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Dual-consistency study for Green–Gauss gradient schemes in an unstructured Navier–Stokes method

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A multi-pass reconstruction method for the discrete-adjoint residual is presented that computes the adjoint of the viscous fluxes based on Green–Gauss gradients in an unstructured finite-volume RANS method. The intermediate discrete-adjoint multipliers of the multi-pass reconstruction are the dual viscous stresses containing the dual Green–Gauss gradients. Since the latter are explicitly evaluated on the fly, meaningful discrete-adjoint operators can be identified and compared against their primal counterparts. Numerical experiments are carried out for a 1D diffusion problem, 2D and 3D RANS cases on a sequence of grids to verify the consistency of the dual Green–Gauss gradients. They are compared against a rediscretisation of the adjoint Green–Gauss gradients known from the continuous-adjoint approach. In that sense, the multi-pass residual reconstruction method provides a deeper insight into the effective dual discretisation, an important part of which is the dual Green–Gauss gradient.

1. Introduction

Adjoint CFD methods can be constructed in a derive-then-discretise strategy pursuing the continuous-adjoint approach [15,16,31,36,32] or in a discretise-then-derive manner following the discrete-adjoint approach [8,9,27,21,25,4,13,33,10].

Given the adjoint partial differential equations (PDE) are appropriately discretised in a continuous-adjoint implementation, the method is expected to consistently converge against the solution of the adjoint PDE with mesh refinement. However, unlike the discrete-adjoint method, the continuous-adjoint approach does not provide the exact derivative of the discrete objective functional on a given mesh in general, which is the price to pay for the convenience of independently rediscretising the adjoint PDE.

Discrete-adjoint methods, on the contrary, do not necessarily lead to dual-consistent adjoint schemes, which can be considered a valid approximation to the adjoint PDE. The adjoint boundary treatment is known to be very sensitive to inconsistencies stemming from incompatible discrete definitions of numerical fluxes and force-objective functionals, both of which contribute to the discrete-adjoint residual. This has been addressed in the literature for discretisations of finite-volume [7,35,33], Discontinuous-Galerkin [21,10] or finite-differencing [12,13] type. The dual consistency of interior-flux discretisations is analysed for finite-volume and finite-difference upwind discretisations for the advection equation by Liu and Sandu [20].

Ideally, a numerical adjoint approach should ensure both that the adjoint solution consistently convergences towards a grid-independent solution of the adjoint PDE and that discrete duality is preserved on a given mesh. In principle, the

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combination of both very desirable properties can be sought from both the continuous- and the discrete-adjoint starting point. However, the prior property is traditionally associated with the continuous-adjoint approach, whereas the latter is naturally linked to the discrete-adjoint approach.

Remote-stencil operations that exceed the compact numerical stencil are often a key ingredient in the construction of second-order accurate finite-volume schemes. The construction and analysis of their dual counterparts is particularly involving compared to compact operators, which are often simplified or first-order accurate approximations. Typically, remote-stencil operations are found in central convection schemes including a numerical dissipation term based on undivided fourth differences [14], in upwind schemes with gradient-based reconstructions [19], in non-compact pressure switches [14] or limiters locally adapting the numerical scheme to the flow and in different non-compact viscous-flux formulations [22–24,11,30]. In unstructured-grid methods, remote-stencil information is often evaluated in two or more passes since only the immediate face-neighbours can be directly accessed: in a first face loop, intermediate quantities such as gradients or undivided Laplacians are computed from direct face-neighbour data alone. In a subsequent face loop, these intermediate quantities are picked up from the direct face neighbours to calculate the second-order flux contributions to the residual.

By reusing many of the modules of the underlying non-linear CFD method, continuous-adjoint implementations on unstructured grids usually inherit the multi-pass approach. By construction of the continuous-adjoint method, the intermediate continuous-adjoint variables are directly associated with the underlying terms of the adjoint PDE and are considered meaningful approximations to these expressions. Gradient discretisation schemes, which are reportedly a key component of (non-linear) viscous finite-volume methods [22–24,11,30], are expected to play a similar role in the corresponding rediscretised continuous-adjoint problem. A by-product of reapplying the residual reconstruction in multiple passes in the continuous-adjoint implementation is that the continuous-adjoint method inherits welcome features like the memory efficiency (no explicit storage of the flux Jacobian required) and the distributed-memory parallel concept based on a one-cell-layer exchange of the intermediate variables such as (Green–Gauss) gradients.

Likewise, in the discrete-adjoint context, the Jacobian matrix of the second-order accurate remote-stencil discretisation does not need to be explicitly stored to compute the discrete-adjoint residual. Instead, the linearised counterparts of the individual residual evaluation steps in the non-linear flow solver can be systematically carried out in backward mode. The issue has previously been addressed by Nielsen et al. [27] in the context of efficiently computing the adjoint residual. They present a finite volume-based implicit discrete-adjoint RANS approach that ensures primal-dual consistency of the solution, which is referred to as duality here. One option suggested by the authors is to explicitly reconstruct the remote-stencil contributions of the linearised upwind scheme in a matrix-free way in multiple (two) passes. A similar two-pass approach is pursued by Mavriplis [25] for the backward linearisation of a RANS method with the focus on the remote-stencil operations of a matrix-dissipative central convection scheme. Peter and Dwight [28] also comment on the benefits of on-the-fly evaluations of the adjoint residual from a memory- and CPU-consumption point of view. Automatic differentiation, e.g. [5,2], applies a similar strategy directly on the code level; forward-against-backward checks are a standard code verification procedure to ensure exact duality of automatically differentiated codes. However, when the program code is obtained by source-to-source precompilation, particularly the reverse-mode linearisation is usually not easily readable, so that it is difficult to investigate and interpret the discrete-adjoint operators from a dual-consistency perspective.

In that sense, the multi-pass reconstruction of the discrete-adjoint residual – pursued here in conjunction with an unstructured discrete-adjoint finite-volume method – helps to recover and exploit some the above-mentioned benefits granted by the continuous-adjoint method. This article focuses on the fully-differentiated viscous fluxes of the RANS equations using Green–Gauss gradients. The discrete-adjoint stresses that include the adjoint Green–Gauss gradients are explicitly evaluated in the first reverse pass. This facilitates to assess and verify the discrete-adjoint gradient scheme from a dual-consistency point of view, since the important remote-stencil part of the dual discretisation is no longer hidden in the (transposed) Jacobian matrix of the viscous-flux discretisation.

The paper is organised as follows: in Section 2, the multi-pass reconstruction method is applied to investigate the primal-dual properties of a baseline finite-volume discretisation for a 1D diffusion problem. It serves as a simplified prototype for the discretisation of the viscous Navier–Stokes fluxes, which are addressed and analysed in Section 3. The method is verified for 2D and 3D RANS problems on a sequence of grids in Section 4, followed by the conclusions drawn in Section 5.

2. An introductory study for a 1D diffusion problem

An elementary 1D diffusion equation was considered first with its scalar diffusion operator being a very simple prototype of the viscous diffusion terms of the Navier–Stokes equations presented in Section 3. The 1D discretisation was set up using the focused Green–Gauss gradient scheme applied in the Navier–Stokes method. The derivative with respect to a variable is denoted by a subscript following a comma. The indefinite integral of a function g is denoted by G, i.e.

$$\int_0^1 g\,\mathrm{d}x = -G(0) + G(1) = [G]_0^1 = [G]_0 + [G]^1 \,. \tag{1}$$

Note that the negative normal on the left-hand side is included in the notation $[G]_0 = -G(0)$.