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A practical discrete-adjoint method for high-fidelity compressible turbulence simulations

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ABSTRACT

Methods and computing hardware advances have enabled accurate predictions of complex compressible turbulence phenomena, such as the generation of jet noise that motivates the present effort. However, limited understanding of underlying physical mechanisms restricts the utility of such predictions since they do not, by themselves, indicate a route to design improvements. Gradient-based optimization using adjoints can circumvent the flow complexity to guide designs, though this is predicated on the availability of a sufficiently accurate solution of the forward and adjoint systems. These are challenging to obtain, since both the chaotic character of the turbulence and the typical use of discretizations near their resolution limits in order to efficiently represent its smaller scales will amplify any approximation errors made in the adjoint formulation. Formulating a practical exact adjoint that avoids such errors is especially challenging if it is to be compatible with state-of-the-art simulation methods used for the turbulent flow itself. Automatic differentiation (AD) can provide code to calculate a nominally exact adjoint, but existing general-purpose AD codes are inefficient to the point of being prohibitive for large-scale turbulence simulations. Here, we analyze the compressible flow equations as discretized using the same high-order workhorse methods used for many high-fidelity compressible turbulence simulations, and formulate a practical space–time discrete-adjoint method without changing the basic discretization. A key step is the definition of a particular discrete analog of the continuous norm that defines our cost functional; our selection leads directly to an efficient Runge–Kutta-like scheme, though it would be just first-order accurate if used outside the adjoint formulation for time integration, with finite-difference spatial operators for the adjoint system. Its computational cost only modestly exceeds that of the flow equations. We confirm that its accuracy is limited by computing precision, and we demonstrate it on the aeroacoustic control of a mixing layer with a challengingly broad range of turbulence scales. For comparison, the error from a corresponding discretization of the continuous-adjoint equations is quantified to potentially explain its limited success in past efforts to control jet noise. The differences are illuminating: the continuous-adjoint is shown to suffer from exponential error growth in (reverse) time even for the best-resolved largest turbulence scales. Implications for jet noise reduction and turbulence control in general are discussed.

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1. Introduction

Adjoint-based methods are attractive and have been used for several purposes in conjunction with simulations of fluid flow, including optimal flow control [1], aerodynamic shape design [2,3], goal-oriented mesh refinement [4], sensitivity-based uncertainty quantification [5], and stability and global mode analysis [6,7]. Our specific efforts are currently directed towards control optimization for turbulent aeroacoustic flows [8], and our demonstration simulations are motivated by this application, which we discuss in some detail. The present work develops an exact space–time adjoint formulation that is practical in that it incurs a computational cost comparable to the flow equations or a direct discretization of their continuous-adjoint. It is also compatible with high-order finite-difference schemes that are the "workhorse" methods for a wide range of compressible flow simulations, including turbulent free-shear flows [9–11], boundary-layer flows [12], and combustion [13]. We show that an exact adjoint is surprisingly important for accurately predicting the sensitivity at all turbulence scales, and that our formulation is computationally efficient and extensible.

The control of sound generation by turbulence provides a particularly challenging target application due to its complexity and the relative subtlety of its noise-generation mechanisms. In aeroacoustic simulations, the computational challenge of representing a range of turbulence scales and the relatively low-amplitude fluctuations is well documented [14,15]. Without a reduced model of noise generation mechanisms to provide guidance, predictions by themselves do not indicate routes to design improvement. Adjoint-based optimization methods used in conjunction with predictive simulations have been proposed and demonstrated to circumvent this complexity by providing gradient information that can be harnessed to achieve noise reductions [8]. In essence, the adjoint carries sensitivity information with respect to an arbitrarily large number of control parameters, which enables the optimization of noise-controlling actuation or geometries. Building on efforts in aerodynamic optimization [16] and incompressible turbulence control [1], Wei and Freund [17] achieved 11 dB noise reduction of far-field sound with internal energy control of a direct numerical simulation (DNS) of a two-dimensional compressible shear layer. Though the method has been demonstrated to also work in genuinely turbulent three-dimensional flows [18], it has not been so remarkably successful in this case. For example, with an approximate adjoint, Kim et al. [19] reduced the noise from a Mach 1.3 large-eddy simulation turbulent jet by 3.5 dB, which would seem to be a relatively modest amount given the flexibility of their actuation. It is not possible in this case to decouple the limits of control from numerical imprecision.

A straightforward approach to computing the adjoint is to start at the PDE level, derive the analytic adjoint PDE, and discretize the two systems independently. However, this is understood to introduce a particular kind of truncation error since the calculus identities used in the derivation of the adjoint are only approximated by their discrete counterparts. The most obvious approximation is the product rule of differentiation used in the formulations, but in general, boundary treatments and geometric transformations also introduce approximations that lead to an inconsistent adjoint. Thus, the predicted gradient is not fully compatible with the numerical solution; it no longer provides an exact gradient of the discrete system. This issue was previously identified for aerodynamics applications by Nadarajah and Jameson [20], who compare this continuous approach with a discrete-adjoint method, designed to be compatible with the discrete forward model. However, their discretization would not perform well for turbulence simulations. Carnarius et al. [21] showed that discretization errors in the continuous-adjoint-based gradient led to an over-prediction in the minimum drag coefficient for flow around a rotating cylinder. For the chaotic Lorenz system, Lea et al. [22] showed that the adjoint-based gradient suffers from cumulative error growth when the cost functional is a time-averaged quantity over an interval longer than the predictability time scales of the system. This is expected to be an important factor for the turbulent flow we consider, both because turbulence is chaotic and because efficient simulations usually employ resolutions close to the limits of the discretization. The resulting truncation errors will thus be relatively large to start with, before they amplify via the chaotic character of the system. In such situations, the discrete-adjoint method is expected to significantly accelerate and improve optimization. Developing a practical discrete-adjoint method, in the sense that it does not require operation counts or memory much beyond direct discretization of the continuous-adjoint, and demonstrating it on a challenging large-scale turbulent flow simulation are our goals. An inherent limitation of conventional continuous- and discrete-adjoint based formulations is their inability to overcome the chaos of turbulence indefinitely. Fortunately, they can be useful for finite-time-horizon control, and means of reformulating the overall problem to overcome this limitation is a subject of ongoing investigation [5].

In this paper, we derive an exact adjoint of the three-dimensional compressible flow equations discretized with the same high-order schemes commonly used in aeroacoustic simulations, and verify that it provides an exact (aside from finite-precision errors) gradient of the cost functional for the sound radiated by a compressible turbulent mixing layer. These schemes are not locally conservative, but are attractive and effective for the class of flows we consider, particularly because of their resolution. To do this, we make some key advances that facilitate implementation for such discretizations. This is an important step beyond the algorithms that have been developed to do this for aerodynamic simulations. For example, Rumpfkeil and Zingg [23] derived the discrete-adjoint equation for unsteady flows governed by the Euler equations integrated using implicit Euler and second-order backward difference (BDF2) methods; Yamaleev et al. [24] formulated a discrete-adjoint method for optimization using the three-dimensional Reynolds-averaged Navier–Stokes (RANS) equations on dynamic unstructured grids; Wang et al. [25] derived the discrete-adjoint equation for the two-dimensional compressible Euler equations with high-order discontinuous Galerkin discretization and an implicit fourth-order Runge–Kutta scheme; Roth and Ulbrich [26] developed a discrete-adjoint approach based on the sparse forward mode of automatic differentiation for a shape optimization problem incorporating various turbulence models; and Nielsen and Diskin [27] tested the