A hybrid adjoint approach applied to RANS equations

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1. Motivation and objectives

Since being first introduced to aerodynamic applications by Jameson (Jameson 1988) in the late 1980s, adapting ideas from more general work by Lions (Lions 1971) on optimal control of systems governed by partial differential equations (PDEs), the adjoint method has been used in a wide variety of areas. These include shape optimization of wing geometries (Reuther & Jameson 1995; Jameson *et al.* 1998; Reuther *et al.* 1999*a*,*b*), sensitivity analysis (Baysal & Eleshaky 1991; Martins & Hwang 2012), uncertainty quantification (Duraisamy & Alonso 2012; Duraisamy & Chandrashekar 2012; Palacios *et al.* 2012; Pierce & Giles 2004), and goal-oriented numerical error estimation and mesh adaptation (Giles *et al.* 2003*a*; Venditti & Darmofal 2002; Giles & Pierce 1998, 1999; Nemec *et al.* 2008; Wintzer *et al.* 2008).

Traditionally there are two different approaches to formulating the numerical system of adjoint equations: the discrete method, which derives the adjoint equations from the discretized residual equations used to numerically solve for the flow and the continuous method, which starts from the continuous form of the governing equations, and only discretizes the problem when finally solving the continuous adjoint equations.

Both techniques are found to have relative advantages and disadvantages over each other. In theory, a discrete method can handle PDEs of arbitrary complexity without significant mathematical development and can treat arbitrary functionals. However, this method requires the evaluation of discrete Jacobians, which we denote as $\mathscr{D}()/\mathscr{D}()$ to distinguish from their continuous alternatives $\partial()/\partial()$, and there are two main ways to do this. The first is to analytically derive these terms from the discretized forms of the flow residuals and then develop code based on this. The second is to use algorithmic Automatic Differentiation (AD), either via source code transformation (Hascoët & Pascual 2004) or operator overloading (Griewank *et al.* 1996). The former, the analytical approach, requires significant development, more than that generally required in the continuous method (Nadarajah & Jameson 2000), while the latter can be computationally expensive.

In comparison, the continuous adjoint method requires significant theoretical development but is better connected to the underlying physics and can be solved in a method independent of the flow solution scheme. However, it is more limited in the types of functionals and governing equations that can be treated, and the gradient calculated will differ more substantially from the discrete gradient (which can be accurately computed by the discrete adjoint method).

Taylor et al. considered using a third, hybrid approach, that combines elements of both the discrete and continuous methods(Taylor *et al.* 2012*a*), deriving the adjoint equation from a mixture of the discretized residual equations and the continuous governing equations (Taylor *et al.* 2012*a*).

In this brief we build on that previous work, which used quasi-one-dimensional flow with a combustion model as a test case, and extend the theory to handle two- and three-dimensional turbulent flows. To demonstrate one of the key advantages of this new approach we develop a hybrid method in which the continuous part, the mean flow, is model-independent. This means that the turbulence model can be switched without incurring additional development cost, noting that the intention is always to handle the discrete parts using AD. Also, it allows this model to be applied in situations where the turbulence model may be difficult or impossible to handle via the continuous adjoint approach.

To investigate the properties of the hybrid adjoint, application is extended to a case of an airfoil in transonic turbulent flow (Cook *et al.* 1979; Haase *et al.* 1993).

Section 2 provides a general introduction to the adjoint method, including the discrete, continuous, and hybrid approaches. Section 3 introduces the Favre-Averaged Navier-Stokes equations, which are then used to develop the general turbulent hybrid adjoint in Section 4. Results and discussion of the application of the hybrid adjoint method to the optimization of transonic turbulent flow over airfoils is presented in Section 5.

2. Introduction to adjoint methods

Adjoint equations can be conveniently formulated in a framework to calculate the sensitivity of a given objective function, $\mathcal{J}$, to parameters, α, in a problem governed by the set of equations that can be represented by $\mathcal{G}(U, \alpha) = 0$, where U is the primal solution.

The adjoint variables can be used purely as a mathematical tool to find the required sensitivities, but, as discussed by Giles & Pierce (Giles & Pierce 2000) and Belegundu & Arora (Belegundu & Arora 1985), they can also be interpreted as representing the sensitivity of the objective function to perturbations in the governing equations, or the influence on the objective function of an arbitrary source function.

The additional computational cost of solving the adjoint problem is typically of the order of one additional flow solution (Anderson & Venkatakrishnan 1999), and the adjoint variables represent the sensitivities of $\mathcal{J}$ to changes in all of the parameters that define the problem at every point in the domain. In contrast, although finite difference methods can also be used to find these sensitivities, they are in general significantly more expensive, requiring at least one additional flow solution to find the gradient of the objective function to any parameter in the domain. There are two main approaches used to derive the adjoint equations: the Primal-Dual Equivalence Theorem and an optimization framework using Lagrange multipliers (Giles & Pierce 2000; Belegundu & Arora 1985). In this brief, we consider the latter method, and, using this, handle the discrete and continuous parts of the hybrid adjoint derivation in an identical context. The following sections summarize the three different methods via this approach, but for a more complete discussion see Taylor (Taylor *et al.* 2012*a*,*b*; Taylor 2013).

2.1. *Discrete adjoint approach*

In the discrete adjoint approach, the governing equations that we wish to enforce are the residuals, at every point in the domain, from the flow solution, $\mathcal{R}_p$, i.e., $\mathcal{G} = \{\mathcal{R}_p\} = 0$. This gives the Lagrangian

$$\mathcal{L} = \mathcal{J}_D + \sum_{p=1}^{N} \psi_p^T \mathcal{R}_p, \tag{2.1}$$

where ψ are the Lagrange multipliers, or discrete adjoint variables, and the discrete perturbation to $\mathcal{L}$ is

$$\Delta\mathcal{L} = \Delta\mathcal{J}_D + \sum_{p=1}^{N} \psi_p^T \Delta\mathcal{R}_p. \tag{2.2}$$

After expanding and manipulating terms we define the adjoint equation, so as to remove the dependence on the flow perturbation, as

$$\sum_{q=1}^{N} \left(\frac{\mathscr{D}\mathcal{R}_q}{\mathscr{D}U_p}\right)^T \psi_q = -\left(\frac{\mathscr{D}\mathcal{J}_D}{\mathscr{D}U_p}\right)^T, \tag{2.3}$$

where we define the discrete Jacobian to be $\frac{\mathscr{D}()}{\mathscr{D}()}$, and the perturbation to the objective function is now

$$\Delta\mathcal{J}_D = \sum_{p=1}^{N} \psi_p^T \frac{\mathscr{D}\mathcal{R}_p}{\mathscr{D}\alpha}\Delta\alpha + \frac{\mathscr{D}\mathcal{J}_D}{\mathscr{D}\alpha}\Delta\alpha, \tag{2.4}$$

where it is seen that once the discrete adjoint Eq. (2.3) is solved, we can determine sensitivities of the objective function to any α relatively cheaply, needing only to consider the explicit dependence of $\mathcal{J}$ and $\mathcal{R}$ on α.

2.2. *Continuous adjoint approach*

In the continuous adjoint approach, we enforce the analytical form of the flow equations, $\mathcal{N}$, i.e., $\mathcal{G} = \{\mathcal{N}\} = 0$. The Lagrangian is thus

$$\mathcal{L} = \mathcal{J}_C - \int_\Omega \phi^T \mathcal{N} d\Omega, \tag{2.5}$$

where ϕ are the Lagrange multipliers, or continuous adjoint variables, and the continuous perturbation to this now becomes

$$\delta\mathcal{L} = (\mathcal{J}_C' - \mathcal{J}_C) - \left(\int_{\Omega'} \phi^T \mathcal{N}' d\Omega - \int_\Omega \phi^T \mathcal{N} d\Omega\right), \tag{2.6}$$

where we note that perturbations to the parameter α may cause perturbations to both the flow, U, and the domain, Ω, and its bounding surface, Γ.

The next step is again to manipulate and rearrange terms such that the direct dependence of this quantity on the flow perturbations, δU, is removed, while retaining those terms dependent on perturbations to α and/or the domain and boundary surface. As these remaining terms are either known or easily determinable, the perturbation to the objective function can then readily be found with respect to those perturbations. This process will lead to the continuous adjoint equation and its boundary conditions, but its derivation and final form are intimately connected to the form of the governing equations, the flow boundary conditions, and the objective function, and cannot be shown generally as in the discrete case above.

2.3. *Hybrid adjoint approach*

The main motivation behind a hybrid adjoint is to combine the best qualities of the discrete and continuous approaches. The general goal is to aim for the convergence and robustness properties of the continuous method, with the flexibility to handle arbitrarily complex PDEs of the discrete adjoint, but additional qualities of each, such as the existence of a surface formulation for gradients in the continuous adjoint approach, are also desirable. While there have been approaches that attempt to combine the continuous and discrete methods taken before, such Giles et al. where continuous-like boundary conditions are used to improve the quality of the discrete adjoint solution near walls with strong boundary conditions (Giles *et al.* 2003*b*), the method discussed in this brief attempts to build a more general, true hybrid.

In our approach, we split the governing equations into those that will be enforced continuously and those that will be enforced discretely, i.e., $\mathcal{G} = \{\{\mathcal{N}\}_C, \{\mathcal{R}_p\}_D\} = 0$.

The equations that will be treated continuously will be those that will not change when making minor adjustments to the flow equations, such as when changing the source terms, and that are easily differentiable (e.g., the Euler equations for a perfect gas), whereas the terms treated discretely will include those that are not easily differential, and those that we may wish to change and experiment with (e.g., chemical source terms and turbulence models). One of the main intentions is that once the derivation for the continuous part is performed, substantial changes do not need to be made in the future, thus significantly lowering the development cost for additional problems.

Additionally, we define the objective function as one of either the discrete or continuous objective functions. We combine these by writing as a sum,

$$\mathcal{J}_H = \beta \mathcal{J}_C + (1-\beta)\mathcal{J}_D, \tag{2.7}$$

where β can be set equal to 0 or 1 in order to recover either the discrete or continuous functionals, respectively. Writing it in this way is useful so that both types of objective functions can be carried through the derivations simultaneously. It should be noted that it is also possible to create a weighted sum of both functionals, but that this has not been considered here. The idea of choosing between the discrete or continuous functionals is meant to allow us to choose the most suitable objective function for a specific problem, avoiding the disadvantages of the other, and a blend of both would therefore be counterproductive. However, one option not considered in this brief would be to switch between the discrete and continuous functionals at different points within the domain.

The Lagrangian now becomes

$$\mathcal{L} = \beta \mathcal{J}_C + (1-\beta)\mathcal{J}_D - \int_\Omega \varphi_C^T \mathcal{N}_C d\Omega + \sum_{p=1}^{N} \varphi_{D,p}^T \mathcal{R}_{D,p}, \tag{2.8}$$

where φ_C and φ_D are the Lagrange multipliers, or hybrid adjoint variables, and the hybrid perturbation can thus be written as

$$\begin{aligned} \{\delta,\Delta\}\mathcal{L} \;=\;& \beta\,(\mathcal{J}_C' - \mathcal{J}_C) + (1-\beta)\Delta\mathcal{J}_D \\ & - \left(\int_{\Omega'} \varphi_C^T \mathcal{N}_C' d\Omega - \int_\Omega \varphi_C^T \mathcal{N}_C d\Omega\right) + \sum_{p=1}^{N} \varphi_{D,p}^T \Delta\mathcal{R}_{D,p}. \end{aligned} \tag{2.9}$$

The next steps in this derivation are similar to those introduced previously for the discrete and continuous parts, mathematically manipulating the equation so as to remove the explicit dependence of the perturbation on δU, and in so doing generating the adjoint equation and boundary conditions for φ_C and φ_D. Due to the dependence of this method on the actual analytical form of the continuous part, this cannot be shown generally.

However, we can make a general observation about the hybrid boundary conditions. When solving the discrete adjoint equations, no such conditions need to be explicitly enforced, because they are already enforced within the calculation of the flow residuals. However, this is not the case for the hybrid approach, which now requires hybrid conditions relating the continuous, φ_C and discrete φ_D, variables from the hybrid adjoint solution. This more closely mirrors the fully continuous than the fully discrete approach.

When deriving and calculating the hybrid adjoint for a specific problem, two important choices will need to be made. The first deals with exactly which governing equations are treated discretely and continuously, and the second is to decide whether to use the discrete or continuous objective function.

An interesting feature to be noted is that the discrete and continuous approaches are, in fact, special cases of the more general hybrid approach. By setting $\beta = 0$ and defining $\{\mathcal{R}\}_D = \mathcal{R}$, and thus $\{\mathcal{N}\}_C = \emptyset$, we recover the pure discrete method, and by setting $\beta = 1$ and defining $\{\mathcal{N}\}_C = \{\mathcal{N}\}$, and thus $\{\mathcal{R}\}_D = \emptyset$, we get the pure continuous method.

However, we are no longer limited to just those two options. It is possible to create a continuous adjoint that has a discrete functional, allowing non-differentiable cost functions to be considered in the continuous approach, or vice versa, and many other combinations in between.

3. Governing equations of the primal problem

The governing equations considered in this brief are the standard Reynolds-Averaged Navier-Stokes equations (Wilcox 2006) for compressible flow along with a required turbulence model, and together these can be written

$$\mathcal{N}(U, \partial_j U, \alpha) = \begin{pmatrix} \mathcal{N}_L \\ \mathcal{N}_T \end{pmatrix} = 0, \quad \text{in } \Omega, \tag{3.1}$$

where the variables, U, consist of mean flow variables, U_L, and turbulence variables, U_T,

$$U = \begin{pmatrix} U_L \\ U_T \end{pmatrix}, \tag{3.2}$$

and $\partial_j U$ are the gradients of the flow variables and α is an undefined parameter that we wish to find sensitivities relative to.

3.0.1. *Reynolds-Averaged Navier-Stokes equations*

The mean flow equations are

$$\mathcal{N}_L(U, \partial_j U, \alpha) = \partial_i \left(F_i - \mu^{v1} F_i^{v1} - \mu^{v2} F_i^{v2} \right) = 0, \quad \text{in } \Omega, \tag{3.3}$$

subject to the boundary conditions

$$\begin{aligned} &u_i = 0, && \text{on } S, \\ &\hat{n}_i \partial_i T = 0, && \text{on } S, \\ &(W)_+ = W_\infty, && \text{on } \Gamma_\infty, \end{aligned} \tag{3.4}$$

where the mean flow variables are

$$U_L = \begin{pmatrix} \rho \\ \rho u_i \\ \rho E \end{pmatrix}, \tag{3.5}$$

and the convective and viscous flux vectors are given by

$$F_i = \begin{pmatrix} \rho u_i \\ \rho u_i u_j + p\delta_{ij} \\ \rho u_i H \end{pmatrix}, \quad F_i^{v1} = \begin{pmatrix} 0 \\ \tau_{ij} \\ u_k \tau_{ik} \end{pmatrix}, \quad F_i^{v2} = \begin{pmatrix} 0 \\ 0 \\ C_p \partial_i T \end{pmatrix}, \tag{3.6}$$

where the temperature and stress are

$$T = \frac{p}{R\rho}, \quad \tau_{ij} = (\partial_j u_i + \partial_i u_j) - \frac{2}{3}\delta_{ij}\partial_k u_k. \tag{3.7}$$

We also define the viscosity terms in Eq. (3.3) as

$$\mu^{v1} = \mu + \mu_T, \quad \mu^{v2} = \frac{\mu}{Pr} + \frac{\mu_T}{Pr_T}, \tag{3.8}$$

where Pr and Pr_T are the laminar and turbulent Prandtl numbers, respectively, and the laminar viscosity, μ, is given by Sutherland's law,

$$\mu = \frac{\mu_1 T^{\frac{3}{2}}}{T + \mu_2}. \tag{3.9}$$

Finally, the eddy viscosity, μ_T, is assumed to be the sole coupling term between the turbulence model and the mean flow equations, and the specific form of μ_T depends on the exact turbulence model being used.

3.0.2. *General turbulence model*

A set of governing equations for a general turbulence model can be written

$$\mathcal{N}_T(U, \partial_j U, \alpha) = \partial_i F_{T_i} - S_T = 0, \quad \text{in } \Omega, \tag{3.10}$$

where the flux, F_{T_i}, and source, S_T, may be functions of U, $\partial_j U$, and α.

The solution of this turbulence model will allow us to calculate the eddy viscosity, μ_T, which will then couple into the RANS governing Eqs. (3.3) through the viscosity terms μ^{v1} and μ^{v2}. It is important to note that the form of μ_T will depend on the model being considered, but that it could generally be a function of U, $\partial_j U$, and α. However, one important boundary condition that applies to a general turbulence model is that on a viscous wall, $\mu_T = 0$.

4. Hybrid adjoint equations

To derive a general set of hybrid adjoint equations for turbulent flow, we consider the hybrid objective function,

$$\mathcal{J}_H = \beta \left(\int_\Omega j_\Omega d\Omega + \int_\Gamma j_\Gamma d\Gamma \right) + (1 - \beta) \frac{\mathscr{D}\mathcal{J}_D}{\mathscr{D}\alpha} \Delta\alpha, \tag{4.1}$$

where by appropriate choice of β (0 or 1), we may select either a discrete or continuous objective function, and through definition of j_Ω, j_Γ, and $\mathcal{J}_D$ the objective function may be defined in the domain, on the boundary, or both.

Also, one of the key goals of applying the hybrid adjoint approach to turbulent flow is that the mean flow equations can be handled continuously and turbulence models discretely. Using Automatic Differentiation to obtain the required terms in the discrete approach will then mean that the turbulence models can be treated as black boxes, and that the models can be switched in and out without the need to perform any additional analytical development. However, it can be seen in Eq. (3.8) that the viscosity terms in the mean flow equations (Eq. 3.3) depend explicitly on the eddy viscosity, μ_T. Additionally, the form of μ_T depends on the exact turbulence model being used and thus there is a model-dependence in the mean flow equations.

This model-dependence can, however, be removed by the introduction of a dummy governing equation for the eddy viscosity,

$$\mathcal{N}_{\mu_T}(U, \partial_j U, \alpha) = \mu_T - f = 0, \quad \text{in } \Omega, \tag{4.2}$$

where

$$f(U, \partial_j U, \alpha) = \mu_T. \tag{4.3}$$

Treating this dummy governing equation discretely will allow the explicit dependence on the form of the eddy viscosity to be moved from the continuous part of the hybrid adjoint equations to the discrete part.

We now enforce the mean flow governing equations, $\mathcal{N}_L$, and the eddy viscosity and turbulence model numerical residuals, $\mathcal{R}_{\mu_T}$ and $\mathcal{R}_T$, respectively, by introducing the modified Lagrangian

$$\begin{aligned}\mathcal{L} \;=\; & \beta\left(\int_\Omega j d\Omega + \int_\Gamma j_\Gamma d\Gamma\right) + (1-\beta)\,\frac{\mathscr{D}\mathcal{J}_D}{\mathscr{D}\alpha}\Delta\alpha \\ & - \int_\Omega \varphi_C^T \mathcal{N}_L d\Omega - \sum_{p=1}^{N} \varphi_{\mu_{T_p}}^T \mathcal{N}_{\mu_{T_p}} \Delta\Omega_p + \sum_{p=1}^{N} \varphi_{D_p}^T \mathcal{R}_{T_p},\end{aligned} \tag{4.4}$$

where $\varphi = \{\varphi_C, \varphi_{\mu_T}, \varphi_D\}$ are the Lagrange multipliers (or hybrid adjoint variables).

Taking the perturbation of the Lagrangian to a change in some parameter α we then get, after linearization and appropriate manipulation,

$$\begin{aligned}\{\delta,\Delta\}\mathcal{L} \;=\; & \int_\Omega \left(\beta\frac{\partial j}{\partial\alpha}\delta\alpha - \varphi_C^T \partial_i\left(\left(\frac{\partial F_i}{\partial\alpha} - \mathcal{A}_1 - \mathcal{A}_4 - \mathcal{B}_1\right)\delta\alpha\right)\right) d\Omega \\ & + \int_\Gamma \beta\frac{\partial j_\Gamma}{\partial\alpha}\delta\alpha d\Gamma + (1-\beta)\,\frac{\mathscr{D}\mathcal{J}_D}{\mathscr{D}\alpha}\Delta\alpha \\ & + \sum_{p=1}^{N} \varphi_{\mu_{T_p}}^T \frac{\mathscr{D} f_p}{\mathscr{D}\alpha}\Delta\alpha\Delta\Omega_p + \sum_{p=1}^{N} \varphi_{D_p}^T \frac{\mathscr{D}\mathcal{R}_{T_p}}{\mathscr{D}\alpha}\Delta\alpha \\ & - \int_\Omega \left(L_\Omega^*(\varphi_C) - \beta\left(\frac{\partial j_\Omega}{\partial U}\right)^T\right)^T \delta U d\Omega \\ & - \int_\Gamma \left(\left(L_\Gamma^*(\varphi_C) - \beta\left(\frac{\partial j_\Gamma}{\partial U}\right)^T\right)^T \delta U - \varphi_C^T\left(\mathcal{A}_3 + \mathcal{B}_3\right)\delta(\partial_j U)\hat{n}_i\right) d\Gamma \\ & - \int_\Omega \left(\partial_i \varphi_C^T\right) \mathcal{C}_1 \delta\mu_T d\Omega + \int_\Gamma \varphi_C^T \mathcal{C}_1 \hat{n}_i \delta\mu_T d\Gamma \\ & + (1-\beta)\sum_{p=1}^{N} \frac{\mathscr{D}\mathcal{J}_D}{\mathscr{D}U_p}\Delta U_p + \sum_{p=1}^{N}\sum_{q=1}^{N} \varphi_{D_q}^T \frac{\mathscr{D}\mathcal{R}_{T_q}}{\mathscr{D}U_p}\Delta U_p \\ & + \sum_{p=1}^{N}\sum_{q=1}^{N} \varphi_{\mu_{T_q}}^T \frac{\mathscr{D} f_q}{\mathscr{D}U_p}\Delta U_p \Delta\Omega_q - \sum_{p=1}^{N} \varphi_{\mu_{T_p}}^T \Delta\mu_{T_p}\Delta\Omega_p,\end{aligned} \tag{4.5}$$

where the adjoint linear operators are

$$L_{\Omega}^{*}(\varphi_C) = -\left(\frac{\partial F_i}{\partial U} - \mathcal{A}_2 - \mathcal{A}_5 - \mathcal{B}_2\right)^T \partial_i \varphi_C - \partial_j \left((\mathcal{A}_3 + \mathcal{B}_3)^T \partial_i \varphi_C\right), \tag{4.6}$$

and

$$L_{\Gamma}^{*}(\varphi_C) = \left(\left(\frac{\partial F_i}{\partial U} - \mathcal{A}_2 - \mathcal{A}_5 - \mathcal{B}_2\right)\hat{n}_i\right)^T \varphi_C + \left((\mathcal{A}_3 + \mathcal{B}_3)\,\hat{n}_j\right)^T \partial_i \varphi_C. \tag{4.7}$$

The adjoint equations are then defined so as to remove the dependence of $\{\delta, \Delta\}\mathcal{L}$ on the flow and eddy viscosity perturbations. We can first remove the terms containing either $\delta\mu_T$ or $\Delta\mu_T$ from Eq. (4.5) by asserting that

$$\int_{\Omega} \left(\partial_i \varphi_C^T\right) \mathcal{C}_1 \delta\mu_T d\Omega + \sum_{p=1}^{N} \varphi_{\mu_{T_p}}^T \Delta\mu_{T_p} \Delta\Omega_p - \int_{\Gamma} \varphi_C^T \mathcal{C}_1 \hat{n}_i \delta\mu_T d\Gamma = 0. \tag{4.8}$$

Noting that at a true far field we can neglect the viscous flux contributions and that at a viscous wall the eddy viscosity is zero, and thus $\delta\mu_T = 0$, we can remove the boundary term from Eq. (4.8), giving,

$$\int_{\Omega} \left(\partial_i \varphi_C^T\right) \mathcal{C}_1 \delta\mu_T d\Omega + \sum_{p=1}^{N} \varphi_{\mu_{T_p}}^T \Delta\mu_{T_p} \Delta\Omega_p = 0. \tag{4.9}$$

Discretizing the domain integral into a sum of the integrals over each cell, and then making the assumption that this condition is not just true within the whole domain, but also within each cell, we obtain, for cell p,

$$\int_{\Omega_p} \left(\partial_i \varphi_C^T\right) \mathcal{C}_1 \delta\mu_T d\Omega + \varphi_{\mu_{T_p}}^T \Delta\mu_{T_p} \Delta\Omega_p = 0. \tag{4.10}$$

Now, under the assumption that $\delta\mu_T$ is a step-wise constant within each cell, we may factor it out of the integral, and, if we also assume that $\delta\mu_{T_p} \approx \Delta\mu_{T_p}$, we may cancel out the dependence on the perturbation to the eddy viscosity, giving, after rearrangement,

$$\varphi_{\mu_{T_p}}^T \Delta\Omega_p = -\int_{\Omega_p} \left(\partial_i \varphi_C^T\right) \mathcal{C}_1 d\Omega. \tag{4.11}$$

Next, to remove the terms containing either δU or ΔU from Eq. (4.5) we write

$$\begin{aligned} &\int_{\Omega} \left(L_{\Omega}^{*}(\varphi_C) - \beta \left(\frac{\partial j_{\Omega}}{\partial U}\right)^T\right)^T \delta U d\Omega \\ &+ \int_{\Gamma} \left(\left(L_{\Gamma}^{*}(\varphi_C) - \beta \left(\frac{\partial j_{\Gamma}}{\partial U}\right)^T\right)^T \delta U - \varphi_C^T \left(\mathcal{A}_3 + \mathcal{B}_3\right) \delta(\partial_j U)\hat{n}_i\right) d\Gamma \\ &- (1-\beta) \sum_{p=1}^{N} \frac{\mathscr{D}\mathcal{J}_D}{\mathscr{D}U_p} \Delta U_p - \sum_{p=1}^{N}\sum_{q=1}^{N} \varphi_{D_q}^T \frac{\mathscr{D}\mathcal{R}_{T_q}}{\mathscr{D}U_p} \Delta U_p \\ &- \sum_{p=1}^{N}\sum_{q=1}^{N} \varphi_{\mu_{T_q}}^T \frac{\mathscr{D} f_q}{\mathscr{D}U_p} \Delta U_p \Delta\Omega_q \quad = \quad 0. \end{aligned} \tag{4.12}$$

The boundary terms can be removed by requiring that

$$\begin{aligned}\int_{\Gamma}\left(\left(L_{\Gamma}^{*}(\varphi_C)-\beta\left(\frac{\partial j_{\Gamma}}{\partial U}\right)^{T}\right)^{T}\delta U-\varphi_C^{T}\left(\mathcal{A}_3+\mathcal{B}_3\right)\delta(\partial_j U)\hat{n}_i\right)d\Gamma & \\ -(1-\beta)\sum_{p=1}^{N_S}\sum_{q=1}^{N_S}\frac{\mathscr{D}j_{\Gamma_q}}{\mathscr{D}U_{T_p}}\Delta\Gamma_q\Delta U_{T_p}-\sum_{p=1}^{N_\Gamma}\sum_{q=1}^{N_\Gamma}\varphi_{D_q}^{T}\frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D}U_p}\Delta U_p &= 0,\end{aligned} \tag{4.13}$$

where the boundary flux of the turbulence model has been separated out from the residual in order to create a fully hybrid boundary condition. This modification of the residual can be written as

$$\mathcal{R}_{T_p}=(\hat{F}_T)_{\Gamma_p}+\mathcal{R}_{T_p}^{*}. \tag{4.14}$$

We also note that the discrete objective function on the surface in Eq. (4.13) has been written as

$$\mathcal{J}_{D_\Gamma}=\sum_{q=1}^{N_S}j_{\Gamma_q}\Delta\Gamma_q. \tag{4.15}$$

At the far field, considering objective functions not defined along that boundary and neglecting flow gradients and viscosity contributions, Eq. (4.13) will reduce to the Euler far field boundary condition,

$$-\int_{\Gamma_\infty}\phi^{T}\frac{\partial F_i}{\partial U}\hat{n}_i\delta U d\Gamma=0. \tag{4.16}$$

At the viscous wall, discretizing the surface integral in Eq. (4.13) into a sum of the integrals over the wall for each boundary cell, and then making the assumption that this condition is not just true over the whole surface, but also for each cell, we obtain, for cell p,

$$\begin{aligned}\int_{\Gamma_p}\left(\left(L_{\Gamma}^{*}(\varphi_C)-\beta\left(\frac{\partial j_{\Gamma}}{\partial U}\right)^{T}\right)^{T}\delta U-\varphi_C^{T}\left(\mathcal{A}_3+\mathcal{B}_3\right)\delta(\partial_j U)\hat{n}_i\right)d\Gamma & \\ -(1-\beta)\sum_{q=1}^{N_S}\frac{\mathscr{D}j_{\Gamma_q}}{\mathscr{D}U_{T_p}}\Delta\Gamma_q\Delta U_{T_p}-\sum_{q=1}^{N_\Gamma}\varphi_{D_q}^{T}\frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D}U_p}\Delta U_p &= 0.\end{aligned} \tag{4.17}$$

After some manipulation, including the assumption that the perturbations in the flow quantities are step-wise constant along the wall in each cell, this then becomes

$$
\begin{aligned}
\beta\left(\int_{S_p}\frac{\partial j_\Gamma}{\partial U}d\Gamma\right)\delta U_p+(1-\beta)\sum_{q=1}^{N_S}\frac{\mathscr{D}j_{\Gamma_q}}{\mathscr{D}U_p}\Delta\Gamma_q\Delta U_p \\
-\left(\int_{S_p}\varphi_{C_{\rho u_j}}^T\hat{n}_i\right)\delta p_p+\sum_{q=1}^{N_S}\varphi_{D_q}^T\left(\frac{\rho_p}{p_p}\frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D}\rho_p}+\frac{1}{\gamma-1}\frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D}(\rho E)_p}\right)\Delta p_p \\
+\left(\int_{S_p}\left(\varphi_{C_{\rho u_j}}^T\tau_{ij}\frac{\partial\mu}{\partial T}+\mu\left(\partial_i\varphi_{C_{\rho E}}\right)\frac{C_p}{Pr}\right)\hat{n}_i d\Gamma\right)\delta T_p-\sum_{q=1}^{N_S}\frac{\rho_p}{T_p}\varphi_{D_q}^T\frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D}\rho_p}\Delta T_p \\
+\left(\int_{S_p}\varphi_{C_{\rho u_j}}^T\mu\hat{n}_i d\Gamma\right)\delta\tau_{ij_p} \\
+(1-\beta)\sum_{q=1}^{N_S}\frac{\mathscr{D}j_{\Gamma_q}}{\mathscr{D}U_{T_p}}\Delta\Gamma_q\Delta U_{T_p}+\sum_{q=1}^{N_S}\varphi_{D_q}^T\frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D}U_{T_p}}\Delta U_{T_p} &= 0,
\end{aligned}
\tag{4.18}
$$

which, given the additional assumption that the continuous perturbations are equal to the discrete ones, i.e., $\delta()_p \approx \Delta()_p$, implies that if the perturbation to the objective function can be written in the form

$$
\frac{\partial j_\Gamma}{\partial U}\delta U=\frac{\partial j_\Gamma}{\partial p}\delta p+\frac{\partial j_\Gamma}{\partial\tau_{ij}}\delta\tau_{ij}+\frac{\partial j_\Gamma}{\partial T}\delta T+\frac{\partial j_\Gamma}{\partial U_T}\delta U_T, \tag{4.19}
$$

the δp, $\delta\tau_{ij}$, δT, and δU_T dependencies can be removed, producing adjoint boundary conditions on the wall.

With these boundary terms removed, and using Eq. (4.11) to remove the eddy viscosity adjoint variable, Eq. (4.12) becomes

$$
\begin{aligned}
\int_\Omega\left(L_\Omega^*(\varphi_C)-\beta\left(\frac{\partial j_\Omega}{\partial U}\right)^T\right)^T\delta U d\Omega \\
-(1-\beta)\sum_{p=1}^{N}\frac{\mathscr{D}\mathcal{J}_{D\Omega}}{\mathscr{D}U_p}\Delta U_p-\sum_{p=1}^{N}\sum_{q=1}^{N}\varphi_{D_q}^T\frac{\mathscr{D}\mathcal{R}_{T_q}^{(*)}}{\mathscr{D}U_p}\Delta U_p \\
+\sum_{p=1}^{N}\sum_{q=1}^{N}\frac{\mathscr{D}f_q}{\mathscr{D}U_p}\Delta U_p\int_{\Omega_q}\left(\partial_i\varphi_C^T\right)\mathcal{C}_1 d\Omega &= 0.
\end{aligned}
\tag{4.20}
$$

Discretizing the domain integral into a sum of the integrals over each cell, and then making the assumption that this condition is not just true within the whole domain, but also within each cell, we obtain, for cell p,

$$
\begin{aligned}
\int_{\Omega_p}\left(L_\Omega^*(\varphi_C)-\beta\left(\frac{\partial j_\Omega}{\partial U}\right)^T\right)^T\delta U d\Omega \\
-(1-\beta)\frac{\mathscr{D}\mathcal{J}_{D\Omega}}{\mathscr{D}U_p}\Delta U_p-\sum_{q=1}^{N}\varphi_{D_q}^T\frac{\mathscr{D}\mathcal{R}_{T_q}^{(*)}}{\mathscr{D}U_p}\Delta U_p \\
+\sum_{q=1}^{N}\frac{\mathscr{D}f_q}{\mathscr{D}U_p}\Delta U_p\int_{\Omega_q}\left(\partial_i\varphi_C^T\right)\mathcal{C}_1 d\Omega &= 0.
\end{aligned}
\tag{4.21}
$$

The final step is then to again assume the continuous flow perturbations are step-wise constant within each cell, and that $\delta U_p \approx \Delta U_p$, allowing them to be cancelled out. This gives the hybrid adjoint equation for viscous flow with a general turbulence model:

$$\int_{\Omega_p}\left(L^*_\Omega(\varphi_C)-\beta\left(\frac{\partial j_\Omega}{\partial U}\right)^T\right)d\Omega-(1-\beta)\sum_{q=1}^{N}\left(\frac{\mathscr{D}j_q}{\mathscr{D}U_p}\right)^T\Delta\Omega_q$$
$$-\sum_{q=1}^{N}\left(\frac{\mathscr{D}\mathcal{R}^{(*)}_{T_q}}{\mathscr{D}U_p}\right)^T\varphi_{D_q}+\sum_{q=1}^{N}\left(\frac{\mathscr{D}f_q}{\mathscr{D}U_p}\right)^T\int_{\Omega_q}\mathcal{C}_1^T\partial_i\varphi_C d\Omega = 0. \quad (4.22)$$

With this definition, the perturbation to the objective function, given by Eq. (4.5) can thus be written

$$\begin{aligned}\{\delta,\Delta\}\mathcal{J}_H=\{\delta,\Delta\}\mathcal{L} &= \int_\Omega\left(\beta\frac{\partial j_\Omega}{\partial\alpha}\delta\alpha-\varphi_C^T\partial_i\left(\left(\frac{\partial F_i}{\partial\alpha}-\mathcal{A}_1-\mathcal{A}_4-\mathcal{B}_1\right)\delta\alpha\right)\right)d\Omega\\ &+\int_\Gamma\beta\frac{\partial j_\Gamma}{\partial\alpha}\delta\alpha d\Gamma+(1-\beta)\frac{\mathscr{D}\mathcal{J}_D}{\mathscr{D}\alpha}\Delta\alpha\\ &-\sum_{p=1}^{N}\frac{\mathscr{D}f_p}{\mathscr{D}\alpha}\Delta\alpha\int_{\Omega_p}\mathcal{C}_1^T\partial_i\varphi_C d\Omega+\sum_{p=1}^{N}\varphi_{D_p}^T\frac{\mathscr{D}\mathcal{R}_{T_p}}{\mathscr{D}\alpha}\Delta\alpha.\end{aligned} \quad (4.23)$$

5. Results

Before applying the turbulent hybrid adjoint approach developed above to an appropriate test case, it is useful to first make some observations based on the theory:

(*a*) The hybrid adjoint Eqs. (4.22) are already written in finite volume form because of the need to discretize the domain integral.

(*b*) By considering a continuous objective function defined on a surface, which does not explicitly depend on the turbulence model variables, such as the drag on an airfoil, and splitting Eq. (4.22) into the adjoint equations for the mean flow and for the turbulence model gives a continuous-like adjoint PDE with discrete and mixed source terms for the mean flow,

$$\int_{\Omega_p}L^*_\Omega(\varphi_C)d\Omega=\sum_{q=1}^{N}\left(\frac{\mathscr{D}\mathcal{R}^{(*)}_{T_q}}{\mathscr{D}U_p}\right)^T\varphi_{D_q}-\sum_{q=1}^{N}\left(\frac{\mathscr{D}f_q}{\mathscr{D}U_p}\right)^T\int_{\Omega_q}\mathcal{C}_1^T\partial_i\varphi_C d\Omega, \quad (5.1)$$

and a discrete-like linear system with mixed source terms for the turbulence model,

$$\sum_{q=1}^{N}\left(\frac{\mathscr{D}\mathcal{R}^{(*)}_{T_q}}{\mathscr{D}U_p}\right)^T\varphi_{D_q}=\sum_{q=1}^{N}\left(\frac{\mathscr{D}f_q}{\mathscr{D}U_p}\right)^T\int_{\Omega_q}\mathcal{C}_1^T\partial_i\varphi_C d\Omega, \quad (5.2)$$

noting that the chosen objective function influences the coupled system only through the hybrid boundary conditions on the viscous wall, i.e.,

$$\int_{S_p}\left(\frac{\partial j_\Gamma}{\partial p}-\varphi^T_{C_{\rho u_j}}\hat{n}_i\right)d\Gamma+\sum_{q=1}^{N_S}\varphi^T_{D_q}\left(\frac{\rho_p}{p_p}\frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D}\rho_p}+\frac{1}{\gamma-1}\frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D}(\rho E)_p}\right)=0, \quad (5.3)$$

$$\int_{S_p}\left(\frac{\partial j_\Gamma}{\partial T}+\left(\varphi^T_{C_{\rho u_j}}\tau_{ij}\frac{\partial\mu}{\partial T}+\mu\left(\partial_i\varphi_{C_{\rho E}}\right)\frac{C_p}{Pr}\right)\hat{n}_i\right)d\Gamma-\sum_{q=1}^{N_S}\frac{\rho_p}{T_p}\varphi^T_{D_q}\frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D}\rho_p}=0, \quad (5.4)$$

$$\int_{S_p} \left(\frac{\partial j_\Gamma}{\partial \tau_{ij}} + \varphi^T_{C_{\rho u_j}} \mu \hat{n}_i \right) d\Gamma = 0, \tag{5.5}$$

and

$$\sum_{q=1}^{N_S} \varphi^T_{D_q} \frac{\mathscr{D}(\hat{F}_T)_{\Gamma_q}}{\mathscr{D} U_{T_p}} = 0. \tag{5.6}$$

The form of Eqs. (5.1) and (5.2) implies that the former should be solved as a PDE and the second as a linear system.

(*c*) While the summation signs in the hybrid adjoint equations (4.22) and wall boundary conditions (4.18) are written as either over all the cells in the mesh, or over all the cells along the surface, it is not typically required to consider the explicit dependence of every cell in the mesh to every other cell. The numerical scheme usually considers a smaller stencil for calculating the flow (and gradients) for any particular cell, and it is this stencil that is most important when handling parts of the hybrid approach discretely. The same is generally true of the calculation of the eddy viscosity.

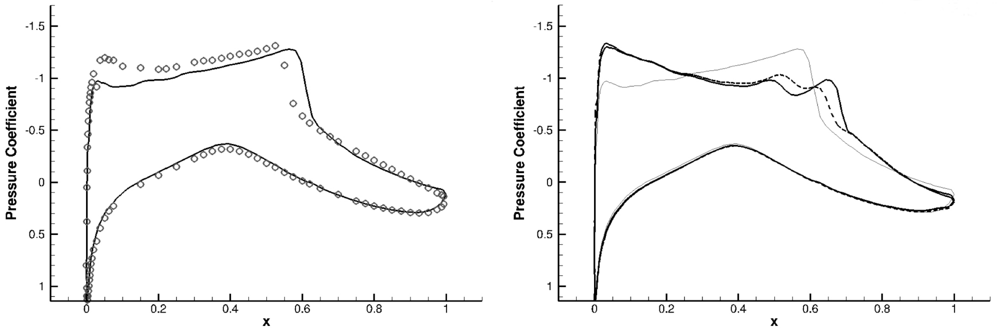
(*d*) The continuous-like treatment of the boundary conditions in the hybrid adjoint derivation implies that, at least on a viscous wall, the choice of objective function in the hybrid adjoint is restricted in a way similar as to the continuous adjoint. This means that only functionals of the pressure, temperature, stress, and turbulence adjoint variable should be considered. However, within the domain, there is the possibility of using a more varied selection of objective functions.

(*e*) An important result from the hybrid derivation shown previously is that no derivatives of the eddy viscosity appear in the continuously treated parts of the hybrid adjoint equations or boundary conditions, and, instead, these model-dependent derivatives are handled discretely. Because the turbulence model is treated discretely, and all required derivatives in the discrete implementation are derived using Automatic Differentiation (AD), this means that, given the only coupling from the turbulence model to the mean flow is via μ_T, the mathematical form of the hybrid adjoint is general for any turbulence model.

(*f*) The derivation of the hybrid adjoint in this brief considered only viscous wall and far field boundary conditions. Some additional work therefore may be required to apply the resulting PDE to other boundary conditions, such as inlets and outlets, and if the outer boundary is not sufficiently far away that viscous terms cannot be neglected.

(*g*) Though shape of the wall S was held fixed in the above derivations of the frozen-viscosity continuous adjoint and hybrid adjoint, the adjoint equations derived, and the adjoint variables that come from their solution, are in fact general and can be used to evaluate the sensitivities to changes in this shape. Assuming there is no explicit dependence of the objective function on the turbulence variables, the objective function depends only on the forces on S and some constant projection vector, and that the surface is either smooth or δS is zero where it is singular, it is possible to write the perturbation to the objective function with respect to shape perturbations as (Bueno-Orovio *et al.* 2012)

$$\begin{aligned} \delta \mathcal{J} \;\; = \;\; & \int_S \Bigg(\hat{n}_i \left(\partial_j \phi_{\rho u_i} + \partial_i \phi_{\rho u_j} - \frac{2}{3} \delta_{ij} \partial_l \phi_{\rho u_l} \right) \partial_k u_k \hat{n}_j \\ & -\mu^{v2} C_p \left(\partial_i(\phi_{\rho E}) - \partial_j(\phi_{\rho E}) \hat{n}_j \hat{n}_i \right) \left(\partial_i(T) - \partial_j(T) \hat{n}_j \hat{n}_i \right) \Bigg) \delta S d\Gamma. \end{aligned} \tag{5.7}$$



(a) (b)

FIGURE 1. (a) Pressure coefficient along the RAE 2822 airfoil compared with experimental results. (b) Coefficient of pressure along baseline and optimized (15th design step) RAE 2822 airfoils (solid grey, baseline; solid black, frozen continuous; dashed, hybrid).

This result can be used to evaluate the sensitivity of objective functions such as the coefficients of lift and drag on an airfoil with respect to changes in its surface shape.

The test case used to investigate the frozen continuous and full hybrid adjoints was transonic flow over the RAE 2822 airfoil a at non-zero angle-of-attack. The flow conditions used, corresponding to AGARD AR 138 case 10 (Cook *et al.* 1979; Haase *et al.* 1993), were:

- Freestream Mach number, $M_\infty = 0.754$,
- Freestream temperature, $T_\infty = 273.15K$,
- Angle-of-attack, $\alpha = 2.57^o$,
- Reynolds number, $Re = 6.2 \times 10^6$,

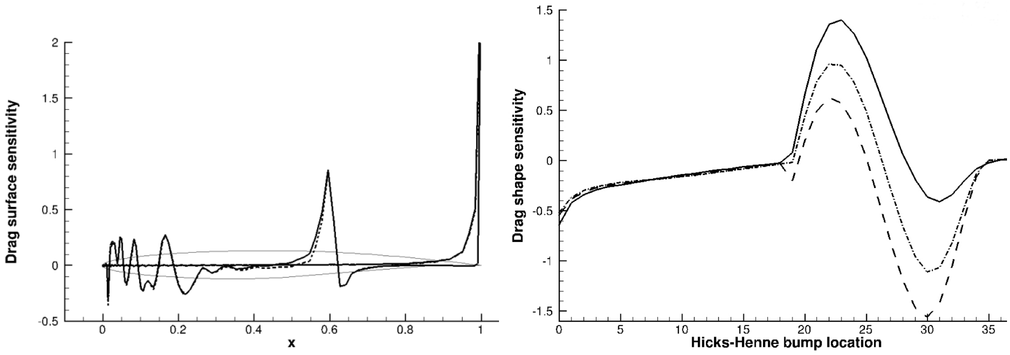
and the grid for this case contains a total of 13,937 points, including 192 on the surface of the airfoil. The turbulence model used was the Spalart-Allmaras one-equation turbulence model, and the resulting surface pressure coefficients are shown in Figure 1(a).

5.0.3. *Surface sensitivity*

Figure 2(a) shows the sensitivity of the coefficient of drag to changes in the surface of the RAE 2822 airfoil obtained using the frozen continuous and hybrid adjoint approaches. It can be seen that there is no significant difference in the sensitivity on the lower surface, but on the upper surface, near the location of the shock, the frozen continuous and hybrid results noticeably differ.

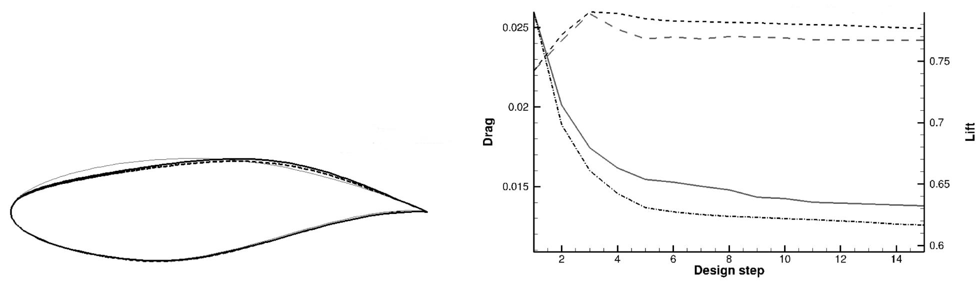
5.0.4. *Shape sensitivity*

The airfoil shape was parameterized using 38 Hicks-Henne bump functions (Hicks & Henne 1978) and the sensitivity of the airfoil drag to changes in the surface was then calculated by projecting these bump functions onto the surface of the airfoil. These bumps were numbered from the lower side of the trailing edge clockwise toward the leading edge (0 to 18) and then backward from the leading edge along the upper surface to the trailing edge (19 to 37), and positioned at intervals of 0.05 of the chord along the x-axis. The sensitivities obtained by finite differencing, the frozen-viscosity continuous adjoint, and the hybrid adjoint are shown in Figure 2(b). A marked difference is seen between the frozen-viscosity continuous adjoint, the hybrid adjoint and the results from finite differencing on the upper surface of the airfoil. To validate the finite difference



(a) (b)

FIGURE 2. (a) Surface sensitivity of coefficient of drag along the RAE 2822 airfoil (solid, frozen continuous; dotted, hybrid). (b) Shape sensitivity of coefficient of drag along the RAE 2822 airfoil (solid, finite differences; dashed, frozen continuous; dash-dotted, hybrid).



(a) (b)

FIGURE 3. (a) Shape comparison of baseline and optimized (10th design step) RAE 2822 airfoils. Note that the shape has been stretched so that $x : y = 0.5 : 1$ (solid grey, baseline; solid black, frozen continuous; dashed, hybrid). (b) Shape optimization of the RAE 2822 airfoil, aiming to minimize the coefficient of drag while constraining the coefficient of lift above 0.74 (solid, C_D frozen continuous; dash-dotted, C_D hybrid; long dashed, C_L frozen continuous; short dashed, C_L hybrid).

results, the finite difference step in the shape was varied from $1e^{-2}$ to $1e^{-8}$, but over this range no significant change was seen in the finite difference results.

5.0.5. *Shape optimization*

Using the above results for surface sensitivities, and the parametrization of the airfoil using 38 Hicks-Henne bump functions, both adjoint methods were then applied to a problem of gradient-based optimization of the shape of the RAE 2822 airfoil with the objective of reducing the drag, while keeping the lift constant. A quasi-Newton method was used to enable the optimization. Figure 3(b) shows the evolution of the drag and lift values at each design step.

Application of the hybrid adjoint to the optimization showed a significant difference from the frozen-viscosity continuous method. After 15 design steps the frozen-viscosity approach gave a drag coefficient of 53.1% of the original value with a lift-to-drag ratio of 55.6 (the baseline was 28.6), and the hybrid gave a drag coefficient of 48.4% and a lift-to-drag ratio of 61.8. The resulting surface pressures is shown in Figure 1(b), indicating that the optimizer is able to reduce the strong shock on the upper surface. The oscillatory nature of the coefficient of pressure profiles is expected to be caused by the relatively coarse discretization of the airfoil into 38 Hicks-Henne bump functions. Using a greater number of bumps would be expected to smooth out the profiles. Finally, Figure 3(a) shows the modified airfoil surfaces produced.

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