \rangle dA = - \int_S \langle E'_c(S), \Theta \rangle dA, \quad \forall \Theta \in C_0^\infty(S, \mathbb{R}^3). \]

This is the starting point of finite element method. Then GPDE is

\[ \frac{\partial \mathbf{x}}{\partial t} = -E'_c(S) \in \mathbb{R}^3. \]
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\[ \frac{\partial \mathbf{x}}{\partial t} = -E'_c(S) \in \mathbb{R}^3. \]
A General Approach

First-order energy (second-order equation):

$$E_1(S) = \int_S h(x, n) dA$$

Second-order energy (fourth-order equation):

$$E_2(S) = \int_S f(H, K) dA$$

Third-order energy (sixth-order equation):

$$E_3(S) = \int_S \| \nabla_s g(H, K) \|^2 dA$$

and their combinations:

$$E(S) = \alpha E_1(S) + \beta E_2(S) + \gamma E_3(S)$$
For first-order energy

\[ E_1(S) = \int_S h(x, n)dA, \]

we obtain second-order equation

\[
\begin{align*}
\frac{\partial x}{\partial t} &= -\nabla_x h - \text{div}_s(\nabla_n h)n - \nabla_s n \nabla_n h + \text{div}_s(h\nabla_s x), \\
S(0) &= S_0.
\end{align*}
\]
For the second-order energy

$$\mathcal{E}_2(S) = \int_S f(H, K) dA,$$

we obtain fourth-order equation

$$\begin{cases} \frac{\partial x}{\partial t} = -\Box(f_K \mathbf{n}) - \frac{1}{2} \Delta_s(f_H \mathbf{n}) + \text{div}_s(f_H \nabla_s \mathbf{n}) + \text{div}_s((f - 2Kf_K) \nabla_s x), \\ S(0) = S_0, \end{cases}$$
For the third-order energy

$$\mathcal{E}_3(S) = \int_S |\nabla_S g(H, K)|^2 dA,$$

we obtain sixth-order equation

$$\frac{\partial \mathbf{x}}{\partial t} = \left[ \Delta_S (g_H \Delta_S g \mathbf{n}) + 2\Box (g_K \Delta_S g \mathbf{n}) - 2 \text{div}_S [g_H \Delta_S g \nabla_S \mathbf{n}] 
- 2Kg_K \Delta_S g \nabla_S \mathbf{x} \right] + 2 \text{div}_S [\mathbf{R} \nabla_S g(\mathbf{R} \nabla_S g)^T] - \text{div}_S [||\nabla_S g||^2 \nabla_S \mathbf{x}],$$

where

$$\mathbf{R} = \frac{1}{\sqrt{g}} \left[ -\mathbf{x}_v, \mathbf{x}_u \right] \left[ \mathbf{x}_u, \mathbf{x}_v \right]^T.$$
Special Examples

1. Mean Curvature Flow [Mullins, 1956], (Minimal surface, Euler, 1744).
   
   \[ f(H, K) = 1 \]
   \[ \mathcal{E}_n^l(S) = -2H \]

2. Surface Diffusion Flow [Mullins, 1957].
   
   \[ f(H, K) = 1 \]
   \[ \mathcal{E}_n^l(S) = 2\Delta_s H \]
   — in the sense \((\cdot, \cdot)_{H^{-1}}\).

3. Sixth-order Flow [Xu, Pan and Bajaj, 2006].
   
   \[ f(H, K) = 1 \]
   \[ \mathcal{E}_n^l(S) = -2\Delta_s^2 H \]
   — in the sense \((\cdot, \cdot)_{H^{-2}}\).
\[ h(x, n) = \gamma(n) \]
\[ \mathcal{E}_n'(S) = \nabla_s n : (\nabla^2_{nn} \gamma) \]

5. Gaussian Curvature Flow [Firey, 1974].
\[ f(H, K) = H \]
\[ \mathcal{E}_n'(S) = K \]

\[ f(H, K) = H^2 \]
\[ \mathcal{E}_n'(S) = \Delta_s H + 2H(H^2 - K) \]

Willmore functional is initially introduced by Thomsen in 1923.

.......
Explicit solutions of the GPDEs are hard to obtain. Numerical solutions are necessary and feasible.

- Generalized Finite Difference Methods
- Finite Element Methods
- Level-Set Methods
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Generalized Finite Difference Methods

Two Scenarios:

- Normal motion equation
  \[ \mathbf{n}^T \frac{\partial \mathbf{x}}{\partial t} = 2H, \]

- All directions motion equation
  \[ \frac{\partial \mathbf{x}}{\partial t} = \Delta_s \mathbf{x}, \]

Two Pivot Problems:

- Discretization of differential geometry operators
- Boundary treatment
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Mixed Finite Element Methods

Two Scenarios:
- Total variation form
- Normal variation form

Two Pivot Problems:
- Construction of the function spaces of finite element
- Boundary treatment
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Level-Set Methods

Key Techniques:

- Narrow band technique
- Runga-Kutta method with adaptive step size
- Fast computation of higher-order level-set function
- Fast reinitialization
Finite Difference Methods
- Easy to implement
- Low cost
- Depends on the discretization of differential geometric operators

Finite Element Methods
- More stable
- Solid mathematical foundation
- Depends on the construction of the space of finite element
4. Conclusion

- Interdisciplinary, GPDEs Methods relate to
  - differential geometry, manifold, equations
  - variational calculus
  - function approximation
  - computational mathematics
  - computer graphics

- Challenging, GPDEs deep into
  - geometry analysis, manifold theory
  - topology
  - geometric measure theory
  - critical theory

- Practical, GPDEs closely relate to
  - Physics and chemistry settings, the motion of interfaces problems, e.g., dissolution, combustion, erosion
  - Biology field, biomembrane vesicle problem, the construction of protein surface
  - Image processing, edge detection, noise removal, image restoration
  - ......
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Thank you!

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