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An adjoint method for a high-order discretization of deforming domain conservation laws for optimization of flow problems

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ABSTRACT

The fully discrete adjoint equations and the corresponding adjoint method are derived for a globally high-order accurate discretization of conservation laws on parametrized, deforming domains. The conservation law on the deforming domain is transformed into one on a fixed reference domain by the introduction of a time-dependent mapping that encapsulates the domain deformation and parametrization, resulting in an Arbitrary Lagrangian–Eulerian form of the governing equations. A high-order discontinuous Galerkin method is used to discretize the transformed equation in space and a high-order diagonally implicit Runge–Kutta scheme is used for the temporal discretization. Quantities of interest that take the form of space–time integrals are discretized in a solver-consistent manner. The corresponding fully discrete adjoint method is used to compute *exact* gradients of quantities of interest along the manifold of solutions of the fully discrete conservation law. These quantities of interest and their gradients are used in the context of gradient-based PDE-constrained optimization.

The adjoint method is used to solve two optimal shape and control problems governed by the isentropic, compressible Navier–Stokes equations. The first optimization problem seeks the energetically optimal trajectory of a 2D airfoil given a required initial and final spatial position. The optimization solver, driven by gradients computed via the adjoint method, reduced the total energy required to complete the specified mission nearly an order of magnitude. The second optimization problem seeks the energetically optimal flapping motion and time-morphed geometry of a 2D airfoil given an equality constraint on the x-directed impulse generated on the airfoil. The optimization solver satisfied the impulse constraint to greater than 8 digits of accuracy and reduced the required energy between a factor of 2 and 10, depending on the value of the impulse constraint, as compared to the nominal configuration.

1. Introduction

Optimization problems constrained by Partial Differential Equations (PDEs) commonly arise in engineering practice, particularly in the context of design or control of physics-based systems. A majority of the research in PDE-constrained

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optimization has been focused on *steady* or *static* PDEs, with a large body of literature detailing many aspects of the subject, including continuous and discrete adjoint methods [1–5], parallel implementations [6,7], one-shot or infeasible path methods [6,8], and generalized reduced gradient or feasible path methods [1,9]. This emphasis on steady problems is largely due to the fact that (a) static analysis is sufficient for a large class of problems of interest and (b) unsteady analysis is expensive to perform in a many-query setting, such as optimization [10]. However, there is a large class of problems where steady analysis is insufficient, such as problems that are inherently dynamic and problems where a steady-state solution does not exist or cannot be found reliably with numerical methods. Flapping flight is an example of the first type, a fundamentally unsteady problem that has become increasingly relevant due to its application to Micro-Aerial Vehicles (MAVs) [11]. Systems with chaotic solutions, such as those encountered in turbulent flows, are an example of the second type of problems where steady analysis breaks down. Design and control of these types of systems calls for *time-dependent* PDE-constrained optimization of the form

$$\begin{aligned} \underset{\boldsymbol{U},\,\boldsymbol{\mu}}{\text{minimize}} \quad & \int_0^T \int_{\boldsymbol{\Gamma}} j(\boldsymbol{U},\boldsymbol{\mu},t)\,dS\,dt \\ \text{subject to} \quad & \int_0^T \int_{\boldsymbol{\Gamma}} \boldsymbol{c}(\boldsymbol{U},\boldsymbol{\mu},t)\,dS\,dt \leq 0 \\ & \frac{\partial \boldsymbol{U}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{U},\nabla \boldsymbol{U}) = 0 \end{aligned} \tag{1}$$

where the last constraint corresponds to a system of conservation laws with solution $\boldsymbol{U}$, parametrized by $\boldsymbol{\mu}$; the objective and constraint functions of the optimization take the form of space–time integrals of pointwise, instantaneous quantities of interest j and $\boldsymbol{c}$ over the surface of the body $\boldsymbol{\Gamma}$.

In this work, the large computational cost associated with time-dependent PDE-constrained optimization will be addressed by two means. The first is the development of a *globally high-order* numerical discretization of conservation laws on deforming domains.[1] For many important problems, high-order methods have been shown to require fewer spatial degrees of freedom [12] and time steps [13,14] for a given level of accuracy compared to low-order methods. Highly accurate quantities of interest, usually the time-average of a relevant surface- or volume-integrated quantity, is paramount, at least at convergence, since they drive the optimization trajectory through the objective function and constraints. Large errors in quantities of interest will cause the optimization procedure to be driven by discretization errors causing termination at a suboptimal design/control. The second approach to reduce the computational impact of time-dependent optimization is the use of gradient-based optimization techniques due to their rapid convergence properties, particularly when compared to derivative-free alternatives.

An efficient technique for computing derivatives of optimization functionals, required by gradient-based optimization solvers, is the *adjoint method*. It has proven its utility in the context of output-based mesh adaptivity and gradient-based PDE-constrained optimization as only a single linearized dual solve is required to compute the gradient of a single quantity of interest with respect to any number of parameters. In the context of partial differential equations, the adjoint equations can be derived at either the continuous, semi-discrete, or fully discrete level. The fully discrete adjoint method will be the focus of this work as it ensures discrete consistency [5,10] of computed gradients, i.e. the gradient of the discrete solution, including discretization errors, is computed. Discrete consistency is beneficial in the context of gradient-based optimization as inconsistent gradients may cause convergence of black-box optimizers to be slowed or hindered [15], unless specialized optimization algorithms are employed that handle gradient inexactness [16].

In this work, a *globally high-order* numerical discretization of general systems of conservation laws, defined on deforming domains, is introduced and the corresponding fully discrete adjoint equations derived. The goal is to harness the advantages of high-order methods in the context of *gradient-based* optimization. The solution of the adjoint equations – the dual solution – will be used to construct exact gradients of fully discrete quantities of interest. A Discontinuous Galerkin Arbitrary Lagrangian–Eulerian (DG-ALE) method [17] is used for the high-order spatial discretization. Previous work on the adjoint method for conservation laws on deforming domains predominantly considers a Finite Volume (FV) spatial discretization [1–4,18,13,5,19], and recently extended to DG-ALE schemes [20–22]. The DG-ALE discretization is chosen rather than FV due to its stable, high-order discretization of convective fluxes. The Geometric Conservation Law (GCL) is satisfied in the DG-ALE scheme through the introduction of an element-level auxiliary equation. The fully discrete adjoint equations derived in this work fully incorporate this GCL augmentation [23], ensuring discrete consistency is maintained.

High-order temporal discretization will be achieved using a Diagonally Implicit Runge–Kutta (DIRK) [24] method, marking a departure from previous work on unsteady adjoints, which has mostly considered temporal discretization via Backward Differentiation Formulas (BDF) [9,18,13,19,22,25], with some work on space–time DG discretizations [23]. Apart from being limited to second-order accuracy, if A-stability is required, high-order BDF schemes require special techniques for initialization [14]. While DIRK schemes require additional work to achieve high-order convergence in the form of additional nonlinear

[1] As with all works on high-order methods, high-order accuracy relies on sufficient regularity in the solution.