Adjoint-Based Electromagnetic Shape Optimization

Owen Miller
EE 291
How to Represent Shapes

- Boundaries determine the shape
- Rather than parametrizing boundary, more effective to embed boundary as the zero level set of a function, which we call $\phi$

$$\partial \Omega(t) = \{(\vec{x}, t) | \phi(\vec{x}, t) = 0\}$$

Interior: $\phi < 0$
Exterior: $\phi > 0$

$\phi > 0$  $\phi < 0$  $\phi > 0$
How to Represent Shapes

• Boundaries determine the shape

• Rather than parametrizing boundary, more effective to embed boundary as the zero level set of a function, which we call \( \phi \)

\[
\partial \Omega(t) = \{(\vec{x}, t) | \phi(\vec{x}, t) = 0\}
\]

Interior: \( \phi < 0 \)
Exterior: \( \phi > 0 \)

To move boundary,

\[
\frac{d}{dt} \phi(\vec{x}, t) = \frac{\partial \phi}{\partial t} + \frac{d\vec{x}}{dt} \cdot \nabla \phi = 0
\]

\( \vec{V} = \frac{d\vec{x}}{dt} \)

Velocity determines boundary movement!

Hamilton-Jacobi Equation
Application: Photodetector Design

- Ge very effective absorber
- Small channel needed for SNR, bandwidth
  ➔ Need highly efficient waveguide!
Waveguide Simulation

Incident Field → Waveguide Mode

Si

Air

Perfectly Matched Layer

Ge is here
Waveguide Simulation

Incident Field → = Waveguide Mode

Si

Air

Perfectly Matched Layer

φ < 0

O O O O O O O O

φ > 0

This is our design area
Waveguide Simulation

Incident Field → = Waveguide Mode

\[
\begin{aligned}
\nabla^2 + \varepsilon(x, \phi) \frac{\omega^2}{c^2} u &= 0 \quad \text{throughout domain} \\
\frac{\partial u}{\partial n} + au &= b \quad \text{on } \Gamma_R \\
u &= 0 \quad \text{on } \Gamma_D
\end{aligned}
\]
Weak Form of Maxwell’s Eqn.’s

\[ \nabla^2 u + \varepsilon(x, \phi) \frac{\omega^2}{c^2} u = F \]

\[ \int_A \left( \bar{v} \nabla^2 u + \varepsilon(x, \phi) \frac{\omega^2}{c^2} \bar{v} u \right) dA = \int_A \bar{v} F dA \quad \text{Inner product with test function } \bar{v} \]

\[ \int_A \left( -\nabla \bar{v} \cdot \nabla u + \varepsilon(x, \phi) \frac{\omega^2}{c^2} \bar{v} u \right) dA + \int_{\partial A} \bar{v} \frac{\partial u}{\partial n} ds = \int_A \bar{v} F dA \quad \text{Integration by parts} \]

\[ \int_A \left( -\nabla \bar{v} \cdot \nabla u + \varepsilon(x, \phi) \frac{\omega^2}{c^2} \bar{v} u \right) dA - a \int_{\Gamma_R} \bar{v} u ds + b \int_{\Gamma_R} \bar{v} ds = \int_A \bar{v} F dA \quad \text{Insert b.c.’s} \]

\[ a(u, v) = L(v) \quad \forall v \in V \]

*Note: \[ a(u, v) = a(\bar{v}, \bar{u}) \]
Shape Derivatives

Consider the merit function $J = \int_D |u|^2 dA = \int_D uu\overline{d}dA$

$$\delta J = \frac{\partial J}{\partial \varphi} \delta \varphi + \frac{\partial J}{\partial u} \delta u + \frac{\partial J}{\partial \overline{u}} \delta \overline{u} = 2 \text{Re} \int_D \overline{u} \delta udA$$

But our independent variable is the geometry, $\phi$, not $u$
Shape Derivatives

Consider the merit function 

\[ J = \int_D |u|^2 \, dA = \int_D u \bar{u} \, dA \]

But our independent variable is the geometry, \( \phi \), not \( u \).

Define an “adjoint” field \( w \) such that

\[ \delta J = \frac{\partial J}{\partial \phi} \delta \phi + \frac{\partial J}{\partial u} \delta u + \frac{\partial J}{\partial \bar{u}} \delta \bar{u} = 2 \text{Re} \int_D \bar{u} \delta u \, dA \]

Define an “adjoint” field \( w \) such that

\[ \nabla^2 w + \varepsilon(x, \phi) \frac{\omega^2}{c^2} w = 2\bar{u} \chi_D \]

\[ \chi_D = \begin{cases} 
1 & x \in D \\
0 & x \notin D 
\end{cases} \]

\[ \frac{\partial u}{\partial n} + au = 0 \quad \text{on } \Gamma_R \]
Weak form of $u$: $a(u, v) = -b \int_{\Gamma_R} \bar{v} ds$

Take differential: $a(\delta u, v) = -\frac{\omega^2}{c^2} \int_A \bar{v} u \frac{\partial \varepsilon}{\partial \varphi} \, dA \quad v \to \bar{w}$
Weak form of $u$: \[ a(u, v) = -b \int_{\Gamma_R} \vec{v} ds \]

Take differential: \[ a(\delta u, v) = \omega^2 \int_A \vec{v} u \frac{\partial \varepsilon}{\partial \varphi} \delta \varphi \ dA \] \[ v \to \vec{w} \]

Weak form of $w$: \[ a(w, v) = 2 \int_D \vec{v} \bar{u} dA \] \[ v \to \delta \bar{u} \]

\[ a(\vec{w}, \delta \bar{u}) = a(\delta u, w) \quad \Rightarrow \quad 2 \int_D \bar{u} \delta \bar{u} dA = -\frac{\omega^2}{c^2} \int_A uw \frac{\partial \varepsilon}{\partial \varphi} \delta \varphi \ dA \]
Weak form of $u$: \[ a(u, v) = -b \int_{\Gamma_R} \bar{v} ds \]

Take differential: \[ a(\delta u, v) = -\frac{\omega^2}{c^2} \int_A \bar{v} u \frac{\partial \varepsilon}{\partial \phi} dA \quad v \rightarrow \bar{w} \]

Weak form of $w$: \[ a(w, v) = 2 \int_D \bar{v} \bar{u} dA \quad v \rightarrow \delta \bar{u} \]

\[ a(\bar{w}, \delta \bar{u}) = a(\delta u, w) \quad \rightarrow \quad 2 \int_D \bar{u} \delta u dA = -\frac{\omega^2}{c^2} \int_A u w \frac{\partial \varepsilon}{\partial \phi} dA \]

\[ \delta J = 2 \text{Re} \int_D \bar{u} \delta u dA = -\frac{\omega^2}{c^2} \text{Re} \int_A u w \frac{\partial \varepsilon}{\partial \phi} \delta \phi dA \]
Weak form of $u$:  $a(u, v) = -b \int_{\Gamma_R} \bar{v} ds$

Take differential:  $a(\delta u, v) = -\frac{\omega^2}{c^2} \int_{A} \bar{v} u \frac{\partial \varepsilon}{\partial \varphi} \delta \varphi \ dA \quad v \rightarrow \bar{w}$

Weak form of $w$:  $a(w, v) = 2 \int_{D} \bar{v} \bar{u} dA \quad v \rightarrow \delta \bar{u}$

$$a(\bar{w}, \delta \bar{u}) = a(\delta u, w) \quad \rightarrow \quad 2 \int_{D} \bar{u} \delta u dA = -\frac{\omega^2}{c^2} \int_{A} u \bar{w} \frac{\partial \varepsilon}{\partial \varphi} \delta \varphi \ dA$$

$$\delta J = 2 \text{Re} \int_{D} \bar{u} \delta u dA = -\frac{\omega^2}{c^2} \text{Re} \int_{A} u \bar{w} \frac{\partial \varepsilon}{\partial \varphi} \delta \varphi dA$$

$$\delta \varphi = -V_n |\nabla \varphi| dt \quad \text{Hamilton-Jacobi}$$

$$\varepsilon(\varphi) = \varepsilon_{Si} H(-\varphi) + \varepsilon_{Air} H(\varphi) \quad \rightarrow \quad \frac{\partial \varepsilon}{\partial \varphi} = -(\varepsilon_{Si} - \varepsilon_{Air}) \delta(\varphi)$$
Helmholtz Shape Derivative

Putting it all together,

$$\delta J = -\frac{\omega^2}{c^2} (\varepsilon_{Si} - \varepsilon_{Air}) dt \operatorname{Re} \int_{A} uwV_n |\nabla \varphi| \delta(\varphi) dA$$

We can choose $V_n = -\overline{uW}$ and we have an ascent algorithm!

$\delta J > 0$
Shape Optimization Process

Use Comsol – standard FEM software

- Define geometry in Matlab
- Pass geometry to Comsol
- Solve for u, w in Comsol
- Use u, w to define velocity
- Update geometry in Matlab w/ Hamilton-Jacobi
- Loop
Test Run

For many steps, restricted step size to ensure $J_{new} > 0.75*J_{old}$

Factor of 8 improvement in merit function!
Comparison of Initial and Final Iterations
Comparison of Initial and Final Iterations

d \approx 30\text{nm}
Timing

35 iterations took 2 hours
\[\begin{align*}
75 \text{ min for simulations} \\
45 \text{ min for everything else (creating/updating structures, passing data back and forth, etc.)}
\end{align*}\]

Because of 75 % restriction, 35 iterations was really > 100 runs