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Adjoint complement to viscous finite-volume pressure-correction methods

Arthur Stück *, Thomas Rung

Institute for Fluid Dynamics and Ship Theory, Hamburg University of Technology, Schwarzenbergstraße 95C, D-21073 Hamburg, Germany

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ABSTRACT

A hybrid-adjoint Navier–Stokes method for the pressure-based computation of hydrodynamic objective functional derivatives with respect to the shape is systematically derived in three steps: The underlying adjoint partial differential equations and boundary conditions for the frozen-turbulence Reynolds-averaged Navier–Stokes equations are considered in the first step. In step two, the adjoint discretisation is developed from the primal, unstructured finite-volume discretisation, such that adjoint-consistent approximations to the adjoint partial differential equations are obtained following a so-called hybrid-adjoint approach. A unified, discrete boundary description is outlined that supports high- and low-Reynolds number turbulent wall-boundary treatments for both the adjoint boundary condition and the boundary-based gradient formula. The third component focused in the development of the industrial adjoint CFD method is the adjoint counterpart to the primal pressure-correction algorithm. The approach is verified against the direct-differentiation method and an application to internal flow problems is presented.

1. Introduction

Today, decades after the pioneering work of Pironneau [40] and Jameson [18], adjoint methods have reached a wide and growing popularity in applied computational fluid dynamics (CFD) wherever detailed sensitivity information of integral output quantities is required. Though the development of adjoint methods notoriously lags behind the primal CFD, the adjoint sensitivity analysis is successfully used for optimal shape design [19,7,21,1,14,20,44,32,37], topology optimisation [2,10,38,15,37], active and passive flow control [5,26,4], goal-oriented error estimation and grid adaptation [12,16] or convergence error correction [31,29]. These applications are different in the control, but in the majority of works the same engineering output quantities are considered, such as projections of forces and moments [21,1,14,32,36,44,4,16], energy or power-related quantities [37,49,50], homogeneity criteria [38,37,45] or (weighted) deviations [19,21] from predefined states. The adjoint problem can be *either* devised via the continuous [40,18,19,21,43,4,37,49] *or* the discrete-adjoint [1,7,33,34,13,32,36,16] strategy.

1.1. Discretisation

In the *continuous-adjoint* approach, the governing equations and objective functionals are linearised on the level of partial differential equations (PDE) and the corresponding adjoint PDE are developed via integration by parts prior to discretisation. The primal problem being the fluid-dynamic differential constraints (Navier–Stokes equations) and the integral objective

* Corresponding author.
E-mail address: arthur.stueck@tu-harburg.de (A. Stück).

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functional must be compatible so that a continuous-adjoint formulation exists; this is particularly important in the context of boundary conditions and boundary-based objectives. Subsequently, a suitable adjoint discretisation must be chosen, which is often passed over in the literature. Unlike the primal discretisation schemes which have been developed and tuned over the past decades, a comparable experience is usually not available for the adjoint problem. Unless derived with due care (e.g. [28]), the discretisation of the adjoint PDE will not match the transposed (adjoint) of the linearised primal discretisation, so that the calculated derivative will not be the exact derivative of the discrete objective functional calculated by the primal solver on a finite mesh. Simplified adjoint schemes that are of reduced complexity or lower order than the primal discretisation can be chosen to reduce the development time for the adjoint field and boundary operators. Adjoint discretisation schemes can be constructed such that the adjoint solution is stabilised. Moreover, the continuous-adjoint method suggests a boundary-based gradient formula, which is very popular in conjunction with unstructured grids [8,20,43,37]; in that case the boundary deformation does not have to be propagated to the interior mesh.

Alternatively, when a *discrete-adjoint* strategy is pursued, the discrete-adjoint system is directly derived from the linearised discretisation of the primal problem via summation by parts. By definition the exact derivative of the discrete problem is calculated. The discrete-adjoint approach supersedes the search for appropriate discretisation schemes for the adjoint PDE. To reduce the effort associated with a complete linearisation and summation by parts, a simplified version of the primal discrete system can be addressed [6,39]. In the discrete-adjoint approach incompatibilities in the discretisation of the primal problem are directly inherited to the discrete-adjoint problem and can result in an ill-posed discrete-adjoint formulation [28,17]. This may either be a consequence of incompatible definitions—e.g. of governing flow equations and objective functionals—so that a continuous-adjoint representation would not even exist for that problem, or it may be due to inconsistent discretisation schemes though a continuous-adjoint counterpart could generally be formulated. Inconsistent discretisations, for example of the primal boundary conditions and the boundary-defined objective functional, can lead to invalid discrete-adjoint boundary operators [28,30] inducing irregularities into the adjoint solution next to the most sensitive area where the objective functional is defined. This, in turn, can deteriorate the sensitivity prediction. A possible implication that may be already observed in the primal problem is a poor mesh convergence in terms of discrete integral criteria which are incompatible with the flow discretisation [17].

In order to bring together the information from both the continuous-and the discrete-adjoint method, a *hybrid-adjoint* strategy is pursued in this study: The adjoint PDE are derived in the first step. In the second step, the adjoint discretisation schemes for the individual terms of the adjoint PDE are constructed via summation by parts from the primal discretisation. This strategy allows to identify appropriate discretisation schemes for the adjoint PDE. Moreover, the analysis of the adjoint problem can reveal inconsistencies within the primal discretisation and give a feedback to improve its deficiencies. Ideally, if the schemes obtained in the discrete-adjoint way are a consistent approximation to the adjoint PDE, the discretisation schemes obtained in the sequence "derive-then-discretise" equal their "discretise-then-derive" counterparts.

1.2. Solution algorithm

Having found an appropriate adjoint discretisation, an *adjoint algorithm* is required to solve the problem numerically. It is possible (a) to use different solution schemes for the discretised primal and adjoint problems [44,35,39], (b) to reuse the modified primal algorithm to solve the adjoint problem (e.g. [22,49,46]), or (c) to traverse the primal algorithm in reverse. Approaches (a) and (b) can be followed with an adjoint discretisation won via the continuous-adjoint or the discrete-adjoint approach. Option (c) is usually pursued by reverse algorithmic differentiation [11,33,13,34] on the code level, i.e. in the discrete-adjoint way. Alternatively, the solution scheme can be reversed manually [36,32].

This study is concerned with unstructured finite-volume schemes and segregated, pressure-based solution strategies widely used in industry to solve incompressible flow problems (e.g. [3,9]). Such schemes are different from the density-based, coupled solution algorithms predominantly used in aerodynamics and complicate the development of adjoint solution schemes in several ways:

- The discrete system of conservation equations for momentum and continuity is transformed into a system of momentum and pressure (correction) equations.
- The equation systems are solved individually in an iterative pressure-projection algorithm, so that an approximation to the Jacobian matrix of the coupled system is available at no time. To reuse the primal solution strategy for the adjoint problem, an iterative sequence of transposed operations is required.
- An incomplete Picard linearisation for the convection of momentum is used in the semi-implicit flow solver. A complete linearisation must be supplemented in transposed form in the adjoint code. An explicit coupling is required in the corresponding segregated, adjoint solution algorithm.
- Compact finite-volume schemes are easily transposed via summation by parts. To achieve second-order accuracy on unstructured grids, an explicit deferred-correction based on an extended molecule is often applied, e.g. to approximate the full viscous stress tensor, to correct non-orthogonality errors, or for (limited) higher-order interpolation of the convective fluxes.

For these reasons, the purpose of this study was to exploit the knowledge of both the continuous-adjoint (Section 2) and the discrete-adjoint method. Manageable, consistent-adjoint schemes suitable for adjoint production codes are derived in a