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Sandia National Laboratories

The Strip Method for Shape Derivatives

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MS21 - Advances in Shape Optimization Algorithms - Part I of III

SIAM Conference on Optimization (OP21)

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Outline

Challenges of Shape Optimization

Shape gradient computation

- Finite Differences (slow, inaccurate)
- Automatic Differentiation (great if we can use it)
- Volume Method, Boundary Method (may be difficult to implement)
- Strip Method (Preprint: http://dx.doi.org/10.13140/RG.2.2.32766.82246)

Constraint formulation

- Smoothness (may be necessary for existence of solutions)
- Symmetry; manufacturability by a given process
- Contact

Interplay with optimization algorithms

- Free-form design: large number of inequality constraints
- Limitations of a priori parametrization

Mesh quality

- Elliptic smoothing
- Explicit reconnection based on remeshing

Model Problem: Square to Circle

$$\min_{\Omega} \mathcal{J}(\Omega) := \int_{\Omega} j(u)\, dx, \tag{1a}$$

where u in (1a) solves the PDE

$$\begin{cases} -\Delta u &= f \quad \text{in} \quad \Omega \\ u &= 0 \quad \text{on} \quad \partial\Omega. \end{cases} \tag{1b}$$

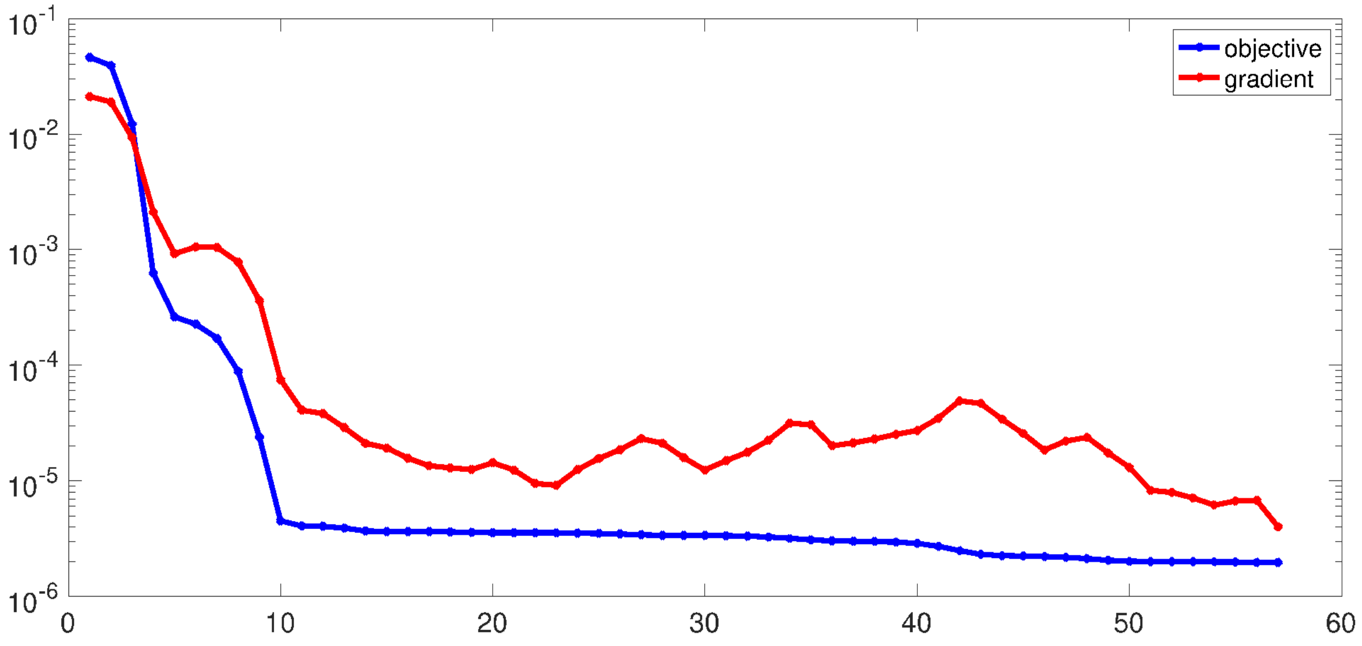
- Initial domain (unit square): $\Omega_0 = (0,1)^2$
- Tracking target: $j(u) = \frac{1}{2}(u - u_*)^2$, $f = \lambda^2 u_*$

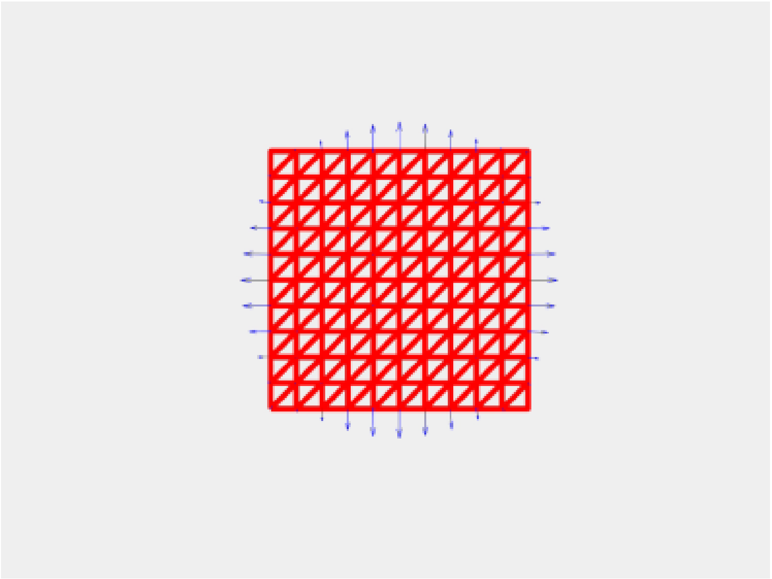
$$u_*(x) = J_0\left(\lambda \left| x - \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix}^\top \right|_2 \right)$$

- Optimal domain (circumscribing circle):

$$\Omega_* = \left\{ x \in \mathbb{R}^2 \ : \ \left| x - \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix}^\top \right|_2 < \frac{\sqrt{2}}{2} \right\}.$$

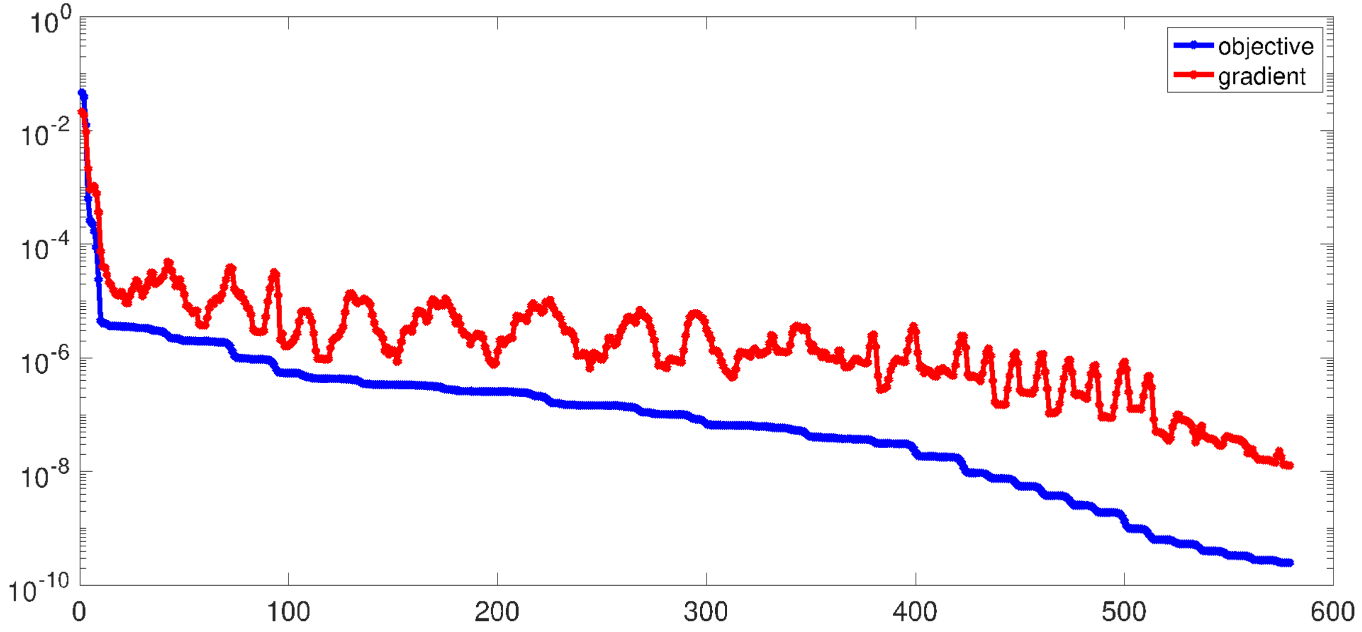
Numerical Results

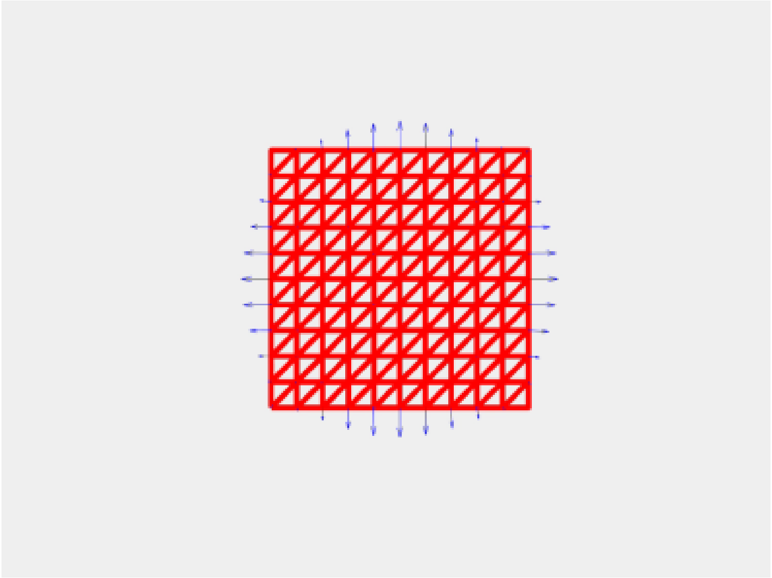




- Discretize (1) with piecewise-linear finite elements.
- Optimization variables: coordinates of the mesh nodes.
- Compute the gradient $d\mathcal{J}$ using adjoint calculus.
- Looks like things are going well.

Numerical Results - Lower Tolerance





- Objective drops by a further three orders of magnitude!
- What happened to the mesh?

The Volume Method

We model perturbations of Ω using the map

$$\mathbb{R}^N \ni x \mapsto x + \boldsymbol{V}(x),$$

where $\boldsymbol{V} \in \mathcal{D}^1$ (continuously differentiable with compact support). The volume form is

$$\langle \boldsymbol{G}_\Omega, \boldsymbol{V} \rangle_{(\mathcal{D}^1)', \mathcal{D}^1} = \int_\Omega \Big(\nabla u \cdot \left(\nabla \boldsymbol{V} + \nabla \boldsymbol{V}^\top \right) \nabla p + p(\boldsymbol{V} \cdot \nabla f) \\ + \operatorname{div} \boldsymbol{V} \left(j(u) - \nabla u \cdot \nabla p + pf \right) \Big) \, dx,$$

where p solves the adjoint equation

$$\begin{cases} -\Delta p = j_u(u) & \text{in} \quad \Omega \\ \quad\;\; p = 0 & \text{on} \quad \partial\Omega. \end{cases}$$

- Support of $\boldsymbol{G}_\Omega$ is contained in $\partial\Omega$. https://epubs.siam.org/doi/book/10.1137/1.9780898719826
- Discretization of the volume method is equivalent to differentiation of the discretization (with suitable subspace for $\boldsymbol{V}$).
- Volume method traditionally favored by engineers.
- Initial example: optimization of discretization error.

The Boundary Method

The gradient can also be expressed on the boundary.

$$\langle \boldsymbol{G}_{\partial\Omega}, \gamma_{\partial\Omega}(\boldsymbol{V}) \cdot \boldsymbol{\nu} \rangle_{C^1(\partial\Omega)', C^1(\partial\Omega)} = \int_{\partial\Omega} (\boldsymbol{V} \cdot \boldsymbol{\nu}) \left(j(u) + \partial_{\boldsymbol{\nu}} p \partial_{\boldsymbol{\nu}} u \right) \, d\sigma.$$

- Boundary method traditionally favored by mathematicians.
- Derivative of solution $(\partial_{\boldsymbol{\nu}} p, \partial_{\boldsymbol{\nu}} u)$ not derivative of operator $(\nabla \boldsymbol{V}, \operatorname{div} \boldsymbol{V})$.

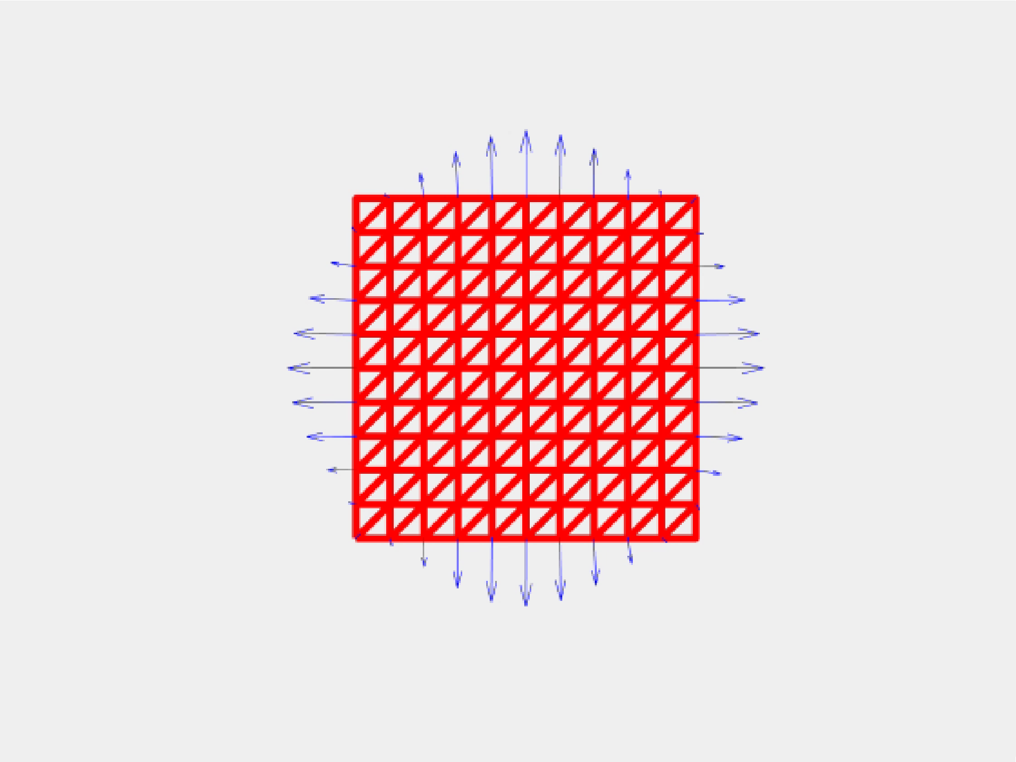
The *Hadamard Structure Theorem* states the equivalence of the two methods:

$$\langle \boldsymbol{G}_{\partial\Omega}, \gamma_{\partial\Omega}(\boldsymbol{V}) \cdot \boldsymbol{\nu} \rangle_{C^1(\partial\Omega)', C^1(\partial\Omega)} = \langle \boldsymbol{G}_{\Omega}, \boldsymbol{V} \rangle_{(\mathcal{D}^1)', \mathcal{D}^1}, \quad \text{for all } \boldsymbol{V} \in \mathcal{D}^1.$$

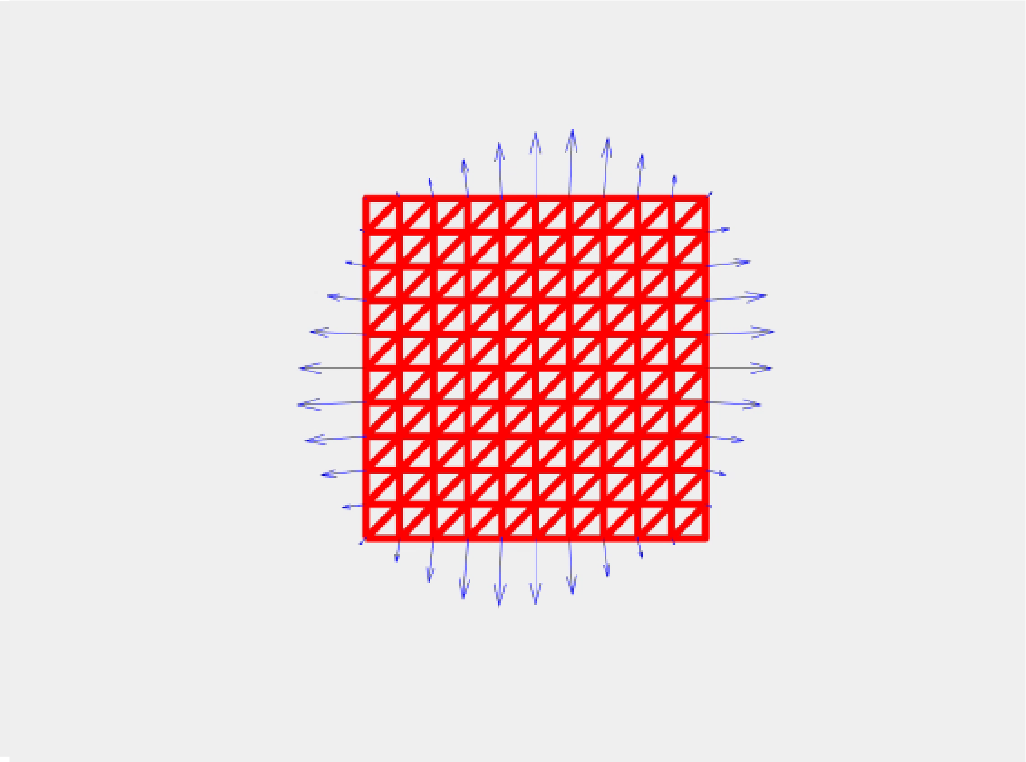
- **Main idea:** integration by parts
- Numerically, they are not equivalent: see Hiptmair et al. (2015)

Accuracy of the Boundary Method

Volume Method (16 iterations)



Boundary Method (41 iterations)



Boundary method is less accurate:

- $O(h)$ vs $O(h^2)$ for the volume method
- On the other hand, it still converges. . .
- Does it have any other advantages?

Disadvantages of Existing Methods

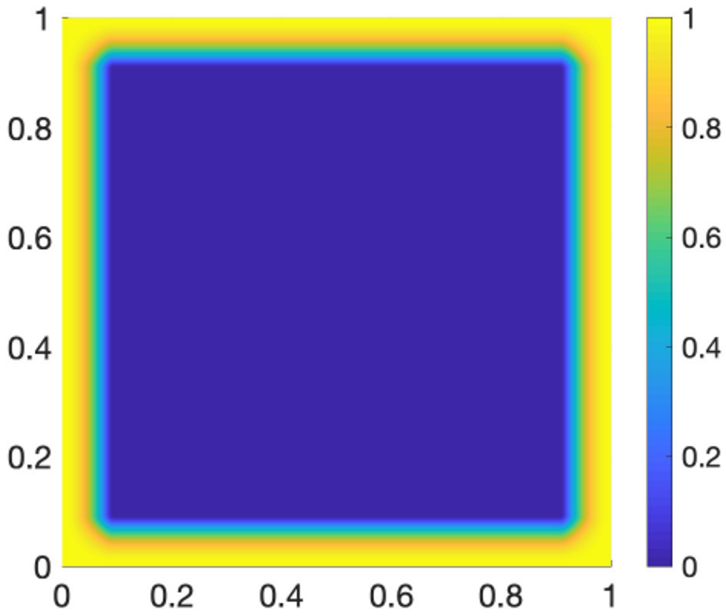
Method	Accuracy	Speed	Implementation Cost
Finite Differences	X	X	✓
Automatic Differentiation	✓	✓	X
Volume Method	✓	✓	X
Boundary Method	X	✓	✓

- No method is ideal.
- Main issue with implementation cost: invasiveness to existing codes.
- Want a method with high accuracy that *is not invasive.*

The Strip Gradient

Let the strip $\Sigma \subseteq \Omega$ be a fixed open set with $\partial\Omega \subsetneq \partial\Sigma$. We define the smooth cut-off function $\psi : \mathbb{R}^N \to [0,1]$ to be infinitely differentiable and satisfy

$$\psi(x) \in \begin{cases} \{1\} & \text{if } x \in \mathbb{R}^N \setminus \Omega \\ (0,1) & \text{if } x \in \Sigma \\ \{0\} & \text{if } x \in \Omega \setminus \Sigma \end{cases} .$$



We can thus decompose any $\boldsymbol{V} \in \mathcal{D}^1$ as

$$\boldsymbol{V} = \psi\boldsymbol{V} + (1-\psi)\boldsymbol{V}.$$

By the Hadamard Structure Theorem,

$$\langle \boldsymbol{G}_\Omega, \boldsymbol{V} \rangle_{(\mathcal{D}^1)',\mathcal{D}^1} = \underbrace{\langle \boldsymbol{G}_\Omega, \psi\boldsymbol{V} \rangle_{(\mathcal{D}^1)',\mathcal{D}^1}}_{\equiv \langle \boldsymbol{G}_\Sigma, \boldsymbol{V} \rangle_{(\mathcal{D}^1)',\mathcal{D}^1}} + \underbrace{\langle \boldsymbol{G}_\Omega, (1-\psi)\boldsymbol{V} \rangle_{(\mathcal{D}^1)',\mathcal{D}^1}}_{=0} .$$

The Strip Method: Error Analysis

- Let $u_h, p_h \in \mathbb{V}_h$ solve the discrete state and adjoint equations

$$\int_\Omega \nabla u_h \cdot \nabla v_h \,\mathrm{d}x = \int_\Omega f v_h \,\mathrm{d}x \quad \forall v_h \in \mathbb{V}_h,$$
$$\int_\Omega \nabla p_h \cdot \nabla v_h \,\mathrm{d}x = \int_\Omega j_u(u_h) v_h \,\mathrm{d}x \quad \forall v_h \in \mathbb{V}_h.$$

- The (semi-)discretized representations of $\boldsymbol{G}_\Omega$ and $\boldsymbol{G}_{\partial\Omega}$ are

$$\langle \boldsymbol{G}^h_\Omega, \boldsymbol{V} \rangle_{(\mathcal{D}^1)', \mathcal{D}^1} = \int_\Omega \Big(\nabla u_h \cdot (\nabla \boldsymbol{V} + \nabla \boldsymbol{V}^\top) \nabla p_h - f \boldsymbol{V} \cdot \nabla p_h + \operatorname{div} \boldsymbol{V} \, (j(u_h) - \nabla u_h \cdot \nabla p_h) \Big) \,\mathrm{d}x$$

and

$$\langle \boldsymbol{G}^h_{\partial\Omega}, \gamma_{\partial\Omega}(\boldsymbol{V}) \cdot \boldsymbol{\nu} \rangle_{C^1(\partial\Omega)', C^1(\partial\Omega)} = \int_{\partial\Omega} (\boldsymbol{V} \cdot \boldsymbol{\nu}) \, (j(u_h) + \partial_{\boldsymbol{\nu}} p_h \partial_{\boldsymbol{\nu}} u_h) \,\mathrm{d}\sigma \,.$$

- $\mathbb{V}_h$ is the finite element space of piecewise-linear (on simplices) or bilinear (on cubes) elements that are globally continuous.

The Strip Method: Error Analysis

Theorem (Hiptmair et al., 2015)

Let Ω be convex or $C^{1,1}$ and f be the restriction of an $H^1(\mathbb{R}^N)$ function onto Ω. If $(u,p) \in H_0^1(\Omega) \times H_0^1(\Omega)$ and $(u_h, p_h) \in \mathbb{V}_h \times \mathbb{V}_h$ respectively solve the continuous and discrete state and adjoint equations then:

$$\left| \langle \boldsymbol{G}_\Omega - \boldsymbol{G}_\Omega^h, \boldsymbol{V} \rangle_{(\mathcal{D}^1)', \mathcal{D}^1} \right| \leq C_1(\Omega, u, p, f) h^2 \|\boldsymbol{V}\|_{W^{2,4}(\Omega)}.$$

In addition, if

$$\|u\|_{W^{2,p}(\Omega)} \leq C \|f\|_{L^p(\Omega)}$$

for some $p > N$ and a positive constant C, then

$$\left| \langle \boldsymbol{G}_{\partial\Omega} - \boldsymbol{G}_{\partial\Omega}^h, \gamma_{\partial\Omega}(\boldsymbol{V}) \cdot \boldsymbol{\nu} \rangle_{C^1(\partial\Omega)', C^1(\partial\Omega)} \right| \leq C_2 h \|\boldsymbol{V} \cdot \boldsymbol{\nu}\|_{L^\infty(\partial\Omega)},$$

where the constant $C_2 > 0$ is independent of h.

The Strip Method: Error Analysis

Corollary (Hardesty et al., 2021)

Let $\Psi : \boldsymbol{V} \mapsto \psi \boldsymbol{V}$ *define a continuous linear operator from* $W^{2,4}(\Omega)$ *into* $W^{2,4}(\Omega)$. *Then, we have*

$$\left| \langle \boldsymbol{G}_\Sigma - \boldsymbol{G}_\Sigma^h, \boldsymbol{V} \rangle_{(\mathcal{D}^1)', \mathcal{D}^1} \right| \leq C_1(\Omega, u, p, f) h^2 \|\Psi\|_{W^{2,4}(\Omega)} \|\boldsymbol{V}\|_{W^{2,4}(\Omega)},$$

where C_1 *is the constant in the theorem.*

- Can easily apply analysis of Hiptmair et al. (2015).
- The strip method retains the higher accuracy of the volume method.
- No need to construct ψ in practice.
- Note we still have a continuous $\boldsymbol{V}$; how do we use this in a discretization?

Discrete Gradients

- Consider a coarse mesh $\mathcal{M}_c$ with Lagrange basis functions $\{\varphi_i^c : i = 1, \ldots, N_c\}$, and a finer mesh $\mathcal{M}_f$ with Lagrange basis functions $\{\psi_i^f : i = 1, \ldots, N_f\}$.
- Let

$$\boldsymbol{V}^c(x) = \begin{pmatrix} \sum_{i=1}^{N_c} \varphi_i^c(x) v_{1,i}^c \\ \sum_{i=1}^{N_c} \varphi_i^c(x) v_{2,i}^c \end{pmatrix}, \qquad \boldsymbol{V}^f(x) = \begin{pmatrix} \sum_{i=1}^{N_f} \varphi_i^f(x) v_{1,i}^f \\ \sum_{i=1}^{N_f} \varphi_i^f(x) v_{2,i}^f \end{pmatrix}.$$

- This results in gradient vectors ($\alpha = 1 \text{ or } 2$).

$$\hat{g}_\alpha^c \in \mathbb{R}^{N_c}, \qquad \hat{g}_\alpha^f \in \mathbb{R}^{N_f}.$$

- With mass matrices

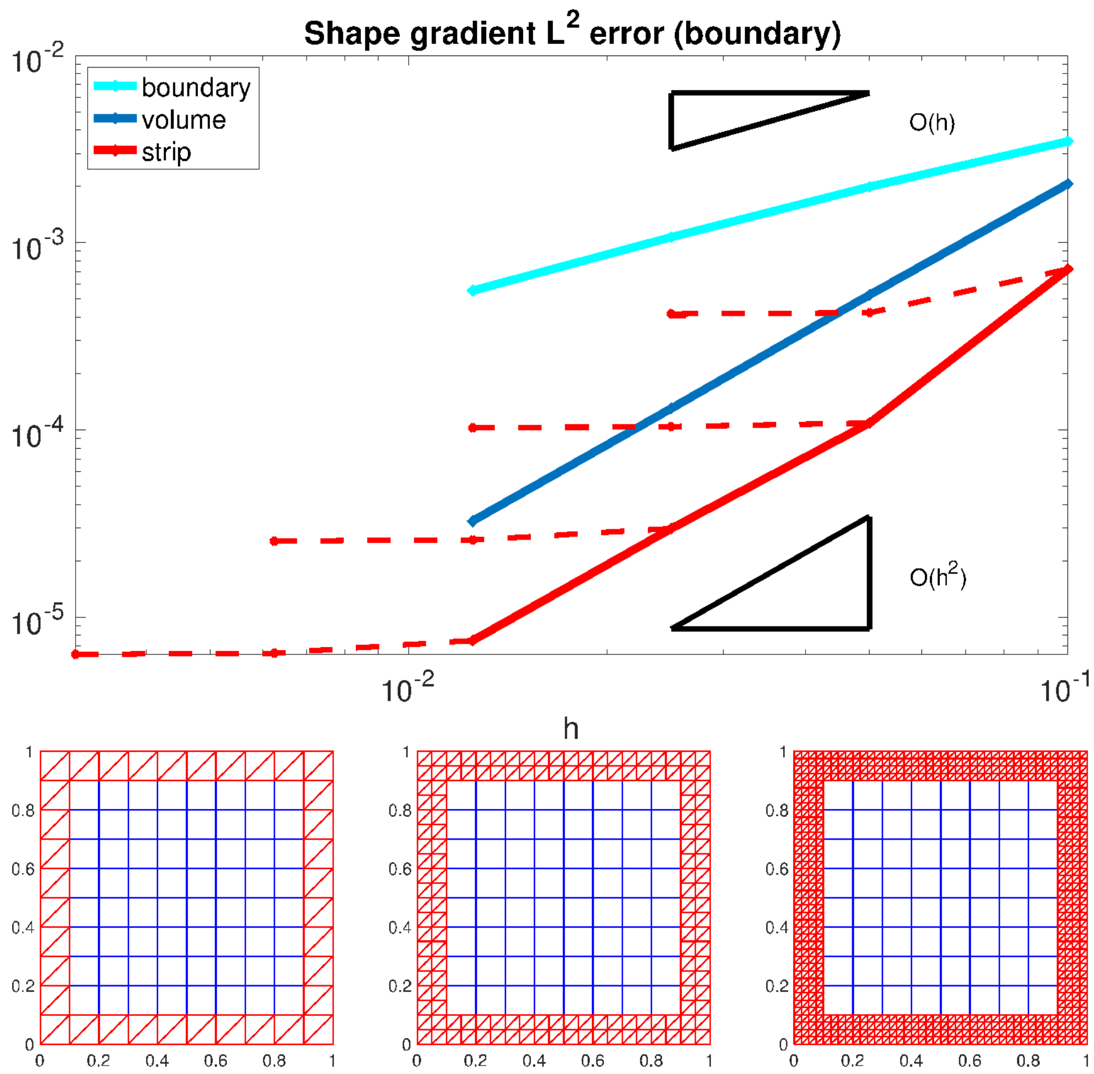
$$(M_{\mathrm{ff}})_{ij} = \int_\Sigma \psi_i^f(x) \psi_j^f(x) \, \mathrm{d}x, \qquad (M_{\mathrm{fc}})_{ij} = \int_\Sigma \psi_i^f(x) \varphi_j^c(x) \, \mathrm{d}x,$$

  the gradient on the fine mesh can be coarsened via L^2 projection:

$$\hat{g}_\alpha^c = M_{\mathrm{fc}}^\top M_{\mathrm{ff}}^{-1} \hat{g}_\alpha^f.$$

Strip Method: Summary

- Volume method in a strip near the boundary
- Accuracy of the volume method
- Speed of the boundary method
- Just needs state and adjoint at quadrature points
- Meshes can be independent
- Codes can be independent
- Adaptive refinement of strip mesh can increase accuracy
- Can implement it using automatic differentiation



Conclusion

Many issues in shape optimization remain research topics.

- We now have much greater understanding of how to select a problem-appropriate strategy for shape gradients.
- Software engineering: strip method makes working with legacy codes possible.
- Still useful for parameterized calculations: faster, more accurate than FD.
- Following parameterization from CAD to mesh to optimization: simple in principle, but requires cross-team cooperation and organization.
- Supporting general shape changes is a large project with many moving parts.