High-Order Mesh Adaptivity Using Goal-Oriented Error Estimation

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Abstract

We explore a new approach to goal-oriented mesh optimization in PDE-driven computational simulations. Targeting high-order mesh adaptivity, the approach combines geometric quality optimization with control of the PDE solution error. By leveraging the Target-Matrix Optimization Paradigm (TMOP) in conjunction with adjoint sensitivity analysis, the method employs a goal-oriented error estimation framework to optimize the mesh adaptively. We demonstrate that the optimized mesh simultaneously achieves good geometric quality and reduces the PDE solution error in regions critical to a predefined computational objective.

1 Introduction

Traditional mesh optimization methods primarily aim to improve geometric quality, often assuming this will lead to better accuracy in solving a PDE on the optimized mesh. However, geometric properties alone do not necessarily guarantee the most accurate PDE solutions. Existing approaches that incorporate solution fields tend to focus on interpolation errors [5, 7] or impose ad-hoc size control based on solution features [8, 9, 6, 3]. In this note, we explore an alternative strategy: optimizing a given starting mesh by directly minimizing the PDE error on the resulting mesh through adjoint sensitivity analysis. This approach is integrated with the Target-Matrix Optimization Paradigm (TMOP) to maintain high geometric quality while enhancing solution accuracy.

2 Optimization Approach

Let u(x) be the finite element solution of the PDE of interest with respect to mesh positions x. Our optimization problems minimize a multi-objective formulation, namely:

$$\min_{\mathrm{x}} \quad w_\mu \mathcal{F}_\mu(\mathrm{x}) + w_{\mathrm{u}} \mathcal{F}_{\mathrm{u}}(\mathrm{x}, \mathrm{u}(\mathrm{x})), \tag{2.1}$$

where $\mathcal{F}_\mu$ is a mesh quality term, $\mathcal{F}_{\mathrm{u}}$ a measure for the finite element error, and the weights w_μ are w_{u} are constants that control the balance between the terms. The mesh quality $\mathcal{F}_\mu$ and finite element error term $\mathcal{F}_{\mathrm{u}}$ are defined as follows:

$$\mathcal{F}_\mu(\mathrm{x}) = \int_\Omega \mu(\mathrm{x}) \; d\Omega \tag{2.2}$$

and

$$\mathcal{F}_{\mathrm{u}}(\mathrm{x}, \mathrm{u}(\mathrm{x})) = \int_\Omega (\mathrm{u}(\mathrm{x}) - \mathrm{u}^*)^2 \; d\Omega, \tag{2.3}$$

where $\mu(\mathrm{x})$ is a mesh quality metric and u^* is the exact solution of the PDE of interest.

2.1 Sensitivity analysis In the adjoint, i.e. reverse mode sensitivity analysis, we compute the sensitivities for both objective contributions. The derivative of a performance measure $\mathcal{F}$ with respect to the node coordinates x_i is

$$\frac{d\mathcal{F}(\mathrm{u}(\mathbf{x}), \mathbf{x})}{d\mathrm{x}_i} = \frac{\partial \mathcal{F}}{\partial \mathrm{x}_i} + \left(\frac{\partial \mathcal{F}}{\partial \mathrm{u}}\right)^T \frac{\partial \mathrm{u}}{\partial \mathrm{x}_i}. \tag{2.4}$$

The explicit dependence of the performance measure on the shape $\frac{\partial \mathcal{F}}{\partial \mathrm{x}_i}$ is accounted for by the first term of the right hand side, while the implicit dependence on the displacement derivative $\frac{\partial \mathrm{u}}{\partial \mathrm{x}_i}$ is accounted for by the second term. Because the physical field u satisfies the Residual equation $\mathcal{R}^{\mathrm{U}}(\mathrm{u}; \mathbf{x}) = 0$, the sensitivity $\frac{\partial \mathrm{u}}{\partial \mathrm{x}_i}$ is annihilated from Eq. 2.4 by evaluating the adjoint variable λ_u that solves

$$\left(\frac{\partial \mathcal{R}^{\mathrm{U}}}{\partial \mathrm{u}}\right)^T \lambda_{\mathrm{u}} = \frac{\partial \mathcal{F}}{\partial \mathrm{u}} \tag{2.5}$$

and then computing

$$\frac{d\mathcal{F}(\mathrm{u}(\mathbf{x}), \mathbf{x})}{d\mathrm{x}_i} = \frac{\partial \mathcal{F}}{\partial \mathrm{x}_i} - \lambda_{\mathrm{u}}^T \frac{\partial \mathcal{R}^{\mathrm{U}}}{\partial \mathrm{x}_i}. \tag{2.6}$$

The Jacobian $\frac{\partial \mathcal{R}^{\mathrm{U}}}{\partial \mathrm{u}}$ is the stiffness matrix used to solve the physical problem and $\frac{\partial \mathcal{R}^{\mathrm{U}}}{\partial \mathrm{x}_i}$ is obtained using the material derivative, cf. [4]. Note that the mesh quality performance measure $\mathcal{F}_\mu$ is not a function of the physical field u and consequently this term's implicit dependency is zero.

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3 Numerical Results

We present preliminary numerical results using simple meshes and a diffusion PDE to illustrate the fundamental concept of the method. All optimization problems are solved by employing the non-linear programming Method of Moving Asymptotes (MMA) [10] and the MFEM finite element library [1, 2].

3.1 Good initial mesh We use a diffusion problem with a manufactured solution to measure the error. The finite element PDE solver finds a temperature field $\mathrm{u} \in \mathcal{H} = \{\mathrm{u} \in H^1(\Omega) : \mathrm{u} = 0 \text{ on } \Gamma_D\}$ such that

$$
\begin{aligned}
0 &= \mathcal{R}^{\mathrm{U}}(\mathrm{u}) \\
&= \textstyle\int_\Omega (\nabla\delta\kappa\nabla\mathrm{u} + \delta\cdot f)\ d\Omega,
\end{aligned}
\tag{3.7}
$$

for all $\delta \in \mathcal{H}$ with conductivity $\kappa = 1$. The exact solution for this problem is $\mathrm{u}^* = \sin(\pi\mathrm{x})\cdot\sin(2\pi\mathrm{y})$.

The finite element errors over the domain Ω, before and after optimization, are presented in Figure 1. As the finite element error is small compared to the mesh quality term, we choose $w_{\mathrm{u}} = 10^6$ and $w_\mu = 1$.

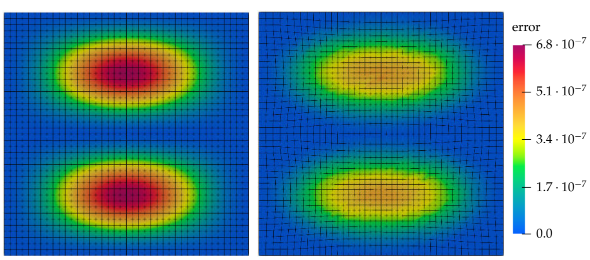

Figure 1: Finite element error before(left) and after(right) mesh optimization

3.2 Randomly perturbed initial mesh The previous example is repeated with a randomly perturbed initial mesh. The finite element errors over the domain Ω, before and after optimization, are presented in Figure 2. The convergence of the objective value as well as its scaled contributions $\mathcal{F}_\mu$ and $w_{\mathrm{u}}\mathcal{F}_{\mathrm{u}}(\mathrm{x},\mathrm{u}(\mathrm{x}))$ are presented in Figure 3.

3.3 Alternative Objective Norms The method is not restricted to the objective formulation of $\mathcal{F}_{\mathrm{u}}$ given in (2.3). We have explored alternative norms, including cases involving error estimators when the exact solution is unknown — a critical capability for practical computations. Next we outline several alternative objective formulations we have implemented.

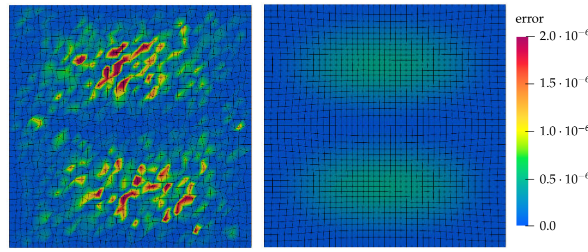

Figure 2: Meshes and finite element errors before (left) and after (right) mesh optimization.

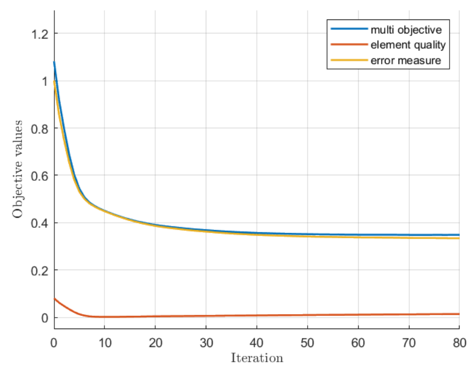

Figure 3: Convergence of optimization problem

H^1-semi norm

$$
\mathcal{F}_{\mathrm{u}}(\mathrm{x},\mathrm{u}(\mathrm{x})) = \int_\Omega (\nabla\mathrm{u} - \nabla\mathrm{u}^*)^2\ d\Omega,
\tag{3.8}
$$

with derivatives

$$
\begin{aligned}
\frac{\mathcal{F}_{\mathrm{u}}}{d\mathrm{u}} &= \int_\Omega 2\cdot(\nabla\mathrm{u} - \nabla\mathrm{u}^*)\,\frac{dN}{d\mathrm{x}}\ d\Omega \\
&= \int_\Omega 2\cdot\left(\frac{dN}{d\mathrm{x}}\hat{\mathrm{u}} - \nabla\mathrm{u}^*\right)\frac{dN}{d\mathrm{x}}\ d\Omega.
\end{aligned}
\tag{3.9}
$$

Zienkiewich-Zhu norm When the exact solution u^* is not known, a common practice is to employ error estimators, such as the Zienkiewicz-Zhu norm, defined as:

$$
\mathcal{F}_{\mathrm{u}}(\mathrm{x},\mathrm{u}(\mathrm{x})) = \int_\Omega (\nabla\mathrm{u} - \mathcal{G}(\mathrm{u}))^2\ d\Omega,
\tag{3.10}
$$

with

$$
\mathcal{G}(\mathrm{u}) = \frac{\sum_e \sum_{i\in Nodes\in e} \frac{dN_i}{d\mathrm{x}}\hat{\mathrm{u}}N_i}{\sum_e \sum_{i\in Nodes\in e} N_i}.
\tag{3.11}
$$

The derivatives of $\mathcal{F}_{\mathrm{u}}$ are:

$$\frac{\mathcal{F}_{\mathrm{u}}}{d\mathrm{u}} = \int_\Omega 2\left(\nabla \mathrm{u} - \mathcal{G}(\mathrm{u})\right)\left(\frac{dN}{d\mathrm{x}} - \frac{d\mathcal{G}(\mathrm{u})}{d\mathrm{u}}\right) d\Omega$$
$$= \int_\Omega 2\left(\frac{dN}{d\mathrm{x}}\hat{\mathrm{u}} - N\hat{\mathcal{G}}(\mathrm{u})\right)\left(\frac{dN}{d\mathrm{x}} - N\frac{\sum_{e,i}\frac{dN_i}{d\mathrm{x}}N_i}{\sum_{e,i}N_i}\right) d\Omega. \tag{3.12}$$

Norm based on average element value This is another approach when the exact solution u^* is not known:

$$\mathcal{F}_{\mathrm{u}}(\mathrm{x}, \mathrm{u}(\mathrm{x})) = \int_\Omega (\mathrm{u} - \mathcal{B}(\mathrm{u}))^2 \ d\Omega, \tag{3.13}$$

with scalar $\mathcal{B}(\mathrm{u})$:

$$\mathcal{B}(\mathrm{u})|_{\Omega^e} = \frac{\int_{\Omega^e} u}{\int_{\Omega^e} 1}. \tag{3.14}$$

The derivatives of $\mathcal{F}_{\mathrm{u}}$ are:

$$\frac{\mathcal{F}_{\mathrm{u}}}{d\mathrm{u}} = \int_\Omega 2(\mathrm{u} - \mathcal{B}(\mathrm{u}))\left(N - \frac{d\mathcal{B}(\mathrm{u})}{d\mathrm{u}}\right) \ d\Omega$$
$$= \int_\Omega 2\cdot(N\hat{\mathrm{u}} - \mathcal{B}(\mathrm{u}))\left(N - \frac{\int_{\Omega^e} N}{\int_{\Omega^e} 1}\right) \ d\Omega. \tag{3.15}$$

4 Conclusion

This brief note outlines ongoing work on a mesh adaptation method that integrates the Target-Matrix Optimization Paradigm with adjoint sensitivity analysis. Preliminary results demonstrate the method's potential to reduce PDE solution errors and optimize PDE-dependent metrics. Future efforts will focus on extending the approach to a broader range of PDEs and more complex physical scenarios.

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