SAND2022-13669C

Approximate Shape Gradients with Boundary Element Methods

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20th Söllerhaus workshop on Fast Boundary Element Methods in Industrial Applications

October, 2022

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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 (https://doi.org/10.1002/nme.6908)

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
- Quality-preserving metrics (V. Schulz, R. Herzog)

Model Problem: Square to Circle

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

where u in (2a) solves the PDE

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

- 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):

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

Shape Derivative of the Objective Function

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 shape derivative of the objective can be expressed

$$dJ(\Omega; \boldsymbol{V}) = \int_\Omega j_u(u) u'(\Omega; \boldsymbol{V})\, dx + \int_{\partial\Omega} (\boldsymbol{V} \cdot \boldsymbol{\nu}) j(u)\, dx, \tag{2a}$$

where u' is the shape derivative of the solution to (1b) (see Sokolowski and Zolesio):

$$\begin{cases} -\Delta u' &= 0 \quad \text{in} \quad \Omega \\ u' &= -(\boldsymbol{V} \cdot \boldsymbol{\nu}) \partial_{\boldsymbol{\nu}} u \quad \text{on} \quad \partial\Omega. \end{cases} \tag{2b}$$

The Boundary Method

By defining the adjoint equation

$$\begin{cases} -\Delta p = j_u(u) & \text{in} \quad \Omega \\ \quad\; p = 0 & \text{on} \quad \partial\Omega, \end{cases} \tag{3}$$

we can compute

$$\begin{aligned} \int_\Omega j_u(u)u' \, dx &\overset{(3)}{=} \int_\Omega \nabla p \cdot \nabla u' \, dx - \int_{\partial\Omega} u' \partial_{\boldsymbol{\nu}} p \, dx \\ &\overset{(2b)}{=} \int_{\partial\Omega} (\boldsymbol{V} \cdot \boldsymbol{\nu}) \partial_{\boldsymbol{\nu}} u \partial_{\boldsymbol{\nu}} p \, dx \end{aligned}$$

and thereby express the shape gradient entirely on the boundary:

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

The Volume Method

Let $y(x) = x + \boldsymbol{V}(x)$, and observe that

$$\begin{aligned} \nabla y =& I + \nabla \boldsymbol{V} \\ \det \nabla y =& \text{div } \boldsymbol{V} \\ (I - \nabla \boldsymbol{V})^{-1} =& I + \nabla \boldsymbol{V} + (\nabla \boldsymbol{V})^2 + \cdots . \end{aligned}$$

Thus, we can differentiate the operator $\int_\Omega \nabla u \cdot \nabla v = \int_\Omega f v$ in (1b) as follows:

$$\int_\Omega \nabla u' \cdot \nabla v \, dx - \int_\Omega \nabla u \cdot \left(\nabla \boldsymbol{V} + \nabla \boldsymbol{V}^\top\right) \nabla v \, dx + \int_\Omega \nabla u \cdot \nabla v \text{div } \boldsymbol{V} \, dx = \int_\Omega v(\boldsymbol{V} \cdot \nabla f) + v f \text{div } \boldsymbol{V} \, dx, \tag{4}$$

and thus write

$$\begin{aligned} \int_\Omega j_u(u) u' \, dx &\overset{(3)}{=} \int_\Omega \nabla p \cdot \nabla u' \, dx \\ &\overset{(4)}{=} \int_\Omega \nabla u \cdot \left(\nabla \boldsymbol{V} + \nabla \boldsymbol{V}^\top\right) \nabla p + p(\boldsymbol{V} \cdot \nabla f) + (\text{div } \boldsymbol{V}) \left(-\nabla u \cdot \nabla p + p f\right) \, dx, \end{aligned}$$

The Volume Method

thereby expressing the volume shape gradient:

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

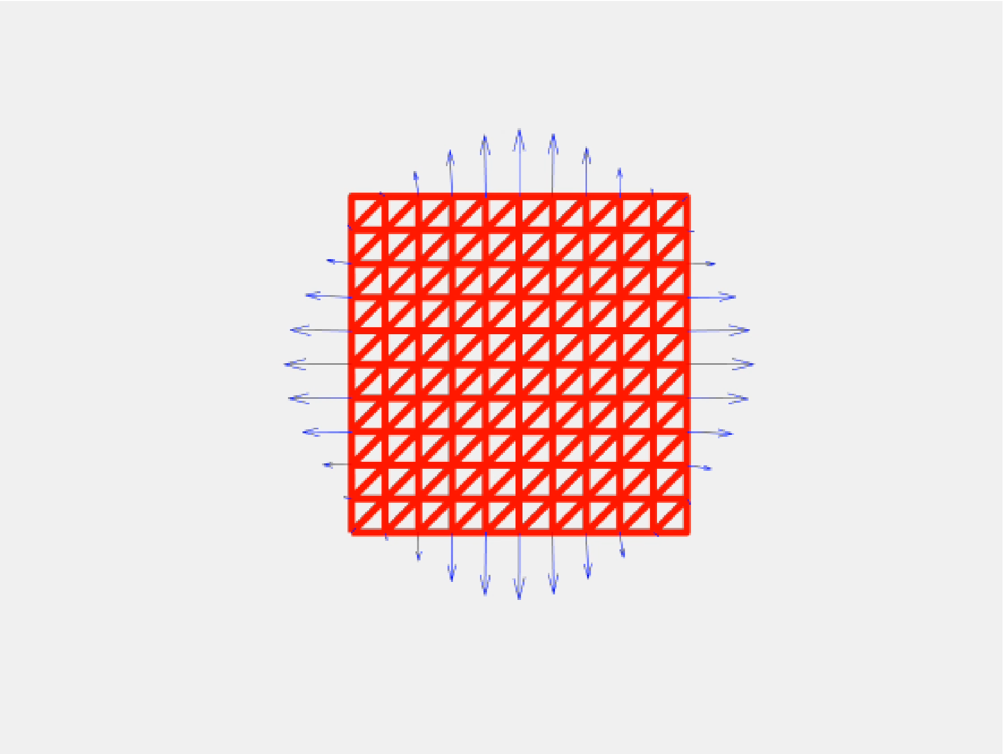
The *Hadamard Structure Theorem* states the equivalence of the two methods:

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

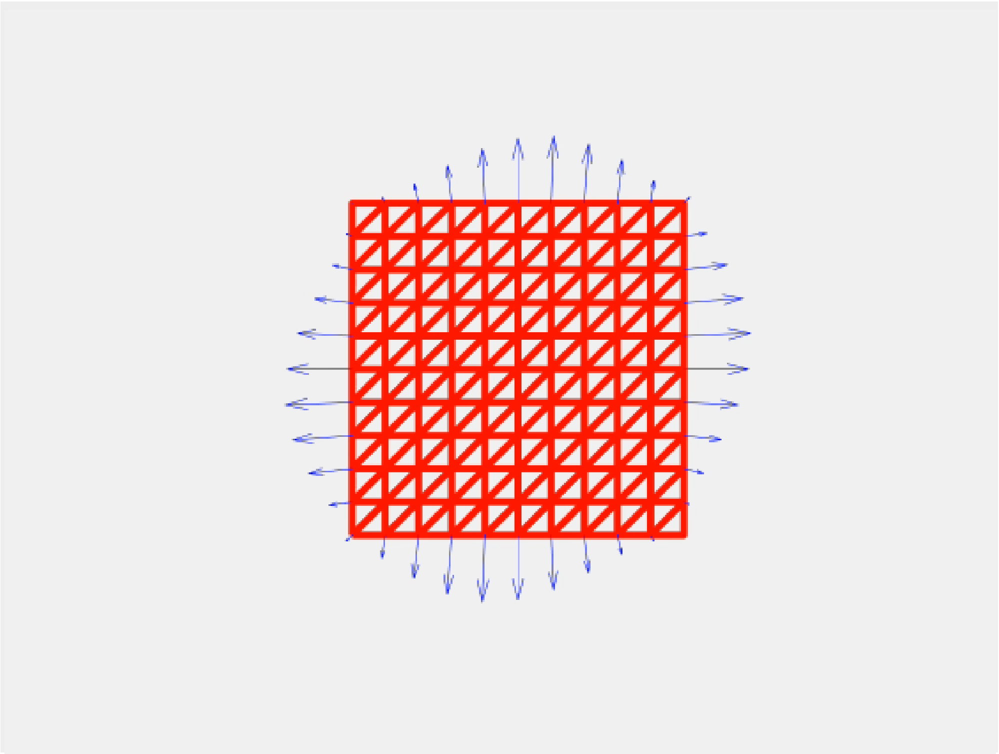
- **Main idea:** integration by parts
- Support of $\boldsymbol{G}_\Omega$ is contained in $\partial\Omega$.
  https://epubs.siam.org/doi/book/10.1137/1.9780898719826
- Discretization of the volume method is equivalent to differentiation of FEM discretization (with suitable subspace for $\boldsymbol{V}$).

Results with Finite Element Method

Volume Method (16 iterations)



Boundary Method (41 iterations)



Hiptmair et al. showed (2015) that they are not equivalent numerically:

- Boundary method is $O(h)$
- Volume method is $O(h^2)$
- Both utilize the same adjoint equation.

The Need for Better Terminology

Boundary method (strong form) for shape gradients

- Derivative of solution $(\partial_{\boldsymbol{\nu}} p, \partial_{\boldsymbol{\nu}} u)$ plus geometric factors $(\boldsymbol{V} \cdot \boldsymbol{\nu})$.
- Data is readily available with boundary element methods.

Volume method (weak form) for shape gradients

- Derivative of operator $(\nabla \boldsymbol{V}, \operatorname{div} \boldsymbol{V})$.
- Boundary element methods will not help us compute volume integrals!

We will consider two approaches. Both rely on solving the state and adjoint equations using BEM.

- **Extraction method**: use "extraction" to get additional required boundary data, use the boundary representation of the shape gradient.
- **Tensor method**: compute operator gradients of integral equations rather than the original PDE.

Boundary Integral Equations

Define the integral operators $K : H^{1/2}(\Gamma) \to H^{1/2}(\Gamma)$, and $V : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ via

$$K\varphi(x) = \frac{1}{4\pi}\int_\Gamma \frac{(x-y)\cdot\boldsymbol{\nu_y}}{|x-y|^3}\varphi(y)\,dy, \quad V\psi(x) = \frac{1}{4\pi}\int_\Gamma \frac{1}{|x-y|}\psi(y)\,dy.$$

Can solve the integral equation

$$V\psi = \left(\tfrac{1}{2}I + K\right)\varphi \tag{5}$$

for the unknown Neumann data $\psi = \partial_{\boldsymbol{\nu}} u|_{\partial\Omega}$. The solution u can then be expressed via the representation formula

$$u(x) = \int_{\partial\Omega} G(x,y)\psi(y) - \partial_{\boldsymbol{\nu_y}} G(x,y)\varphi(y)\,dy,$$

where $G(x,y) = 1/4\pi|x-y|$ is the Green's function for the Laplace equation.

The Extraction Method for a Dirichlet Problem

Consider the (slightly different) model problem

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

1. Solve $V(\partial_{\boldsymbol{\nu}} u) = \left(\frac{1}{2}I + K\right) g$ for $\partial_{\boldsymbol{\nu}} u$.
2. Solve $V(\partial_{\boldsymbol{\nu}} p) = \left(\frac{1}{2}I + K\right) j_u(u)$ for $\partial_{\boldsymbol{\nu}} p$.
3. Evaluate the boundary shape derivative (plus additional terms with $j(u)$ on the boundary):

$$\int_{\partial\Omega} (\boldsymbol{V} \cdot \boldsymbol{\nu}) \partial_{\boldsymbol{\nu}} p \partial_{\boldsymbol{\nu}} u \, dx.$$

The Extraction Method for a Neumann Problem

Now with a Neumann problem

$$\begin{cases} -\Delta u &= 0 \quad \text{in} \quad \Omega \\ \partial_{\boldsymbol{\nu}} u &= g \quad \text{on} \quad \partial\Omega, \end{cases}$$

things get more interesting. The shape sensitivity equation corresponding to (2b) now reads:

$$\begin{cases} -\Delta u' &= 0 \quad \text{in} \quad \Omega \\ \partial_{\boldsymbol{\nu}} u' &= \text{div}_\Gamma((\boldsymbol{V} \cdot \boldsymbol{\nu})\nabla_\Gamma u) + \kappa g(\boldsymbol{V} \cdot \boldsymbol{\nu}) \quad \text{on} \quad \partial\Omega, \end{cases} \tag{6}$$

where κ is the mean surface curvature.

- This only makes sense for smooth surfaces.
- Tangential derivatives $\nabla_\Gamma u$ can be computed via extraction approach of Schwab and Wendland (1999).
- Compute tangential derivatives of $\varphi = u|_\Gamma$ (in local coordinates, with $A = \frac{1}{2}I - K$):

$$A\varphi_\mu = -V\psi_\mu - A_{(\mu)}\varphi - V_{(\mu)}\psi.$$

Another Look at Operator Derivatives

Let $\{\varphi_i : i = 1, \ldots, N_h\}$ be a nodal Lagrange basis for the FEM subspace $\mathbb{V}_h$. Then with

$$u_h(x) = \sum_{i=1}^{N_h} U_i \varphi_i(x),$$

the state equation (1b) can be discretized as

$$KU = F \tag{7}$$

where

$$K_{ij} = \int_\Omega \nabla\varphi_i \cdot \nabla\varphi_j \, dx,$$
$$F_i = \int_\Omega f \varphi_i \, dx.$$

The Discrete Sensitivity Equation

Assume there are $S_h = 2N_h$ nodal coordinates corresponding to shape variables s_k, $k \in \{1, \ldots, S_h\}$. The discrete shape derivative of K for $k \in \{1, \ldots, S_h\}$ is

$$(K')_{ijk} = \frac{\partial K_{ij}}{\partial s_k}.$$

Using this notation, the discrete shape derivative of (7) is

$$K'U + KU' = F',$$

which can be rearranged into the discrete shape sensitivity equation

$$U' = K^{-1}\left(F' - K'U\right).$$

The Discrete Adjoint Equation

With the discrete derivative of $\mathcal{J}(\Omega)$ written

$$G_i = \int_\Omega j_u(u_h)\varphi_i \, dx,$$

the discrete shape sensitivity equation

$$U' = K^{-1}\left(F' - K'U\right)$$

can be used to form the objective function gradient

$$G^\top U' = \underbrace{G^\top K^{-1}}_{=P^\top}\left(F' - K'U\right),$$

where the adjoint state P solves $K^\top P = G$.

- These last few slides have been written for FEM, but apply equally well to BEM.
- The challenge in the BEM case is to compress the tensor K'.
- My paper with Mario Bebendorf (2013) shows how to do it.

Conclusion

Most literature on shape optimization with boundary element methods sticks to cases where extraction is not required, and everything can be computed on the boundary.

- The extraction approach usually requires more analytic work, plus the solution of additional integral equations.
- The tensor approach is general, but requires compression infrastructure.
- Both approaches require numerical integration of the same singular kernels.

No one has addressed their accuracy as Hiptmair did for FEM:

- Accuracy of boundary data computed with BEM.
- Accuracy of extracted tangential and higher-order derivatives.
- Can Hiptmair's analysis be extended to this case?