Topology, Material, and Mechanisms Optimization: Level Set Methods

Michael Y. Wang
Dept. of Automation & Computer-Aided Engineering
The Chinese University of Hong Kong
Shatin, N.T., Hong Kong

05 January 2004
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2. Level-Set Concept
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6. Examples:
   1. Topology Optimization with Multi-Materials
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   3. Compliant Mechanism Design
7. Conclusions
### Motivation

- **Traditional Design**

- **Shape Optimization**
  - Homogenous Materials
  - Fixed Geometric Form
  - Limited Performance

### Topology Optimization

- **Shape & Topology**
- **Heterogeneous Materials**
- **Multi-Physics Domain**
- **High Performance**
• Structural optimization – Michell structures (1904)
• FEM & shape optimization – Shape sensitivity and variations (Haug, Choi, Sokolowski, 70’s and 80’s)
  • Boundary Variation
  • Costly re-meshing
• Topology optimization – Trusses (Prager ’80)
• Homogenization-based methods (Bendsoe ’88)
• Simple Isotropic Material Penalty (SIMP) approach (Sigmund ’90)
• Various evolutionary approach: GA, EA (Xie ‘95)
Homogenization Based Optimization

Design domain

Figure 4.5: The Post-processor form with menu controls and results display
Min\(\rho \ f(\rho)\) of a ‘ground’ structure

s. t \(\sum_{i=1}^{N} \rho_i v_i \leq V^*\)

\(0 < \rho_i \leq 1\)

Problem Relaxation:

- Homogenization-based method (Bendsoe 1988)
- Simple Isotropic Material with Penalty (SIMP)
  \(E = E_0 \times (\rho_i)^n\) (\(n = 2, 3, 4\))

Difficulties:

- Very large number of design variables N
- Various numerical instability & inaccuracy
- Lack of concise geometric boundary description
The Process

- Material starts accumulating first at the supports and loading points.
- Then it gradually spreads to other parts.
SIMP Optimization

Figure 5.3a: Mean compliance case 1

Figure 5.3b: Objective function Versus Time

Figure 5.3c: Optimum structure
• Checker board is attributed to inaccuracy in FE modeling and homogenization relaxation.

• Checker board gives artificially high stiffness.
• Mesh changes the connectivity of the elements.
• Finer meshes tend to create more holes or internal boundaries.
“Gray-Scale” Structure Problem

Figure 6.8a: $\varepsilon = 0.01$; optimized structure

Figure 6.8b: $\varepsilon = 0.07$; optimized and gray scale structures

Figure 6.8c: $\varepsilon = 0.1$; optimized and gray scale structures
Class of Problems

Based on (Haber and Bendsoe 1998) & (Bendsoe 1999)

<table>
<thead>
<tr>
<th>Class 1: Basic Problems</th>
<th>Class 2: Relaxed Problems</th>
<th>Class 3: Restricted Problems</th>
<th>Class 4: Evolutionary Problems</th>
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<tbody>
<tr>
<td>Discrete</td>
<td>Continuous</td>
<td>Continuous</td>
<td>Discrete</td>
</tr>
<tr>
<td>$\Omega \rightarrow {0,1}$</td>
<td>$\Omega \rightarrow [0,1]$</td>
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<td>$\Omega \rightarrow {0,1}$</td>
</tr>
<tr>
<td>Ill-posed</td>
<td>“Regularized” Perforated Designs</td>
<td>Constraints on Admissible Space</td>
<td>Evolutionary Processes</td>
</tr>
<tr>
<td></td>
<td>Homogenization SIMP</td>
<td>Perimeter, Slope, Filtering</td>
<td>“Greedy” method: Hard-Kill, Bi-directional</td>
</tr>
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### Ideal Characteristics

<table>
<thead>
<tr>
<th></th>
<th>Homogenization Based</th>
<th>Evolution Based</th>
<th>Level-Set Based</th>
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<tbody>
<tr>
<td><strong>Topological Flexibility and Robustness</strong>: to represent complex topologies and to evolve gracefully</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td><strong>True Geometric Representation</strong>: boundary representation, geometric attributes (e.g., curvature, derivatives), few design DOF</td>
<td>×</td>
<td>×</td>
<td>✓</td>
</tr>
<tr>
<td><strong>Continuous Parameterization</strong>: to avoid integer programming</td>
<td>✓</td>
<td>×</td>
<td>✓</td>
</tr>
<tr>
<td><strong>Efficient Computation</strong>: with high accuracy and efficiency</td>
<td>×</td>
<td>×</td>
<td>✓</td>
</tr>
<tr>
<td><strong>Separation from Analysis Representation</strong>: independent of FE mesh or coordinate system, independent accuracy control</td>
<td>×</td>
<td>×</td>
<td>✓</td>
</tr>
<tr>
<td><strong>Adaptability</strong>: automatic refinements, adaptive algorithms</td>
<td>×</td>
<td>×</td>
<td>✓</td>
</tr>
<tr>
<td><strong>Shape and Design Sensitivity</strong>: to link design derivative with shape derivatives</td>
<td>×</td>
<td>×</td>
<td>✓</td>
</tr>
</tbody>
</table>
"Color" & "Texture" in Structures

- Key Characteristics:
  - Function and Form Integration
    - e.g., micro-hinges
  - Multi-, Graded-, Textured-Materials & Composition
  - Multi-Physics Domains

Key Attributes:
- Material at right place
- Right material at right place
- Right property for the right material at the right place
1. **Computer Representation:**
   - Heterogeneous Materials in CAD (HKU, UM)
   - “Color” and “Rainbow” CAD

2. **Design Methods:**
   - Homogenization Methods in Mechanics
   - Optimization Methods for Design

3. **Fabrication Technology:**
   - Color SLA (HKU)
   - Shape Deposition Manufacturing (Stanford)
   - Multi-material Diffusion (SMU)
New Models

Combining the Best of the Current Approaches:

- Fixed mesh of homogenization
  - No re-meshing
  - Use adaptive meshing
- General method of shape derivative
  - Any type of problem

Level Set Models
- Kumar 1996
- Sethian & Wiegmann 2000
- Osher & Santosa 2001
- Santosa 2000
- Allaire et al. 2003
- Wang et al. 2003

Phase-Field Models
- Bourdin & Chambolle 2003
- Wang & Zhou 2003

Distance Fields
- CAD community
Concept of Level Sets

\[ Z = \phi(x, y, t_0) \]

\[ Z = \phi(x, y, t_1) \]

\[ Z = \phi(x, y, t_2) \]
**Level Set Model**

- Embedding $x$ into a Scalar Function $\phi$ of a Higher Dimension
- Boundary $\Gamma$ is an “Iso-Surface” (a Level-Set)

$$\Gamma = \{ x : \Phi(x) = 0 \}$$

- $\Phi$ has Fixed Topology
- $\Gamma$ has Variable Topology

**Regional Representation (R-rep):**
- Semi-Explicit
- Global
- Inside & Outside Regions:

$$\begin{align*}
\Phi(x) &> 0 \quad \forall x \in \Omega \setminus \partial \Omega \\
\Phi(x) &= 0 \quad \forall x \in \partial \Omega \\
\Phi(x) &< 0 \quad \forall x \in \Omega \setminus \Omega
\end{align*}$$
Level-Set Propagation

“Iso-Surface”:

\[ \Gamma(t) = \{ x(t) : \Phi(x(t), t) = 0 \} \]

Level-Set Equation:

\[ \frac{\partial \Phi(x)}{\partial t} = -\nabla \Phi(x) \frac{dx}{dt} \equiv -\nabla \Phi(x) \cdot V(x) \]

Hamilton-Jacobi Eq. for Front Propagation:

\[ \frac{\partial \Phi}{\partial t} = V_n |\nabla \Phi| \]

“Normal Velocity”:

- Effective for changes in normal direction only
- Tangential changes are for re-parameterization only

\[ V_n(x) \]
Geometric Evolution

- Boundary Capturing vs. Boundary Tracking:
  - Implicit Method (Euler Method) vs. Explicit Method (Lagrange Method)

- Topologically Flexible:
  - Variable Topology in $\Gamma$
  - Fixed Topology in $\Phi$

- Geometrically Concise:
  - True Geometric Model
  - Normal, Tangent, Curvatures

- Evolution Process for Optimization:
  - $V_n(x)$ is the link
Optimization: \[
\text{Minimize } J(u, \Phi) = \int_{\Omega} F(u) H(\Phi) d\Omega \\
\text{subject to: } \\
a(u, v, \Phi) = L(v, \Phi) \text{ for all } v \in U \\
u = u_0 \text{ on } \Gamma_u \\
V(\Phi) = \int_{\Omega} H(\Phi) d\Omega \leq V_{\text{max}}
\]
\[
a(u, v, \Phi) = \int_{\Omega} E_{ijkl} \varepsilon_{ij}(u) \varepsilon_{kl}(v) H(\Phi) d\Omega \\
L(v, \Phi) = \int_{\Omega} p v H(\Phi) d\Omega + \int_{\Omega} \tau v \delta(\Phi) \left| \nabla \Phi \right| d\Omega
\]

Lagrange Equation: \[
\text{Minimize } \bar{J}(u, \Phi) = J(u, \Phi) + \lambda_+ \cdot (V(\Phi) - V_{\text{max}}) \\
\text{subject to: } \\
a(u, v, \Phi) = L(v, \Phi), u|_{\partial \Delta_u} = u_0 \text{ for all } v \in U \\
\lambda_+ \cdot (V(\Phi) - V_{\text{max}}) = 0 \\
\lambda_+ \geq 0
\]
\[
H(\Phi) = \begin{cases} 
1 & \text{if } \Phi \geq 0 \\
0 & \text{if } \Phi < 0 
\end{cases} \\
\delta(\Phi) = \frac{dH}{d\Phi}
\]
Existence Theory
1. Generally, the minimization problem has no solution.
2. Solution exists with additional conditions:
   - Perimeter constraint
   - Topology constraint

Two Main Elements:
1. Euler derivative of the objective functional with respect to shape changes – Shape Derivatives
2. Transport equations (PDE) for shape evolution and minimization
Shape Sensitivity

Shape Transformation – Perturbation in Diffeomorphism: \( \Omega_t = (I + \psi)\Omega \)

\[ T : x \rightarrow x_t(x), \ x \in \Omega, \quad x_t = T(x, t) \quad \Omega_t = T(\Omega, t) \]

Transformation Velocity:

\[ \frac{dx_t}{dt} = V(x_t, t) \]

Transformation Identity:

\[ x_t = T(x, t) = x + tV(x) \]

\[ V(x) = V(x, 0) \]

Well-Established Methods:

- Murat & Simon 70’s, Haug & Choi 80’s, Sokolowski & Zolesio 90’s
Frechet Derivatives

Material Derivative
- For a given velocity vector in the shape transformation, the material derivative is defined by
  \[ \dot{u}(x; V) = \lim_{t \to 0} \frac{1}{t} [u(x + tV) - u(x)] \]

Shape derivative is the Frechet derivative on the boundary \( \partial \Omega \), depending only on \( V_n \)
\[ J'(\Omega)(V \cdot n) \]

Lemmas (Haug 1986):

Lemma 1: For a regular function \( \psi_1 = \int_\Omega f(x) d\Omega \)
the material derivative is given by
\[ \psi_1' = \int_\Omega f'(x) d\Omega + \int_{\Gamma} f(x)(V \cdot n) d\Gamma \]

Lemma 2: For
\[ \psi_2 = \int_\Gamma g(x) d\Gamma \]
the material derivative is given by
\[ \psi_2' = \int_\Gamma g'(x) d\Gamma + \int_{\Gamma} (\nabla g \cdot n + kg(x))(V \cdot n) d\Gamma \]

Lemma 3: For
\[ \psi_3 = \int_\Gamma g(x) \cdot n d\Gamma \]
the material derivative is given by
\[ \psi_3' = \int_{\Gamma} \left( (g'(x) \cdot n + \text{div } g(x))(V \cdot n) \right) d\Gamma \]
Shape Derivative

Shape Derivative in $V_n$

$$\frac{d\bar{J}(u, \Phi)}{d\Phi} = \int_{\Omega} \delta(\Phi) (\beta(u, w, \Phi) + \lambda_+) V_n d\Omega$$

$$\beta(u, w, \Phi) = F(u) + pw - \tau w \kappa - E_{ijkl} \varepsilon_{ij}(u) \varepsilon_{kl}(w)$$

The Kuhn-Tucker Condition of Optimal Solution:

$$\beta(u, w, \Phi) + \lambda_+ \bigg|_{\partial\Omega} = 0$$

$$\lambda_+ \cdot (V(\Phi) - V_{\text{max}}) = 0$$

$$\lambda_+ \geq 0$$
Gradient Descent/Projected Gradient Method

Construction of the Velocity Field:

\[ V_n(x) = -[\beta(u, w, \Phi) + \lambda_+] \]

\[ \lambda_+ = -\int_{\partial \Omega} \beta(u, w, \Phi) d\Gamma / \int_{\partial \Omega} d\Gamma \]

Gradient-Descent Optimization Process:

\[ \frac{d\bar{J}(u, \Phi)}{d\Phi} = -\int_{\Omega} \delta(\Phi)V_n^2 d\Omega \leq 0 \]

Level-Set Evolution:

\[ \frac{\partial \Phi}{\partial t} = V_n|\nabla \Phi| \quad \text{and} \quad \left. \frac{\partial \Phi}{\partial N} \right|_{\partial \Omega} = 0 \]

Perimeter Regularization

- **Perimeter measure:**  \( E(\Omega) \equiv |\partial \Omega| = \int_{\Gamma} d\Gamma \)

- **Euler derivative:**
  \[
  E'(\Omega) \equiv \frac{dE(\Omega)}{dt} = \int_{\Gamma} \kappa(V \cdot n) d\Gamma = \int_{\Omega} \delta(\Phi) \kappa(\Phi) V_n |\nabla \Phi| d\Omega
  \]

- **Curvature flow:**
  \[
  V_n = V \cdot n = -\kappa
  \]

- **Geometric heat equation:**
  \[
  E'(\Omega) = -\int_{\Omega} \delta(\Phi) \kappa^2 |\nabla \Phi| d\Omega \leq 0
  \]

- **Weighted Total-Variation Scheme:**
  \[
  E_{TV}(\Phi) = \int_{D} I(x) |\nabla \Phi| d\Omega
  \]
  \[
  I(x) = \frac{c_1}{1 + c_2 V_N^2(x)}
  \]
Computations

- PDEs on Rectilinear Grid:
  - Finite Difference Methods
  - Interface Embedded

- Finite Element Method for Mechanics:
  - Independent FD Grid and FE Mesh

- Boundary Recovery:
  - Marching-Cube Methods in Computer Graphics
Numerical Schemes

Robust Schemes:

- Up-wind Scheme of Entropy Solution (Osher & Sethian ’88)

\[
\phi_{ijk}^{n+1} = \phi_{ijk}^n - \Delta t [\max(V_{N_{ij}},0) \nabla^+ + \min(V_{N_{ij}},0) \nabla^- ]
\]

\[
\nabla^+ = \left[ \max(D_{yjk}^{+x},0)^2 + \min(D_{yjk}^{-x},0)^2 \right]^{1/2},
\]

\[
\nabla^- = \left[ \max(D_{yjk}^{+x},0)^2 + \min(D_{yjk}^{-x},0)^2 \right]^{1/2},
\]

- ENO & TVD-RK High Order Schemes (Shu & Osher ’88)
Level-Set Numerics

- Narrow-Band Schemes (Sethian ’99)
- Velocity Extensions
- Re-Initialization
  - Signed Distance Function Schemes (Peng ’99)
- Linear Complexity of Boundary Only:

\[ O(N(\Gamma)) \]

- Well-Documented:
  - Osher & Fedkiw 2003
Enhancements

Conjugate Velocity Mapping:
- Wang et al. '03

\[ \frac{\partial \Phi}{\partial t} = f(V_n) |\nabla \Phi| \]
\[ \frac{\partial \Phi}{\partial N} = 0 \]
\[ f(V_n) = F(V_n) - \mu \text{ for } V_n \in T \]
\[ F(r) = r \left[ \frac{1-\alpha}{2} + \frac{1+\alpha}{2} |r| \right] \]
\[ \mu = \frac{\int_{\Omega} F(V_n) d\Gamma}{\int_{\Omega} d\Gamma} \]

Adaptive Oct-tree Schemes with Semi-Lagrange Method:
- Strain '01

\[ F(x) \]
\[ x \]
**Algorithm**

1. **Step 1**: Initialize the level set function for an initial design in terms of its boundary.
2. **Step 2**: Compute the displacement field and the adjoint displacement field through the linear elastic system.
3. **Step 3**: Calculate the “speed function” on the surface along the normal direction.
4. **Step 4**: Solve the level set equation to update the embedding function.
5. **Step 5**: Check if a termination condition is satisfied. Repeat Steps 2 through 5 until convergence.

\[ J(u) = \int_D E_{ijkl} \varepsilon_{ij}(u) \varepsilon_{kl}(u) d\Omega \]
Two-Bar Example

(1) Initially 90%

(2) Initially 55%
Two-Bar (Video)
Multiple Loading

Fig. 17.3 (a) The Third Michell Type Structure
Multi-Load (Video)
MBB Beam (Video)
Michell Truss

Michell Solution (1904)

Design domain

Non Design domain

(a)  
(b)  
(c)  
(d)  
(e)  
(f)  
(g)  
(h)  

Computational Modeling & Design Laboratory
Department of Automation & Computer Aided Eng.
**Micro-Models**

1. **Single Material:**

\[ E = xE_1 \]

2. **Two Material Mixture:**

\[ E = x_1(E_1 + x_2(E_2 - E_1)) \]

3. **Material Reinforcement:**

\[ E = x_1(E_1 + x_2E_2) \]
Multiphase Materials

- Partitioning level-set model:
  - Phase 1 by Level-set 1
  - Phase 2 by Level-set 2

- Domain partition by m
  Level-sets for m phases
  \( \phi_i \ (i = 1, \ldots, m) \)

- Overlap problem:
  - T-Junction

- Enforcing constraint:
  \[
  \sum_{i=1}^n H(\phi_i(x)) = 1
  \]

\[
\Omega = \bigcup_{i=1}^n \Omega_i
\]

\[
\Omega_i \cap \Omega_j = \emptyset \quad i \neq j
\]
“Color” Level-sets Model

\( m \) level-set functions
(Chan & Vase ’02)

\[
\Phi = [\phi_1, \phi_2, \ldots, \phi_m]
\]

\[
H(\Phi) = [H(\phi_1), H(\phi_2), \ldots, H(\phi_m)]
\]

\( n \) material Phases:

\[
\omega_k = \{x : H(\Phi(x)) = \text{constant vector}, x \in D\}
\]

\[
n = 2^m
\]

\[
D = \bigcup_{k=1}^{n} \omega_k \quad \omega_k \cap \omega_l = \emptyset \quad k \neq l
\]

(Chan & Vase ’02) for Image Segmentation
Optimization with "Color" Level-Set Model

Phase Characteristic Function:

\[ \chi_k(x) = \begin{cases} 1 & \text{if } x \in \omega_k \\ 0 & \text{otherwise} \end{cases} \]

\[ \chi_k(\Phi) = \prod_{i=1}^{m} H_i^k \]

Optimization with Color Level-sets:

Minimize \( J(u, \Phi) = \sum_{k=1}^{n} \int_{D} F^k(u) \chi_k(\Phi) d\Omega \)

subject to: \( G_j(u, \Phi) = \sum_{k=1}^{n} \int_{D} g_j^k(u) \chi_k(\Phi) d\Omega \leq 0 \) \((j = 1, \cdots, r)\)

Level-set PDEs:

\[ \frac{\partial \phi_i}{\partial t} = -P_i(\Phi) |\nabla \phi_i|, \quad x \in D \setminus \partial D \]

\[ \frac{\partial \phi_i}{\partial n} = 0 \quad \text{on } \partial D \]
Three-Materials

- Three Phases Plus Void
- \( P = 30, 15 \)
- Each phase of 10%
- \( E = 200, 100, 50 \)
Convergence
Two Materials

- Two Phases Plus Void
- $P = 80$
- Volume = 10\%, 20\%
- $E = 200, 100$
Convergence
Three Materials

- Three Phases Plus Void
- $P = 80$
- Each phase of 10%
- $E = 200, 100, 50$
Convergence

The graph shows the convergence of material volume ratios and total deformation energy over iterations. The x-axis represents the number of iterations, while the y-axis shows the volume ratio and deformation energy. The graph includes lines for different material volume ratios and a dashed line for total deformation energy.
Material Design

Base Material:  
- Poisson’s ratio = 0.3

Designed Material:  
- Poisson’s ratio = -0.5

Optimization:  
\[
\min \text{imize } \left( E_{1111}^H - E_{1111}^* \right)^2 - \left( E_{2222}^H - E_{2222}^* \right)^2 + \left( E_{1122}^H - E_{1122}^* \right)^2
\]

Y-periodic Cellular Material:
\[
E_{ijkl}^H = \frac{1}{|Y|} \int_Y \left( E_{ijkl} - E_{ijpq} \frac{\partial \kappa_p^{kl}}{\partial y_q} \right) dY
\]
\[
\int_Y E_{ijpq} \frac{\partial \kappa_p^{kl}}{\partial y_q} \frac{\partial v_i}{\partial y_j} dY = \int_Y E_{ijkl} \frac{\partial v_i}{\partial y_j} dY
\]
Material Cell

Fig. 2 Isotropic Microstructure with Poisson’s Ratio Equal to −0.5

(a)  (b)  (c)

(d)  (e)  (f)

Fig. 3 Isotropic Microstructure with Poisson’s Ratio Equal to −0.5
Compliant Mechanisms

- Micro-Griper/Clamp
- MEMS Device
- Flexure Hinges

Fig. (4) Design domain for flexible mechanism
Fig. 6 Evolution Procedure of the Pulled Crunching Mechanism
Convergence

(a) The Mechanical Advantage  (b) The material and displacement constraints

Fig. 5  The pulled Crunching Mechanism
Variational Problems of Free-Discontinuities:

- Mumford-Saha Model (1989):
  \[ J_{MS}(f, \Gamma) = \int_{\Omega} F(f) dx + \alpha \int_{\Omega \setminus \Gamma} \varphi(\nabla f(x)) dx + \beta \int_{\Gamma} dS \]
  - Multiple, distinct regions, each with a continuous (or constant) variable (Material regions)
  - Separated by interfaces (Boundaries)

PDE-driven Geometro-Physical Evolution

- Level-Set PDE Models:
  \[ \frac{\partial \Phi(x,t)}{\partial t} + \nabla \Phi(x,t) \cdot V(x) = 0 \]
  - Physical optimization
  - Regularization on material domain
  - Regularization on geometric domain
  - Topology and geometry control
  \[ V_n = V \cdot n = -\kappa \]
**Constraints**

**Geometric Constraints:**
- Curvature Constraint
  - Circular Holes
- Gradient Constraints

**Topology Constraints:**
- Topology-Preserving

**Manufacturing Constraints:**
- Regional

**Homogenization-Based Methods:**
- Image-Based Post-Processing
- Difficult to Constrain “Pixels”
Conclusions

1. Level-Set Models and Computation:
   - Concise Boundary & Interior Representation
   - Topologically Flexible & Geometrically Accurate
   - Powerful PDE & Variational Numerical Methods

2. Multi-Phase Level-Sets for Optimization:
   - Heterogeneous phases
   - Efficient and Concise Representation
   - Structure, Material and Mechanism Design

3. On-going Research:
   - Geometry-dependent Loading (e.g., Pressure loading)
   - Variational Methods for Topology Optimization
   - Solid Free-Form Design as a Geometro-Physical Evolution Process for Heterogeneous Systems
Acknowledgements

Contributions

- Dr. XM Wang
  (Dalian Univ. of Tech.)
- P Wei, SW Zhou

Collaborations

- Prof. DM Guo
  (Dalian Univ. of Tech.)

Supported by:

- National Science Foundation (USA) (No. CMS-96347717)
- National Science Foundation of China (Nos. 59775065, 50128503)
- Hong Kong Research Grants Council (No. 2050254)