Adjoint-Based Optimization, Uncertainty Quantification, and Data Assimilation of Multiphysics Systems using High-Order Numerical Discretizations

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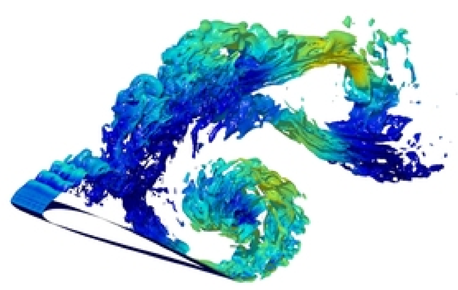
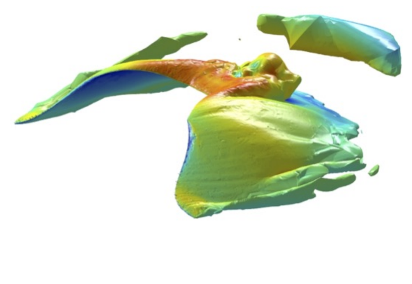
Abstract

An adjoint-based optimization framework for multiphysics problems governed by coupled partial differential equations is presented. High-order spatio-temporal discretizations are used for the underlying PDE and quantity of interest to obtain highly accurate simulations at a reasonable cost. The corresponding fully discrete adjoint equations are used to yield very precise gradients of quantities of interest. The deterministic optimization framework is extended to address the challenges posed by stochastic optimization where the input data for the PDE is not known with certainty. Such problems require an ensemble of primal and adjoint solves at each optimization iteration and dramatically increases the computational cost. To address this issue, a globally convergent multifidelity optimization framework is presented that is capable of reducing the cost of solving stochastic optimization problems by several orders of magnitude. Finally, a novel optimization-based framework is presented for solving PDEs with discontinuous solutions to high-order accuracy.



Motivation and Impact

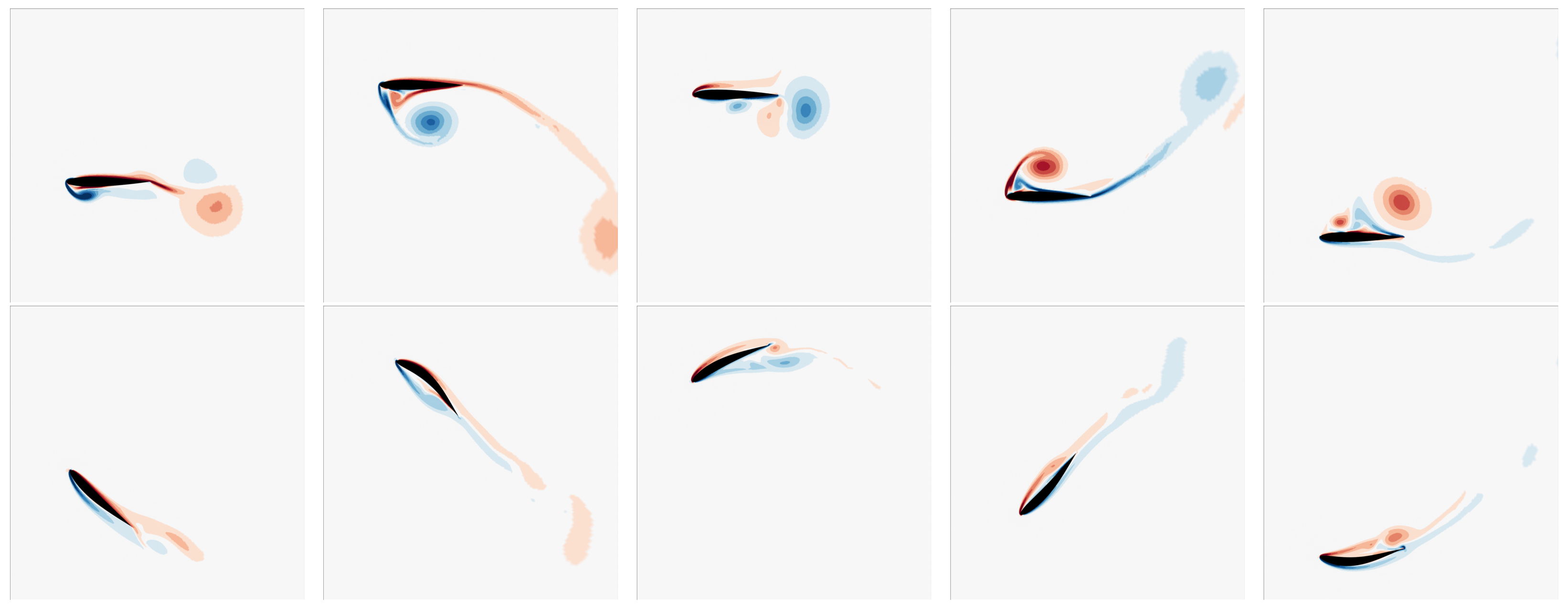
- Optimization problems governed by partial differential equations are ubiquitous in science and engineering and robust, efficient, and effective solutions of these problems can lead to improved designs or discovery not otherwise possible. We have leveraged the proposed methods to study energetically optimal flight and optimal energy harvesting mechanisms, among other problems.
- Outside of the traditional context of design and control, PDE-constrained optimization can lead to improved computational models through *data assimilation*, where the parameters of a model are inferred by optimally matching the simulation result to measured data. The proposed optimization framework has been used to enhance the resolution of magnetic resonance images.
- The combination of optimization and uncertainty quantification is critical since, in reality, we generally seek optimal and *risk-averse* designs that are robust with respect to uncertainties in the operating conditions.



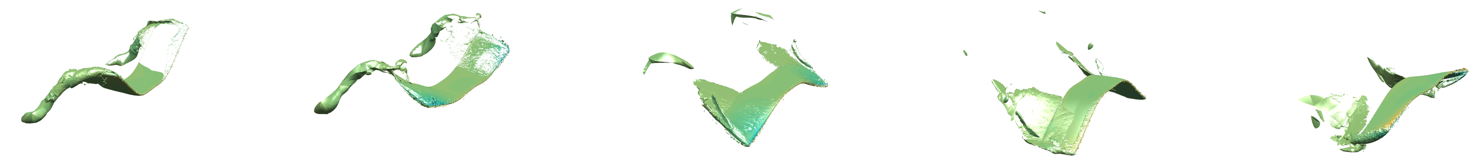
High-Order Adjoint-Based Optimization

- We propose a globally high-order framework for solving optimization problems governed by deforming domain conservation laws using gradient-based methods.
- The conservation law is transformed to a fixed domain using the Arbitrary Lagrangian-Eulerian formulation and discretized to high-order using discontinuous Galerkin in space and diagonally implicit Runge-Kutta in time. Quantities of interest are discretized in solver-consistent manner.
- The corresponding *fully discrete adjoint method* is derived and implemented to yield exact gradients of the optimization functional.

Energetically optimal flapping motions [3, 4]

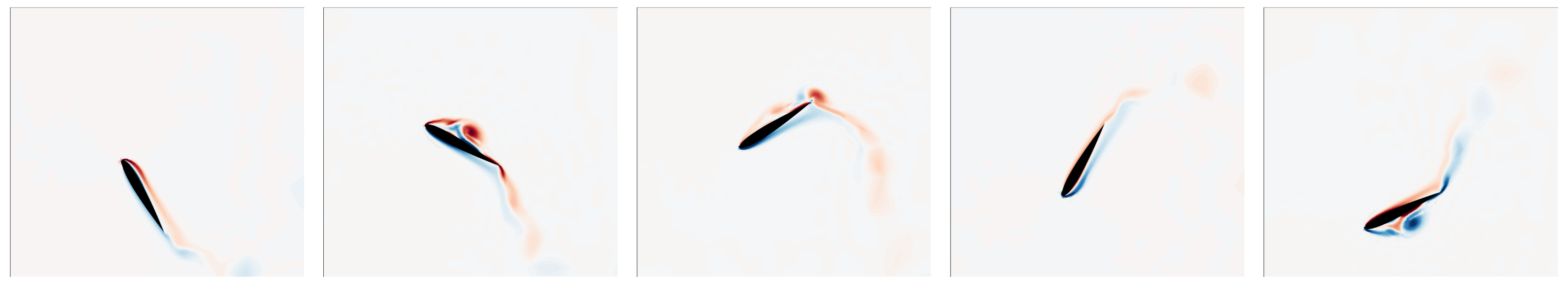


Flow vorticity around flapping airfoil undergoing pure heaving motion (*top*) and an energetically optimal motion under a thrust constraint of $T_x = 2.5$ (*bottom*). Snapshots are taken at five equally spaced time instances.



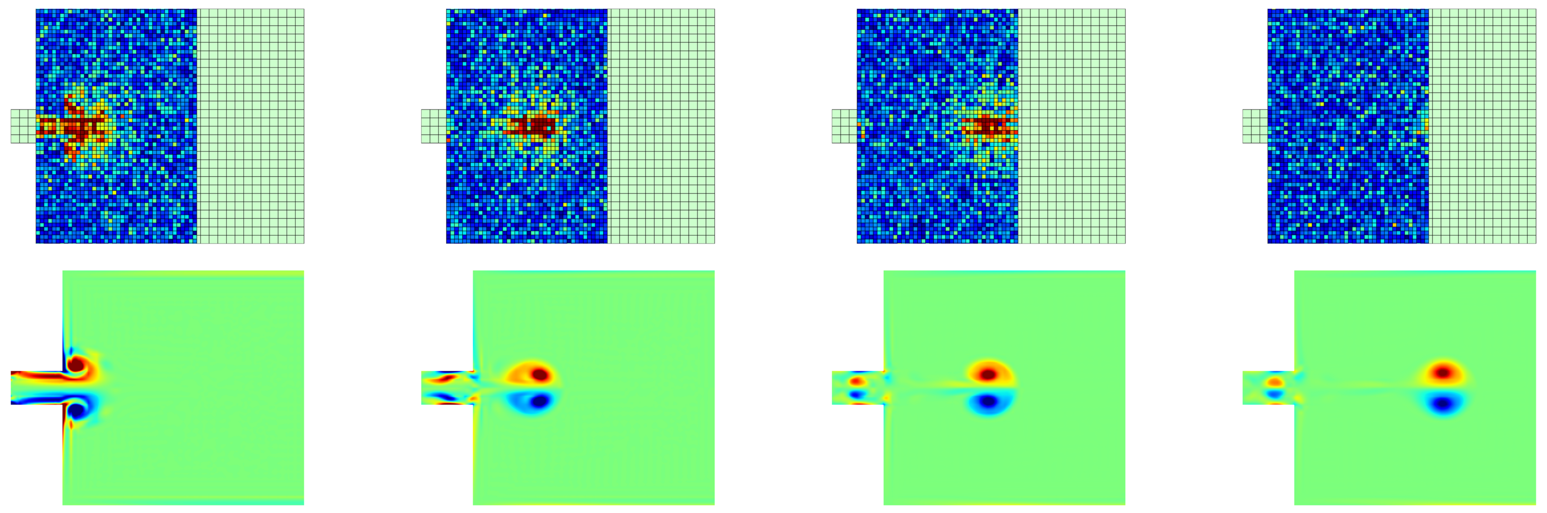
Visualization of the flow field around 3D flapping wing corresponding to the energetically optimal motion at neutral thrust ($T_x = 0$). Snapshots are taken at six equally spaced time instances.

Optimal energy harvesting mechanism



Flow vorticity around flapping airfoil-damper system undergoing an optimal pitching trajectory that maximizes energy stored in the damper given limited available input energy $E_\theta \leq 0.15$. Snapshots are taken at five equally spaced time instances.

Data assimilation to enhance Magnetic Resonance Images (MRIs)

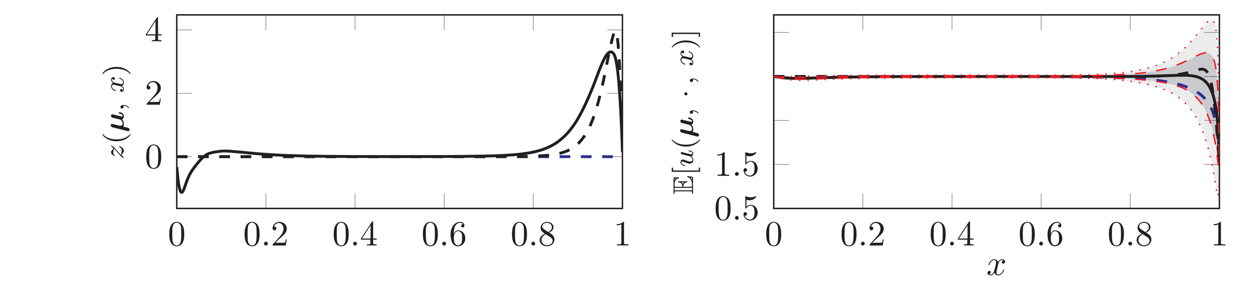


Top: MRI voxel data with 10% noise overlay on vortex tank domain and mesh at 4 instances in time. *Bottom*: Reconstructed flow in vortex tank at same 4 time instances, obtained using adjoint-based optimization framework for data assimilation to determine correct inflow boundary condition.

Stochastic Optimal Control

- In many science and engineering settings, it is not sufficient to merely find an optimal solution, rather an optimal solution that is *risk-averse* or *robust* w.r.t. the uncertainties of the input.
- However, the merging of uncertainty quantification and optimization leads to extremely expensive methods since every optimization iteration requires an *ensemble* of PDE solves to integrate risk measures over the stochastic space.
- We propose a framework that incorporates two sources of inexactness in the stochastic PDE-constrained optimization process to reduce the overall computational burden: anisotropic sparse grids to efficiently approximate integrals over the stochastic dimension and reduced-order models to reduce the cost of PDE solves. Global convergence guaranteed by managing inexactness with trust-region method [1].

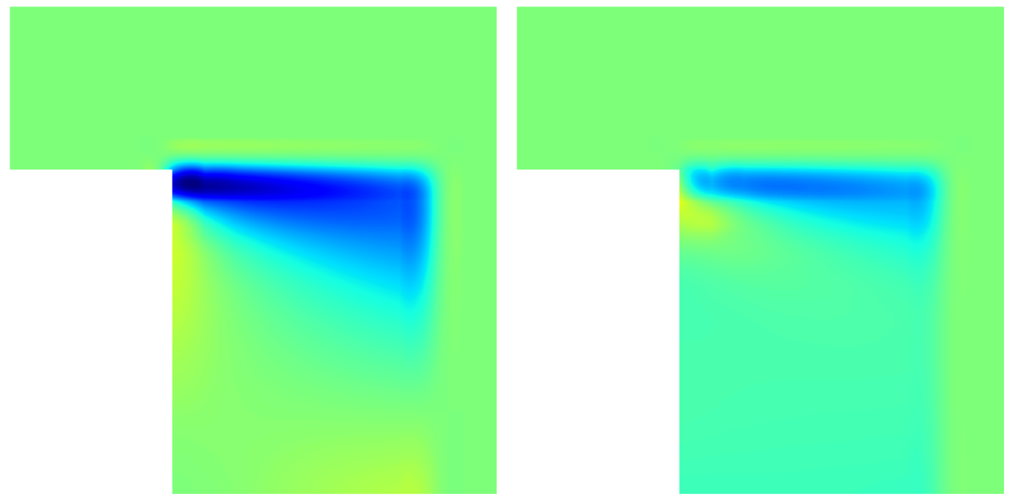
Viscous Burgers' Equation



Left: the control defining the initial guess for the optimal control for the viscous Burgers' equation (- - -), the solution of the deterministic optimal control problem (- - -), and the solution of the stochastic optimal control problem (——). *Right*: the mean solution of the viscous Burgers' equation at the initial control (- - -), optimal deterministic control (- - -), and the optimal stochastic control. One (- - -) and two (······) standard deviations about the mean solution corresponding to the optimal stochastic control are also included.

	#HDM (ndof)	#ROM (mean size)
HDM opt	31064 (500)	-
ROM opt	45 (500)	3320 (42)

Incompressible Navier-Stokes Equation



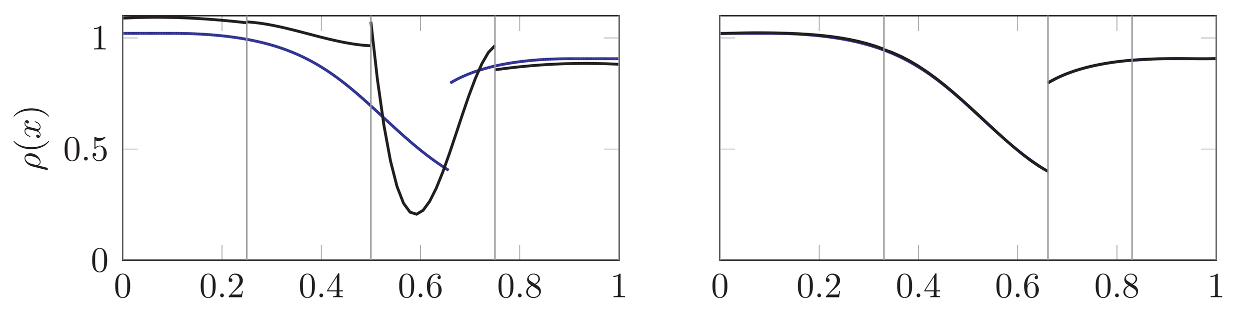
The vorticity of the incompressible Navier-Stokes equations corresponding to a traditional backward-facing step (*left*) and that corresponding to the solution of the risk-neutral optimal boundary control problem that seeks to minimize the magnitude of the vorticity in the re-circulation region by injecting fluid along the vertical edge of the step (*right*).

High-Order Shock Tracking

- The problem of finding (numerically) the solution of conservation laws when the solution contains discontinuities or sharp gradients has been a longstanding difficulty, particularly when high-order methods are used.
- This difficulty usually arises from using a polynomial basis to capture a discontinuous feature, which is likely to exhibit Gibbs' phenomena, particularly for high polynomial orders.
- However, the inter-element solution discontinuities supported by discontinuous Galerkin (dG) and Finite Volume (FV) discretizations provides a convenient way to capture discontinuous features *if the mesh can be aligned with such features.*
- We propose an **optimization-based, r-adaptivity** framework [2] that looks to *find the discretized dG/FV solution* $\boldsymbol{u}$ *and nodal positions of the computational mesh* $\boldsymbol{x}$ *that simultaneously satisfy the discretized conservation law* $\boldsymbol{r}(\boldsymbol{u}; \boldsymbol{x}) = 0$ *and minimize some measure of the Gibbs' phenomena*

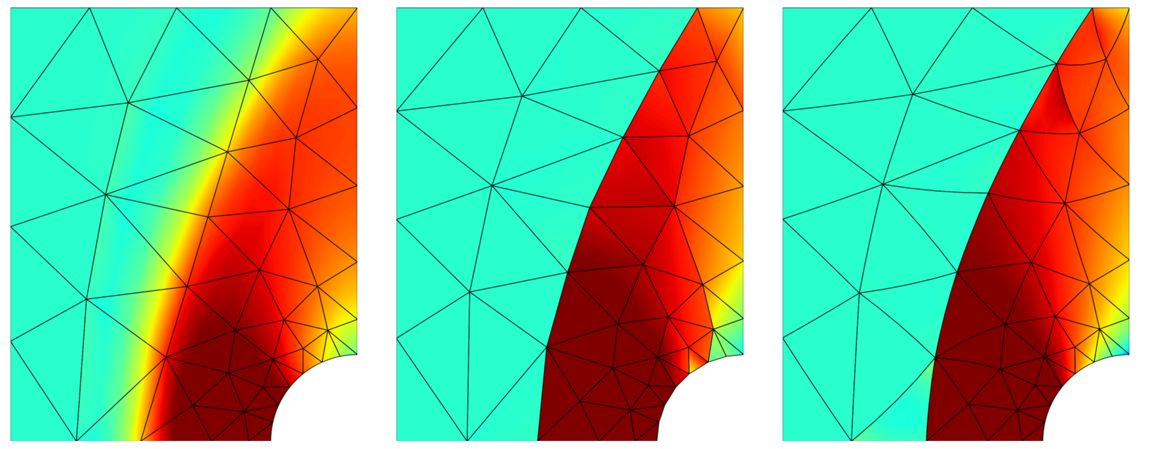
$$\underset{\boldsymbol{u}, \boldsymbol{x}}{\text{minimize}} \quad f(\boldsymbol{u}; \boldsymbol{x}) \qquad \text{subject to} \quad \boldsymbol{r}(\boldsymbol{u}; \boldsymbol{x}) = 0.$$

Quasi-1D Euler Equations



The solution of the quasi-1d Euler equations using 300 linear elements (——) and 4 quartic elements (——). The vertical lines (——) indicate the element boundaries. *Left*: The high-order elements are not aligned with the shock and cause substantial over/under-shoot. *Right*: The high-order dG shock tracking framework is applied to align the high-order elements with the shock and the resulting solution matches the 300 element reference solution very well, with substantially fewer degrees of freedom.

2D Euler Equations, Supersonic Regime



The solution of the 2d Euler equations using: 67 quadratic elements on a mesh not aligned with the shock (*left*), 67 linear elements on a mesh aligned with the shock (*middle*), 67 quadratic elements on a mesh aligned with the shock (*right*). The shock-aligned meshes and corresponding solution were obtained using the high-order dG shock tracking framework.

Conclusions and future work

- This work presented an adjoint-based optimization framework for multiphysics problems using high-order, partitioned spatio-temporal methods.
- A multifidelity framework that leverages adaptive sparse grids and reduced-order models was developed to extend this deterministic framework to stochastic optimization problems. The method is several orders of magnitude faster than traditional approaches to solve such problems.
- A full space PDE-constrained optimization framework was developed to resolve discontinuities with high-order accuracy by aligning the underlying mesh with the discontinuities. This was demonstrated on the quasi-1D and 2D Euler equations, where the entire flow field, including the discontinuity, were very well resolved on extremely coarse, high-order meshes.
- In the upcoming months, we intend to team with application experts to solve relevant science and engineering optimization problems. We also intend to further develop the shock tracking method, which is in its infancy, by devising an efficient full space solver for the optimization problem and test the method of 3D problems.

Technical capabilities and challenges

Capabilities: We currently have a modular, extensible PDE-constrained optimization framework and codebase that can be adopted by other groups. Additionally, we are among the first to successfully align high-order meshes with discontinuous feature and recover high-order convergence for these problems, which should prove useful for groups interested in high-speed conservation laws.
Challenges: The development of the full space nonlinear optimization method required for a large-scale implementation of our shock tracking method would benefit from the expertise of an expert in optimization theory; we are currently uses SNOPT as a solver.

References

[1] Matthew J. Zahr. *Adaptive model reduction to accelerate optimization problems governed by partial differential equations.* PhD thesis, Stanford University, August 2016.

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[3] Matthew J. Zahr and Per-Olof Persson. An adjoint method for a high-order discretization of deforming domain conservation laws for optimization of flow problems. *Journal of Computational Physics*, 2016.

[4] Matthew J Zahr and Per-Olof Persson. Energetically optimal flapping wing motions via adjoint-based optimization and high-order discretizations. In *Frontiers in PDE-Constrained Optimization*. Springer, 2017.

Acknowledgments

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