1 Introduction

Title: Efficient aerodynamic shape optimization using adaptive high-order methods

Outline: this project focuses on the development of an efficient shape optimization framework with applications in aerodynamics. The project builds on two techniques in computational fluid dynamics (CFD). The first is adaptive discontinuous Galerkin (DG) methods, which provide efficient and reliable solution of partial differential equations (PDEs) through rigorous error estimation and adaptive mesh refinement. The second is adjoint-based methods for PDE-constrained optimization, which enable efficient optimization of shape optimization problems involving many free-form geometry-deformation parameters. While each topic has seen significant development in the respective communities, the intersection of the two topics, which a limited number of works have explored, presents an opportunity for more automated and efficient aerodynamic shape optimization. In this work, we explore multi-/variable-fidelity optimization. We will develop algorithms that adaptively control the accuracy of the PDE solver during the optimization process (i) to reduce the PDE solution cost and (ii) to satisfy both the solution accuracy and optimality condition to an arbitrary user-prescribed tolerance at termination. We will formulate, implement, and analyze variable-fidelity optimization strategies and assess the strategies using increasingly difficult aerodynamics shape optimization problems, ranging from the Euler to Reynolds-averaged Navier-Stokes flows, from subsonic to transonic regimes, and from low-dimensional to high-dimensional geometry parametrizations.

Some references. You should be able to find all papers in acelibrary. The references in parentheses are important, but perhaps are not most accessible, so I would start with items not in parentheses.

- CFD vision papers: it is always important to keep a high-level picture of our research goal. These papers provide a review of current state of CFD.
 - NASA review [8]
 - high-order methods review [9]
- FEM, PDEs, and scientific computing: much of the literature requires basic understanding of FEM and scientific computing.
 - FEM: AER1418 lecture notes
 - PDE: ESC384 lecture notes
 - Scientific computing: AER336 lecture notes
 - All notes are available at http://arrow.utias.utoronto.ca/~myano/teaching.html.
- DG:
 - general review [5]
 - most accessible presentation of BR2 [3]
 - (elliptic equations review [1])
 - (aerodynamics review [2])
- output error estimation:
 - aerodynamics review [6]
 - (general review [4])
- optimization
 - textbook [7]

2 Exercise 1. FE approximation of parametrized reaction-diffusion equation

We first introduce a physical domain $\Omega \equiv (0,1) \subset \mathbb{R}^1$ and a parameter domain $\mathcal{D} \equiv (10^{-4},10^{-1}) \subset \mathbb{R}^1$. We then consider the following reaction-diffusion equation with a parametrized diffusion coefficient: given $\mu \in \mathcal{D}$, find $u(\mu) : \Omega \to \mathbb{R}$ such that

$$-\mu \Delta u(\mu) + u(\mu) = 1$$
 in Ω
 $u(\mu) = 0$ on $\partial \Omega$,

and evaluate the output (i.e., quantity of interest)

$$s(\mu) \equiv \int_{\Omega} (1 - u(\mu)) dx.$$

- Q1. Rewrite the problem in weak form. Identify the test and trials spaces, (parametrized) bilinear form, and linear form.
- **Q2.** Is the weak form of the PDE well posed for all $\mu \in \mathcal{D}$?
- Q3. Find an analytical expression for $u(x;\mu)$. How does the solution vary as a function of μ ?
- **Q4.** Write a 1d FEM code that find the solution $u(\cdot, \mu)$ and the output $s(\mu)$ for any given $\mu \in \mathcal{D}$.
- Q5. Repeat the above exercise within the femmat framework.

 Note. Use example/poisson1d_intro.m as the starting example.
- **Q6.** For \mathbb{P}^1 (linear) and \mathbb{P}^2 (quadratic) FE methods and $\mu = 1/100$, evaluate the $H^1(\Omega)$ and $L^2(\Omega)$ norm of the error for a sequence of uniformly refined meshes. Plot error vs dof in log-log scale. Does the observed convergence rate match the theory?
- **Q7.** Repeat the same exercise as the above for the output error $|s(\mu) s_h(\mu)|$.
 - Reading: Chapters 1–4 of the AER1418 notes. I would start with Chapter 1. Then, it might make sense to start reading Chapter 3 and then read parts of Chapter 2 that are required to make sense of Chapter 3 as necessary. Similarly, I would start on femmat implementation and read parts of Chapter 4 as necessary.

3 Exercise 2. Optimization of the reaction-diffusion equation

Throughout this exercise, we consider the following optimization problem:

$$\begin{split} \min_{\mu \in \mathcal{D}} |s_{\text{target}} - s(\mu)|^2 \\ \text{subject to} \quad &- \mu \Delta u(\mu) + u(\mu) = 1 \quad \text{in } \Omega, \\ u(\mu) = 0 \quad \text{on } \partial \Omega. \end{split}$$

Use \mathbb{P}^2 FE with a reasonably refined mesh such that the FE approximation error is small.

- Q1. Solve the optimization problem using (i) the FE discretization and (ii) gradient-free optimizer in Matlab. (This will be slow and require many function evaluations.)
- **Q2.** We wish to solve the problem using (i) the FE discretization and (ii) gradient-based optimization method. To this end, we wish to compute the gradient efficiently using the *adjoint method*. Note that algebraically, we can think of the problem as this:

$$J(\mu) = q(u(\mu); \mu)$$

s.t. $R(u(\mu); \mu) = 0$.

To compute $\frac{\partial J}{\partial u}$, we recognize that

$$\frac{\partial J}{\partial \mu} = \frac{\partial q}{\partial u} \frac{\partial u}{\partial \mu} + \frac{\partial q}{\partial \mu}.$$

But,

$$\frac{\partial R}{\partial u}\frac{\partial u}{\partial \mu} + \frac{\partial R}{\partial \mu} = 0 \qquad \Rightarrow \qquad \frac{\partial u}{\partial \mu} = -\left(\frac{\partial R}{\partial u}\right)^{-1}\frac{\partial R}{\partial \mu},$$

and hence

$$\frac{\partial J}{\partial \mu} = -\frac{\partial q}{\partial u} \left(\frac{\partial R}{\partial u} \right)^{-1} \frac{\partial R}{\partial \mu} + \frac{\partial q}{\partial \mu} = -\psi^T \frac{\partial R}{\partial \mu} + \frac{\partial q}{\partial \mu},$$

where the adjoint ψ satisfies $\left(\frac{\partial R}{\partial u}\right)^T \psi = \left(\frac{\partial q}{\partial u}\right)^T$. Implement the adjoint method to compute the gradient, and validate the implementation against finite difference.

Q3. Solve the problem using (i) the FE discretization and (ii) gradient-based optimization method.

4 Exercise 3. Multi-parameter nonlinear reaction-diffusion equation

We first introduce a physical domain $\Omega \equiv (0,1) \subset \mathbb{R}^1$ and a P-dimensional parameter domain $\mathcal{D} \equiv (10^{-4},10^{-1})^P \subset \mathbb{R}^1$. We in addition introduce P subdomains $\Omega_i = ((i-1)/P,i/P), i=1,\ldots,P$. We then consider the following nonlinear reaction-diffusion equation with a parametrized diffusion coefficient: given $\mu \in \mathcal{D}$, find $u(\mu) \in H_0^1(\Omega)$ such that

$$-\nabla \cdot (\mu_i \nabla u(\mu)) + u(\mu)^3 = 1 \quad \text{in } \Omega_i, \quad i = 1, \dots, P,$$

$$u(\mu) = 0 \quad \text{on } \partial \Omega$$

and evaluate the output (i.e., quantity of interest)

$$s(\mu) \equiv \int_{\Omega} (1 - u(\mu)) dx.$$

- Q1. Write the weak form of the problem.
- **Q2.** Write a 1d FEM code that find the solution $u(\cdot; \mu)$ and the output $s(\mu)$ for any given $\mu \in \mathcal{D}$.
- **Q3.** Optimization ...

References

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