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An adjoint view on flux consistency and strong wall boundary conditions to the Navier–Stokes equations

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ABSTRACT

Inconsistent discrete expressions in the boundary treatment of Navier–Stokes solvers and in the definition of force objective functionals can lead to discrete-adjoint boundary treatments that are not a valid representation of the boundary conditions to the corresponding adjoint partial differential equations. The underlying problem is studied for an elementary 1D advection–diffusion problem first using a node-centred finite-volume discretisation. The defect of the boundary operators in the inconsistently defined discrete-adjoint problem leads to oscillations and becomes evident with the additional insight of the continuous-adjoint approach. A homogenisation of the discretisations for the primal boundary treatment and the force objective functional yields second-order functional accuracy and eliminates the defect in the discrete-adjoint boundary treatment. Subsequently, the issue is studied for aerodynamic Reynolds-averaged Navier–Stokes problems in conjunction with a standard finite-volume discretisation on median-dual grids and a strong implementation of noslip walls, found in many unstructured general-purpose flow solvers. Going out from a base-line discretisation of force objective functionals which is independent of the boundary treatment in the flow solver, two improved flux-consistent schemes are presented; based on either body wall-defined or farfield-defined control-volumes they resolve the dual inconsistency. The behaviour of the schemes is investigated on a sequence of grids in 2D and 3D.

1. Introduction

The finite-volume method is one of the most established approaches to approximately solve the integral Navier–Stokes equations for complex geometries. Most implementations claim to be second-order accurate in space. By construction, the finite-volume method conserves the transported quantities like mass, momentum, energy, etc. on a given mesh locally on the cell level and globally throughout the fluid domain. Unless conservation is lost due to flux inconsistencies between flow solver and post-processing, the outputs (such as integral force components) predicted by the CFD method benefit from the conservation property. Therefore, the discretisation of integral output quantities, which are also referred to as objective functionals, should account for the discretisation used in the flow solver.

The solution of the adjoint problem is the natural connection between the linearisations of the residual and the considered objective functional. Consequently, the adjoint system inherits all the potential inconsistencies lying between the residual and the objective; either on the level of partial differential equations (PDE) when the continuous-adjoint prob-

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lem is constructed in a derive-then-discretise approach [14,15,25,28,26], or on the discrete level when the discrete-adjoint system is set up in a discretise-then-derive strategy [7,6,20,19,3,9].

In the continuous-adjoint method, a set of adjoint PDE is devised via integration by parts from the Lagrange polynomial which is the linearised integral objective functional augmented by the differential governing equations weighted by the adjoint variables. It is important to note that the adjoint PDE and its boundary conditions can only be formulated if the primal field equations, its boundary conditions and the objective functional are compatible. Subsequently, the adjoint system consisting of PDE, boundary conditions and sensitivity equation should be discretised in a consistent way, such that within the asymptotic range the discretisation error converges to zero at a certain order as the mesh is refined. In principle, the discretisations for the adjoint equations and the governing non-linear equations are independent and can be individually chosen. In practice, huge portions of the (non-linear) primal discretisation schemes may be reused for the adjoint problem, particularly for the self-adjoint operators appearing in the PDE. However, consistency only guarantees that the discrete objective functional and the corresponding adjoint-based sensitivity derivative match in the continuous limit. In general, the method does not output the exact derivative of the discrete objective functional on a given mesh.

The starting point for the construction of the discrete-adjoint method is the discretisation of the primal problem and the objective functional. Both are differentiated in a discrete sense. Accordingly, the discrete Lagrange polynomial consists of the discrete objective functional augmented by the algebraic constraints (discretised governing equations) weighted by the corresponding discrete-adjoint multipliers. Summation by parts, the discrete equivalent of integration by parts, yields the transposed or discrete-adjoint equations. The output of the discrete-adjoint approach is the exact derivative of the discrete objective functional on a given mesh, provided the discrete differentiation is complete and correct, the discrete-adjoint equation system is linearised about a fully converged reference solution and is fully converged itself. Instead of solving the discrete-adjoint equations linearised about the converged non-linear steady-state solution, a sequence of linearised algebraic operations in a CFD code can be carried out in reverse order recomputing or restoring the linearisation point in every step. This is possible in a (semi-)automated approach known as adjoint mode of algorithmic differentiation (e.g. [4]). Forward and reverse evaluations should yield the same derivative of the sequence output with respect to the sequence input. Following the ideas of Giles et al. [5,7], Nielsen et al. [20] have manually ensured primal–dual equivalence throughout the iteration process of a linearised, unstructured finite-volume Navier–Stokes method.

Discrete differentiation is a straightforward algebraic exercise but can be tedious when carried out manually for complex problems. Having derived the discrete objective functional and the discrete governing flow equations, the discrete-adjoint problem obtained via summation by parts is simply a consequence of the primal discretisation. As opposed to the continuous-adjoint method, the discrete adjoint can, in principle, be constructed for arbitrary discrete objective functionals, which is very welcome in practical application. However, unlike the forward problem, the discrete-adjoint problem collects influences from the discrete objective functional and the discrete governing equations. Thus, inconsistencies or incompatibilities in the inputs are directly inherited to the discrete-adjoint problem which then becomes a “sensor” revealing such inconsistent definitions present in the primal discretisation. Suffering inconsistent inputs, the discrete-adjoint solution cannot necessarily be considered a valid approximation to the corresponding adjoint PDE.

This has been observed for different discretisation methods, in particular of higher-order. Adjoint-consistent Discontinuous-Galerkin schemes for aerodynamic Euler and Navier–Stokes flow problems are presented for example by Lu [18], Oliver and Darmofal [22] and Hartmann et al. [8,10]. Irregularities and spurious oscillations are observed in the adjoint field solution in conjunction with adjoint inconsistent (wall) boundary formulations [18,8,10]. Such irregularities are eliminated through adjoint-consistent schemes. Moreover, it is demonstrated that the accuracy of functional predictions and of adjoint-based functional error estimators generally increases when adjoint-inconsistent schemes are replaced by adjoint-consistent formulations. In this way, superconvergent outputs of (adjoint-based error corrected) functionals can be achieved which exceed the design-order of the schemes. The concept is carried over to a summation-by-parts finite-differencing discretisation of higher-order by Hicken and Zingg [11–13]. Like for the Discontinuous-Galerkin discretisations, superconvergent functional outputs and an improved effectiveness of functional error estimators are observed for inviscid Euler flow cases. Liu and Sandu [17] systematically investigate the adjoint (in)consistency in finite-volume and finite-difference upwind schemes based on a 1D advection problem. Unlike the above-mentioned studies, the article at hand focuses on the implications of an adjoint (in-)consistency in the context of node-centred, second-order accurate finite-volume Navier–Stokes schemes with strong wall boundary conditions – a combination found in many CFD codes. With a linear face reconstruction used in the finite-volume method, functional superconvergence is not expected for second-order PDE like the Navier–Stokes equations. However, functional accuracy is shown to be directly related to the conservation property of the finite-volume method. Like in the previously mentioned studies, the regularity of the adjoint problem is linked to the flux-consistency of the discretisations of both the governing flow equations and the objective functional.

Adjoint boundary treatments are prone to dual inconsistencies when boundary-based objective functionals are considered, such as integral aerodynamic forces. In that case, both the discrete governing equations and the discrete objective functional contribute to the discrete-adjoint boundary treatment. Unless the discrete boundary flux of momentum in the discrete equations governing the flow exactly matches the discrete definition of the fluid-dynamic force integral in the objective functional [26], a meaningful discrete-adjoint boundary scheme cannot be expected. Since the solver balances numerical fluxes that usually include artificial dissipation contributions, also these terms need to be taken into consideration in the discrete objective functional to arrive at a valid discrete-adjoint boundary dissipation operator. The natural boundary treatment in the finite-volume method is to provide the boundary fluxes to the balances of the cells adjacent to the boundaries.