Advances in CFD Discretisation Schemes and Solution Algorithms for a Stable Discrete Adjoint

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Researchers in the field of CFD adjoint-based optimization are currently facing a number of challenges,[6] regardless of the specific approach. Examples of such difficulties, affecting specifically the adjoint Navier-Stokes equations, are: continuous adjoint solvers suffering from convergence issues, suggesting, among other causes, that the discretisation schemes and algorithms employed in standard CFD are not always suited to the nature of adjoint equations; discrete adjoint solvers also failing to converge in large cases unless a very well converged primal flow field is provided; adjoint codes produced via reverse Automatic Differentiation (AD) being based on hypotheses often not valid, thus producing unreliable gradient values as well as being costly in terms of storage memory. Evidence suggests that convergence issues in adjoint solvers are related to convergence of the CFD itself, meaning that classical Finite Volume (FV) schemes yield a solution that, although acceptable as a mere aerodynamics case study, cannot be used to produce a robust adjoint system. It appears therefore that adjoint solvers could benefit from a well-converged primal flow solution, which in turns requires a) an appropriate, mathematically sound discretisation scheme and b) an adequate solving algorithm. We attempted to tackle both of these aspects, and we summarize our main findings in the present work.

I. Discretisation schemes

In recent years a new family of CFD discretisation schemes, the Virtual Elements Method[1] (VEM) has emerged as a promising alternative to classical schemes such as FV. The aim is to allow for more freedom in the numerical model, most notably in mesh geometry (e.g. the possibility to use strongly non-orthogonal or non-convex elements) and discontinuity of material properties. The method also eliminates certain numerical artefacts typical of FV (e.g. Non-Orthogonal Correctors), thus ensuring robustness and improving convergence properties, without at the same time having to resort to certain somewhat constraining features of classical Finite Elements (FE), such as shape functions. The method is of particular relevance in the context of CFD optimization, as a) it can deal with mesh distortion as typically encountered in shape optimization processes, and b) it might alleviate robustness issues linked with the (continuous or discrete) adjoint Navier-Stokes equations, often used to compute gradients in gradient-based optimization. VEM has been largely and successfully validated for pure anisotropic diffusion operators,[2] convection-diffusion problems and 1st-order Navier-Stokes.[3]

We outline here our own incompressible Navier-Stokes scheme, a VEM-based method we named Mixed Hybrid Finite Volumes (MHFV). Compared to previous literature, our scheme a) features an original approach to derive and stabilize the VEM diffusion operator, b) is extended to 2nd-order accuracy for both velocity and pressure fields, and c) offers a selection of stabilization schemes for convective terms inspired by traditional FV and FE strategies. Results are presented on a series of 2D and 3D benchmark test cases, highlighting in particular how the scheme is reliable even on highly distorted meshes - a further appealing feature when it comes to shape optimization, where FV-compatible mesh quality cannot always be ensured by standard mesh-morphing tools.

II. Solution algorithms

The efficiency of traditional SIMPLE-like preconditioners is debatable: they are somewhat stable but they exhibit a rather poor convergence rate, they are prone to stagnation and they are affected by mesh

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refinement. They mostly owe their popularity to legacy reasons, being amongst the first devised working methods, and to their segregated nature, as they require solving linear systems that are relatively small and easy to deal with compared to the full Oseen-type system typically stemming from the Navier-Stokes discretisation.

Recent progress in computational power and linear solver capabilities led researchers to reconsider some other Navier-Stokes solution schemes, previously investigated but deemed unfeasible in industrial contexts. Research has successfully produced a number of alternative algorithms, although mostly restricted so far to the FE community, such as those based on the so-called approximate commutators.[4] Several interesting comparisons amongst various Navier-Stokes preconditioners have also been published.[8]

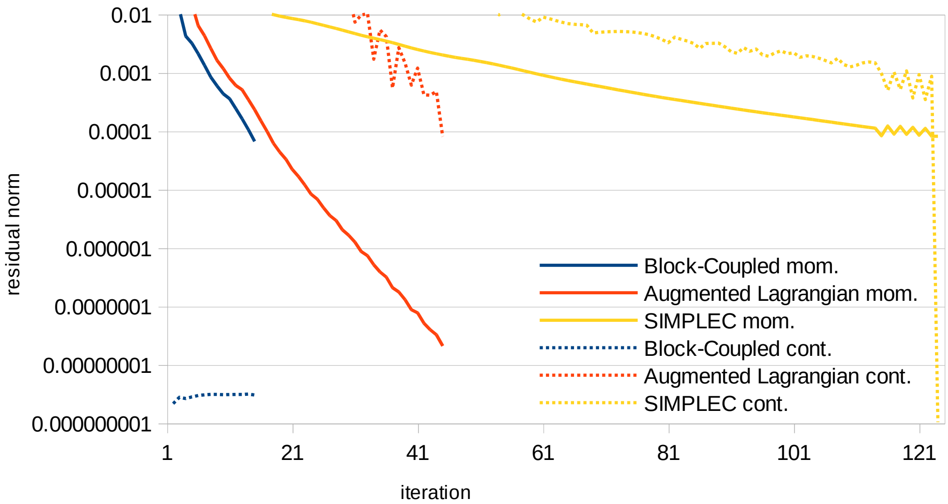

Figure 1. S-Bend 3D test case: convergence history of the primal x-momentum and continuity residuals for different solution algorithms.

We present here our own implementation of a traditional SIMPLE-like scheme as well as some alternative ones, including the Augmented Lagrangian[5] (AL), applied to the above mentioned MHFV Navier-Stokes solver. Performance is assessed via comparisons on a series of test cases (Figure 1).

We also investigate efficient ways of solving the discrete adjoint Navier-Stokes problem itself, which is in essence a linear system similar to the original Oseen, and is therefore affected by the same practical difficulties. We explicitly assemble the adjoint system via our Equational Differentiation[7] (ED) approach, and we devise multiple solution strategies (SIMPLEC, V-Coupled, AL) adapted from the primal. We run a series of adjoint test cases and compare performance of various solution schemes.

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