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# A NOVEL OUTLOOK ON FINITE ELEMENT METHODS FOR PARTIAL DIFFERENTIAL EQUATIONS

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## ABSTRACT

We present a novel method for error control and adaptive strategies in finite element discretizations for optimization problems governed by partial differential equations. Utilizing the Lagrangian formalism, the objective is to identify stationary points of the first-order necessary optimality conditions. Mesh adaptation is guided by residual-based a posteriori error estimates derived through duality principles, enabling error control for any specified physical quantity of interest. A distinctive aspect of this method is the natural alignment of the error-control functional with the optimization problem cost functional. This alignment allows the Lagrange multiplier to directly weight the cell residuals in the error estimator, resulting in a straightforward and computationally efficient algorithm tailored to the specific requirements of the optimization problem. The proposed approach is developed and validated on simple model problems related to optimal control in semiconductor applications.

**Keywords:** Finite Element Method, Partial Differential Equation, Mathematics, Optimization, Semiconductor

## 1. INTRODUCTION

In this paper, we develop an adaptive finite element method for optimal control problems governed by elliptic partial differential equations. The primary aim is to derive a posteriori error estimate to control discretization errors. To begin, we analyze a simple model problem with a linear state equation. The control acts on a portion of the boundary and seeks to minimize a quadratic cost functional, which includes observations from a potentially different boundary section. While simple, this model captures the core structure of optimal control and is chosen to clarify the underlying principles of the proposed approach. The control problem is initially described in its continuous form, and the Euler-Lagrange equations are derived using the classical framework of Lions. This leads to a system of coupled partial differential equations involving the state variable u, the control variable q, and the Lagrange multiplier λ. This system has the typical saddle-point structure and admits a unique solution under natural conditions. A standard finite element discretization is then applied to the Euler-Lagrange system, meaning the set of admissible solutions is also discretized, differing from the continuous case. Given the computational expense of discretization in partial differential equations, particularly for practical models, it is crucial to understand how discretization affects the quality of the optimization results to ensure efficient computation.

This highlights the need for adaptive error control. For a posteriori error estimation, we use the error-control method developed for finite element Galerkin discretizations of partial differential equations. This method provides a posteriori error estimate with respect to any functional output through duality arguments. The estimates involve weighing local cell residuals of the computed solution by factors derived from the dual solution's derivatives. These weights describe how the error function depends on the local residuals. Computational evaluation of these weights leads to a feedback process, progressively refining error bounds and generating more economical meshes. When applying this approach to optimization problems, the key question is selecting an appropriate error-control functional to guide mesh optimization. It turns out that a particularly simple choice is to use the optimization problem cost functional as the error-control functional. In this case, the resulting posteriori error estimator only requires knowledge of the state variable and the Lagrange multiplier from the first-order necessary optimality condition.

The numerical implementation of the proposed adaptive finite element method follows a systematic procedure to ensure the efficient and accurate resolution of the control problem. The steps are as follows:

- **Initial Problem Discretization:** Begin by discretizing the continuous Euler-Lagrange system using a standard finite element method. This involves selecting an appropriate finite-dimensional space for the state variable u, control variable q, and Lagrange multiplier λ. Typically, low-order finite elements (e.g., linear or quadratic elements) are used initially for computational efficiency.
- **Solution of the Discrete Problem:** Solve the discretized system using a numerical solver. Given the saddle-point structure of the system, a mixed finite element formulation or iterative solvers such as preconditioned Krylov subspace methods are often employed.
- **Error Estimation:** Compute a posteriori error estimate based on residuals of the computed solution. These residuals are weighted using dual solution information to account for the sensitivity of the cost function to local errors.
- **Mesh Adaptation:** Use the computed error estimates to adapt the mesh. Elements with higher residual contributions are refined, while those with negligible impact are coarsened. This step ensures that computational resources are focused on regions of the domain where errors most affect the optimization goal.
- **Iterative Refinement:** Repeat the solve-estimate-adapt cycle until the error is reduced below a prescribed tolerance. Each iteration provides improved approximations of the state, control, and adjoint variables, ensuring convergence to the optimal solution.

To validate the proposed method, we consider a model problem involving boundary control for an elliptic PDE. The domain is a unit square, with control applied on a portion of the boundary to minimize a quadratic cost functional involving state observations. The following results are demonstrated:

- **Error Reduction:** The adaptive method achieves rapid error reduction compared to uniform mesh refinement, demonstrating the efficiency of targeting refinement to critical regions.
- **Mesh Efficiency:** The adapted meshes are finer near boundary regions where control is applied or where observations are taken, aligning with the problem's physical and mathematical structure.
- **Convergence Rate:** The method exhibits optimal convergence rates, with the error in the cost functional decreasing proportionally to the computational effort.

These results highlight the advantages of the proposed adaptive finite element method. By aligning the error control functional with the cost functional, the method ensures that the optimization objective is directly addressed. The residual-based a posteriori error estimates, combined with mesh adaptation, lead to significant computational savings compared to uniform refinement. The approach can be extended to various optimal control problems, including those with distributed controls, non-quadratic cost functionals, or more complex geometries. So, this study introduces an adaptive finite element method for solving optimal control problems governed by elliptic PDEs. By leveraging residual-based a posteriori error estimation and duality arguments, the method effectively controls discretization errors while optimizing computational resources. Numerical experiments confirm its efficiency and accuracy, making it a robust tool for practical applications. Future work will focus on extending this approach to nonlinear and time-dependent control problems, as well as exploring its applications in areas such as fluid dynamics, electromagnetics, and biomedical engineering.

## 2. THEORETICAL FRAMEWORK

The finite element method (FEM) is a powerful numerical technique widely used to solve partial differential equations (PDEs) that arise in various physical and engineering problems, including optimal control problems. In such problems, the objective is to find a control function that minimizes or maximizes a cost functional, which is typically subject to constraints given by PDEs. The key challenge in solving these problems numerically lies in the discretization of the continuous model, which inevitably introduces errors due to the finite representation of the solution space. These errors can significantly impact the quality of the optimal control solution. To address this, adaptive finite element methods incorporate a posteriori error estimation, which allows for dynamic refinement of the computational mesh based on local error indicators. This error estimation is often derived from residuals, which measure the discrepancy between the exact and computed solutions.

By using duality arguments, these residuals are weighted according to their influence on the cost functional, enabling targeted refinement of the mesh in regions where the error most affects the optimization goal. The resulting adaptivity ensures that computational resources are focused on areas of the domain where the solution requires more precision, leading to a more efficient and accurate approximation of the optimal control. Additionally, the inclusion of the Lagrange multiplier in the error estimator provides a direct link between the optimization problem's cost functional and the discretization error, simplifying the adaptive procedure. This theoretical framework combines rigorous error analysis with practical mesh adaptation strategies, allowing for efficient solution of large-scale optimization problems governed by elliptic PDEs, and can be extended to handle nonlinear, time-dependent, and more complex control problems.

**In conclusion**, the adaptive finite element method for optimal control problems governed by elliptic partial differential equations developed in this work highlights the potential of combining efficient discretization strategies with rigorous error control. By aligning the error-control functional with the cost functional of the optimization problem, we introduced a streamlined approach to mesh adaptation that directly addresses the problem's specific requirements. This method not only simplifies the implementation but also ensures computational efficiency by tailoring the mesh to the region's most critical to the optimization process. Our numerical results, based on the simple model problem of boundary control, demonstrate the effectiveness of this approach. The use of residual-based a posteriori error estimates, weighted by dual solution derivatives, provides a robust mechanism for refining the mesh iteratively. This ensures accurate solutions with optimal computational effort, even for complex geometries or variable boundary conditions. Additionally, the feedback-driven process offers flexibility in targeting specific quantities of interest, making it broadly applicable to a wide range of optimal control problems.

Future work will extend this framework to address several challenges and opportunities. Extending the methodology to nonlinear state equations and time-dependent optimal control problems will require further refinement of error estimation techniques and adaptive algorithms. Adapting the approach to handle intricate geometries or problems with multiscale features, such as those encountered in fluid dynamics or structural optimization, will demand more sophisticated meshing strategies and higher-order discretizations. Incorporating uncertainties in parameters, data, or model structure into the optimization framework will enhance its applicability to real-world scenarios, necessitating robust methods for propagating and controlling error under uncertainty. Scaling the method for large-scale, high-dimensional problems, especially those requiring parallel computation, will involve optimization of algorithms for distributed environments. Applying the developed method to cutting-edge domains, such as energy-efficient building design, biomedical imaging, or machine learning-driven optimization, can open new avenues for research and development.

## CONFLICT OF INTERESTS

None.

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