Towards a hybrid adjoint approach for complex flow simulations

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1. Motivation and objectives

The adjoint method was first developed for aerodynamic shape optimization applications through the use of control theory by Jameson (1998) in the late 1980s and early 1990s, using ideas adapted from more general work by Lions (1971) on optimal control of systems governed by partial differential equations (PDEs). Over the past two decades, adjoint methods have been used in a variety of applications including shape optimization of wing geometries (Reuther & Jameson 1995), goal-oriented numerical error estimation and mesh adaptation (Giles *et al.* 2003; Venditti & Darmofal 2002), sensitivity analysis, and uncertainty quantification (Duraisamy & Chandrashekar 2012).

Depending on the approach followed for the derivation of the adjoint equations, this method is conventionally characterized as either discrete or continuous. While both of these approaches involve numerical solutions, the difference arises from the order of discretization and linearization of the governing equations. In the discrete adjoint method, the discretized governing equations are used to derive the discrete adjoint equations. In the continuous adjoint method, the adjoint equations are derived from the analytical form of the PDE and then discretized to obtain a discrete representation. This difference is shown in Figure 1, noting that though both paths lead to discretized adjoint equations, unless we have dual consistency these equations and their resultant adjoint variables will not be identical.

The discrete method can employ algorithmic Automatic Differentiation (Mader *et al.* 2008), either via source code transformation, e.g., using TAPENADE (Hascoët & Pascual 2004), or operator overloading, e.g., using ADOL-C (Griewank *et al.* 1996), to calculate partial derivatives and hence, PDEs of arbitrary complexity can be handled with very little mathematical development. However, the resulting system can become highly stiff or ill-conditioned and difficult to solve, and little freedom exists to tailor the scheme for the numerical solution of the problem. On the other hand, the discrete adjoint provides the "exact" gradient of the discretized objective function, and it is able to treat objective functions of arbitrary complexity. It is also possible to analytically derive (by hand) the required partial derivative terms from the discretized forms of the flow residuals and then develop code based on this; however, this requires significant development, possibly more than that generally required in the continuous method (Nadarajah & Jameson 2000). Moreover, there exist complex sets of governing equations for which the hand-differentiation of all terms in the equations is infeasible.

In contrast, the continuous approach allows for a more thorough understanding of the physical significance of the adjoint equations and boundary conditions, but may require significant mathematical development. It is, however, well connected to the original PDE in its analytical form and has a unique form independent of the scheme used to solve the flow-field system. For these reasons, it offers flexibility in choosing the discretization scheme for the adjoint system, and the problem can be well posed. However, this method

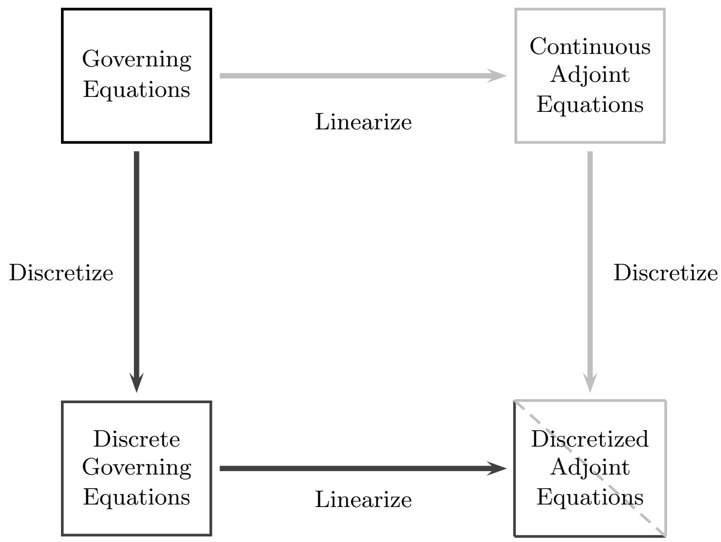

FIGURE 1. General scheme for deriving discrete and continuous adjoints

	Discrete	Continuous
Ease of development	+	−
Compatibility of numerical gradients with the discretized PDE	+	−f
Compatibility of numerical gradients with the continuous PDE	−	+
Surface formulation for gradients	−	+
Ability to handle arbitrary functionals	+	−
Ability to handle non-differentiability	+	−
Computational cost (CPU usage and storage)	−	+
Flexibility in solution	−	+

TABLE 1. Simple comparison between the discrete and continuous adjoint approaches

may result in discrepancies in the gradient of the discretized objective function and may limit the types of functionals that can be treated. Moreover, some limitations exist in the kinds of cost functions that can be treated, and the derivation of the continuous adjoint equations may be infeasible for many complex governing PDEs. Furthermore, for sensitivity analysis, surface gradient formulations exist that do not require the deformation of the volume mesh, thus saving considerable computational time and increasing the robustness of the procedures.

Table 1 shows the relative advantages and disadvantages of using the two standard methods. Where an approach has been given a + sign, this indicates it has favorable characteristics in this respect, and a − sign indicates undesirable characteristics.

The discrete adjoint can be derived via a Lagrange method that enforces the governing equations for the flow discretely, using the flow solution residuals. The continuous adjoint can be derived by enforcing the analytical form of the governing equations. In this work we introduce a hybrid approach that combines these two methods by enforcing part of

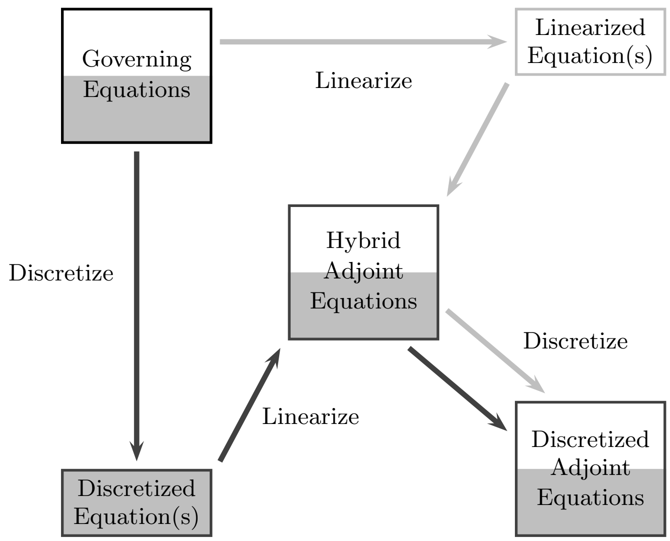

FIGURE 2. General scheme for deriving hybrid adjoint

the governing equations continuously and part discretely. This general hybrid scheme is shown in Figure 2.

The hybrid adjoint approach is intended for problems involving very complex PDEs (such as those involving two or more equation turbulence models, combustion including look-up tables, and multi-species simulations such as those seen in multi-species, multiphase problems). The basic idea is to use a continuous formulation for those portions of the flow problems for which such formulations already exist (in the form of a program or as previously published equations), but to treat discretely those portions of the governing equations that are difficult (or impossible) to handle analytically. The result is intended to be a formulation that produces high-quality adjoint information and that inherits the favorable characteristics of the original methods, while overcoming their drawbacks.

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 which can be represented by $\mathcal{G}(U, \alpha) = 0$, where U is the solution.

The adjoint variables that solve these equations can be used purely as a mathematical tool to find the required sensitivities, but, as discussed by Giles & Pierce (2000) and Belegundu & Arora (1985), they also have a physical meaning. They can 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 of the order of one additional flow solution, and the adjoint variables represent the sensitivities of $\mathcal{J}$ to changes in all parameters that define the problem at every point in the domain. In contrast, though 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 each 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 work we consider the latter method, and present the discrete, continuous and then hybrid derivations in an identical context. The following sections summarize the two existing methods via this approach.

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, $\mathcal{R}_i$, i.e., $\mathcal{G} = \{\mathcal{R}_i\} = 0$. This gives the Lagrangian

$$\mathcal{L} = \mathcal{J}_D + \sum_{i=1}^{N} \psi_i^T \mathcal{R}_i, \tag{2.1}$$

where ψ is the Lagrange multiplier or discrete adjoint variable, and the discrete perturbation to $\mathcal{L}$ is

$$\Delta\mathcal{L} = \Delta\mathcal{J}_D + \sum_{i=1}^{N} \psi_i^T \Delta\mathcal{R}_i. \tag{2.2}$$

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

$$\sum_{j=1}^{N} \left(\frac{\mathfrak{D}\mathcal{R}_j}{\mathfrak{D}U_i}\right)^T \psi_j = -\left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_i}\right)^T, \tag{2.3}$$

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

$$\Delta\mathcal{J}_D = \sum_{i=1}^{N} \psi_i^T \frac{\mathfrak{D}\mathcal{R}_i}{\mathfrak{D}\alpha}\Delta\alpha + \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha}\Delta\alpha, \tag{2.4}$$

where it is seen that once the adjoint equation 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, $\mathcal{N}$, and the boundary conditions, $\mathcal{B}$, i.e., $\mathcal{G} = \{\mathcal{N}, \mathcal{B}\} = 0$. The Lagrangian is thus

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

where ϕ, $\phi_\mathcal{B}$ are the Lagrange multipliers or continuous adjoint variables, and the continuous perturbation to this now becomes

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

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. In doing this we will also express $\phi_{\mathcal{B}}$ in terms of ϕ, leaving just one set of adjoint variables. As the remaining terms in the perturbation to the objective function are either known or easily calculated quantities, this quantity can then 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 objective function, and the boundary conditions and cannot be shown generally as in the discrete case above.

3. Hybrid adjoint methodology

The main motivation behind a hybrid adjoint is to combine the best qualities of the discrete and continuous approaches. The goal is thus to aim for the convergence and robustness properties of the continuous method, with the flexibility to handle arbitrarily complex PDEs of the discrete adjoint. While there have been approaches that attempt to combine the continuous and discrete methods taken before, such as Lozano and Ponsin's use of continuous adjoint variables in a discrete adjoint framework to calculate sensitivities (Lozano & Ponsin 2011), the method discussed in this work (Taylor *et al.* 2012) attempts to build a more general, true hybrid.

In our approach, we will split the governing equations into those that will be enforced continuously and those that will be enforced discretely, i.e., $\mathcal{G} = \{\{\mathcal{N}, \mathcal{B}\}_C, \{\mathcal{R}_k\}_D\} = 0$. We note that the discrete boundary conditions are not explicitly mentioned here because they are already included and applied in the discrete residual calculation.

The equations that will be treated continuously are 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), while 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 will not be needed in the future, thus significantly lowering the development cost for further problems.

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

$$\mathcal{J}_H = \beta \mathcal{J}_C + (1 - \beta)\mathcal{J}_D, \tag{3.1}$$

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.

The Lagrangian now becomes

$$\mathcal{L} = \beta \mathcal{J}_C + (1 - \beta)\mathcal{J}_D - \int_\Omega \nu^T \mathcal{N}_C d\Omega - \int_\Gamma \nu_{\mathcal{B}}^T \mathcal{B}_C d\Gamma + \sum_{i=1}^{N} \mu_i^T \mathcal{R}_{D_i}, \tag{3.2}$$

where ν, $\nu_{\mathcal{B}}$ and μ are the Lagrange multipliers or hybrid adjoint variables, and the hybrid perturbation can thus be written

$$\begin{aligned}\{\delta,\Delta\}\mathcal{L} \quad = \quad & \beta\,(\mathcal{J}_C' - \mathcal{J}_C) + (1-\beta)\Delta\mathcal{J}_D \\ & -\left(\int_{\Omega'} \nu^T \mathcal{N}_C' d\Omega - \int_{\Omega} \nu^T \mathcal{N}_C d\Omega\right) - \left(\int_{\Gamma'} \nu_{\mathcal{B}}^T \mathcal{B}_C' d\Gamma - \int_{\Gamma} \nu_{\mathcal{B}}^T \mathcal{B}_C d\Gamma\right) \\ & + \sum_{i=1}^{N} \mu_i^T \Delta\mathcal{R}_{D_i}.\end{aligned} \tag{3.3}$$

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 removing the boundary condition adjoint variables $\nu_{\mathcal{B}}$ by expressing them in terms of ν, and in so doing generating the adjoint equation and boundary conditions for ν and μ. Due to the dependence of this method on the actual analytical form of the continuous part, this cannot be shown generally.

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

An interesting feature that can be inferred from the above equation 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 $\{\mathcal{N},\mathcal{B}\}_C = \emptyset$, we recover the pure discrete method, and by setting $\beta = 1$ and defining $\{\mathcal{N},\mathcal{B}\}_C = \{\mathcal{N},\mathcal{B}\}$, and thus $\{\mathcal{R}\}_D = \emptyset$, we get the pure continuous.

However, we are no longer limited to just those two options. It is now 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.

4. Application to quasi one-dimensional flow with a simple combustion model

4.1. *Primal problem*

We consider quasi one-dimensional Euler flow (smooth or shocked) in the duct $x \in [x_i, x_e]$ with height $h(x)$. Additionally, inspired by Powers & Aslam (2006), we include a simple combustion model, introducing the reaction progress variable Λ and the additional flow variable $\lambda = \rho\Lambda$.

The analytical governing equations are given as

$$\mathcal{N} \equiv \frac{d}{dx}(hF) - \frac{dh}{dx}P - hQ = 0, \quad x \in [x_i, x_e], \tag{4.1}$$

where

$$U = \begin{pmatrix} \rho \\ m \\ \epsilon \\ \lambda \end{pmatrix}, \quad F = \begin{pmatrix} m \\ \frac{m^2}{\rho} + p \\ mH \\ m\Lambda \end{pmatrix}, \quad P = \begin{pmatrix} 0 \\ p \\ 0 \\ 0 \end{pmatrix}, \quad Q = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \omega \end{pmatrix}, \tag{4.2}$$

$$H = \frac{\epsilon + p}{\rho}, \tag{4.3}$$

$$p = (\gamma - 1)(\epsilon - \frac{m^2}{2\rho} + \lambda q), \tag{4.4}$$

where q is the specific heat release, a constant, and

$$T = \frac{p}{\rho R}. \tag{4.5}$$

We consider two possible forms for the combustion source term ω:
(a) a differentiable, exponential form, $\omega = \rho(1 - \Lambda)e^{-C/RT}$, and
(b) a non-differentiable, Heaviside form, $\omega = b\rho(1 - \Lambda)\mathcal{H}(T - T^*)$.
We also define two objective functions as integrals over the domain:
(a) a differentiable form, $\mathcal{J} = \int_{x_i}^{x_e} p dx$, the 'lift' over the duct, and
(b) a non-differentiable form, $\mathcal{J} = \int_{x_i}^{x_e} |p - p^*| \, dx$, the magnitude of a pressure difference.

Note that the reason for choosing both differentiable and non-differentiable source and objective functions is to allow the hybrid method to be developed, investigated and applied to situations where the continuous adjoint cannot.

4.2. *Discrete adjoint method*

Following the general discrete approach we can write the adjoint equation:

$$\sum_{l=1}^{N} \left(\frac{\mathfrak{D}\mathcal{R}_l}{\mathfrak{D}U_k}\right)^T \psi_l = -\left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k}\right)^T, \tag{4.6}$$

and the perturbation to the objective function:

$$\Delta \mathcal{J}_D = \sum_{k=1}^{N} \psi_k^T \frac{\mathfrak{D}\mathcal{R}_k}{\mathfrak{D}\alpha} \Delta\alpha + \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha} \Delta\alpha, \tag{4.7}$$

where the residuals, $\mathcal{R}_k$, are given in the solution strategy to the primal problem above.

4.3. *Continuous adjoint method*

Without showing in detail the derivation of the continuous adjoint for this case, which is relatively long and, for simple quasi one-dimensional flow, has been well explained by Giles & Pierce (2001), we state that the adjoint equation is

$$L^*(\phi) - \left(\frac{\partial j}{\partial U}\right)^T = 0, \quad x \in [x_i, x_e], \tag{4.8}$$

where

$$L^*(\phi) = -h \left(\frac{\partial F}{\partial U}\right)^T \frac{d\phi}{dx} - \left(\frac{dh}{dx}\left(\frac{\partial P}{\partial U}\right)^T + h\left(\frac{\partial Q}{\partial U}\right)^T\right)\phi, \tag{4.9}$$

with the boundary conditions

$$\left[h\phi^T \frac{\partial F}{\partial U} \delta U\right]_{x_i}^{x_e} = 0, \tag{4.10}$$

giving the perturbation to the objective function

$$\delta \mathcal{J}_C = \int_{x_i}^{x_e} \phi^T \frac{\partial \mathcal{N}}{\partial \alpha} \delta\alpha dx + \int_{x_i}^{x_e} \frac{\partial j}{\partial \alpha} \delta\alpha dx. \tag{4.11}$$

We note also that for shocked flow the objective function needs to be written as an integral on either side of the shock, located at x_s:

$$\mathcal{J}_C = \int_{x_i}^{x_s} j dx + \int_{x_s}^{x_e} j dx, \tag{4.12}$$

and that this generates an additional adjoint boundary condition at the shock

$$h_s \phi_s^T \left[\frac{dF}{dx} \right]_{x_s-}^{x_s+} = - [j]_{x_s-}^{x_s+} . \tag{4.13}$$

4.4. *Hybrid adjoint method*

In the hybrid adjoint approach for this case we choose to continuously enforce the analytical form of the Euler part of the flow equations, $\mathcal{N}_E$, and their boundary conditions, $\mathcal{B}_E$, and discretely enforce the residual for the solution of the combustion model, $\mathcal{R}_{\lambda_k}$, i.e., $\mathcal{G} = \{\{\mathcal{N}_E, \mathcal{B}_E\}_C, \{\mathcal{R}_{\lambda_k}\}_D\}$.

In this simple quasi one-dimensional problem the boundary surface in general will not change, and thus for smooth flow the $\mathcal{B}_E$ term can be ignored. However, in the case of shocked flow we must enforce the Rankine-Hugoniot conditions at the internal shock boundary

$$\mathcal{B}_E = [hF_E]_{x_s-}^{x_s+} = 0, \tag{4.14}$$

and must also admit the effect from the potential movement of this boundary surface within the perturbation of the functional. For this case we have the Lagrangian

$$\begin{aligned} \mathcal{L} \;\; = \;\; & \beta \left(\int_{x_i}^{x_s} j dx + \int_{x_s}^{x_e} j dx \right) + (1-\beta)\mathcal{J}_D \\ & - \int_{x_i}^{x_s} \nu^T \mathcal{N}_E dx - \int_{x_s}^{x_e} \nu^T \mathcal{N}_E dx - \nu_s^T \left[hF_E \right]_{x_s-}^{x_s+} + \sum_{k=1}^{N} \mu_k^T \mathcal{R}_{\lambda_k}, \end{aligned} \tag{4.15}$$

and its perturbation

$$\begin{aligned} \{\delta, \Delta\}\mathcal{L} \;\; = \;\; & \beta \left(\int_{x_i}^{x_s} \delta j dx + \int_{x_s}^{x_e} \delta j dx - [j]_{x_s-}^{x_s+} \right) + (1-\beta)\Delta\mathcal{J}_D \\ & - \int_{x_i}^{x_s} \nu^T \delta\mathcal{N}_E dx - \int_{x_s}^{x_e} \nu^T \delta\mathcal{N}_E dx - \nu_s^T \delta \left([hF_E]_{x_s-}^{x_s+} \right) + \sum_{k=1}^{N} \mu_k^T \Delta\mathcal{R}_{\lambda_k}. \end{aligned} \tag{4.16}$$

Using linearity, the perturbed quantities on the right hand side can be evaluated as

$$\delta j = \frac{\partial j}{\partial U}\delta U + \frac{\partial j}{\partial \alpha}\delta\alpha, \tag{4.17}$$

$$\Delta\mathcal{J}_D = \sum_{k=1}^{N} \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k}\Delta U_k + \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha}\Delta\alpha, \tag{4.18}$$

$$\delta\mathcal{N}_E = L_E(\delta U) - \frac{\partial \mathcal{N}_E}{\partial \alpha}\delta\alpha = 0, \tag{4.19}$$

where

$$L_E(\delta U) = \frac{d}{dx}\left(h \left(\frac{\partial F_E}{\partial U}\delta U \right) \right) - \frac{dh}{dx}\left(\frac{\partial P_E}{\partial U}\delta U \right), \tag{4.20}$$

$$\Delta \mathcal{R}_{D_k} = \sum_{l=1}^{N} \frac{\mathfrak{D}\mathcal{R}_{D_k}}{\mathfrak{D}U_l}\Delta U_l + \frac{\mathfrak{D}\mathcal{R}_{D_k}}{\mathfrak{D}\alpha}\Delta\alpha = 0, \tag{4.21}$$

and

$$\delta\left([hF_E]_{x_s-}^{x_s+}\right) = h_s\left[\frac{\partial F_E}{\partial U}\delta U\right]_{x_s-}^{x_s+} - h_s\left[\frac{dF_E}{dx}\right]_{x_s-}^{x_s+}\delta x_s. \tag{4.22}$$

Incorporating these into Eq. (4.16) and performing integration by parts on the continuous terms, followed by rearrangement, we obtain

$$\begin{aligned}
\{\delta,\Delta\}\mathcal{L} \;=\;& \int_{x_i}^{x_s}\nu^T\frac{\partial \mathcal{N}_E}{\partial\alpha}\delta\alpha dx + \int_{x_s}^{x_e}\nu^T\frac{\partial \mathcal{N}_E}{\partial\alpha}\delta\alpha dx + \sum_{k=1}^{N}\mu_k^T\frac{\mathfrak{D}\mathcal{R}_{\lambda_k}}{\mathfrak{D}\alpha}\Delta\alpha \\
&+\beta\left(\int_{x_i}^{x_s}\frac{\partial j}{\partial\alpha}\delta\alpha dx + \int_{x_s}^{x_e}\frac{\partial j}{\partial\alpha}\delta\alpha dx\right) + (1-\beta)\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha}\Delta\alpha \\
&-\int_{x_i}^{x_s}\left(L_E^*(\nu)-\beta\left(\frac{\partial j}{\partial U}\right)^T\right)^T\delta U dx - \int_{x_s}^{x_e}\left(L_E^*(\nu)-\beta\left(\frac{\partial j}{\partial U}\right)^T\right)^T\delta U dx \\
&+\sum_{k=1}^{N}\left((1-\beta)\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N}\mu_l^T\frac{\mathfrak{D}\mathcal{R}_{\lambda_l}}{\mathfrak{D}U_k}\right)\Delta U_k \\
&-\left(h_s\nu_s^T\left[\frac{dF_E}{dx}\right]_{x_s-}^{x_s+} + [j]_{x_s-}^{x_s+}\right)\delta x_s \\
&-h_s\left(\nu_s^T - \nu^T(x_{s+})\right)\left(\frac{\partial F_E}{\partial U}\delta U\right)\bigg|_{x_s-} + h_s\left(\nu_s^T - \nu^T(x_{s-})\right)\left(\frac{\partial F_E}{\partial U}\delta U\right)\bigg|_{x_s+} \\
&-\left[h\nu^T\frac{\partial F_E}{\partial U}\delta U\right]_{x_i}^{x_e},
\end{aligned} \tag{4.23}$$

where

$$L_E^*(\nu) = -h\left(\frac{\partial F_E}{\partial U}\right)^T\frac{d\nu}{dx} - \frac{dh}{dx}\left(\frac{\partial P_E}{\partial U}\right)^T\nu. \tag{4.24}$$

We then proceed by appropriately restricting the adjoint variables ν and μ such that the explicit dependence of the Lagrangian perturbation on the flow perturbation and shock movement can be removed. Canceling the two lines involving the quantity ν_s leads to

$$\nu_s = \nu, \tag{4.25}$$

and the internal shock boundary condition

$$\nu_2(x_s) = \left(\frac{dh_s}{dx}\right)^{-1}\frac{[j]_{x_s-}^{x_s+}}{[p]_{x_s-}^{x_s+}}. \tag{4.26}$$

The remaining lines with a dependence on δU can then be removed if

$$\begin{aligned}
-\int_{x_i}^{x_s}\left(L_E^*(\nu)-\beta\left(\frac{\partial j}{\partial U}\right)^T\right)^T\delta U dx - \int_{x_s}^{x_e}\left(L_E^*(\nu)-\beta\left(\frac{\partial j}{\partial U}\right)^T\right)^T\delta U dx \\
+\sum_{k=1}^{N}\left((1-\beta)\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N}\mu_l^T\frac{\mathfrak{D}\mathcal{R}_{\lambda_l}}{\mathfrak{D}U_k}\right)\Delta U_k - \left[h\nu^T\frac{\partial F_E}{\partial U}\delta U\right]_{x_i}^{x_e} \;=\; 0.
\end{aligned} \tag{4.27}$$

Unlike in the purely continuous adjoint, we cannot set the last term equal to zero on its own because the Jacobian $\frac{\partial F_E}{\partial U}$ is not square. However, to solve this problem we can extract the boundary flux terms from the numerical residual to complete this matrix and form the inlet and exit hybrid boundary conditions:

$$\begin{pmatrix} h_i \nu_i^T & \mu_1^T \end{pmatrix} \begin{pmatrix} \left.\dfrac{\partial F_E}{\partial U}\right|_i \\ \dfrac{\mathfrak{D}\widehat{hF}_{\lambda_1}}{\mathfrak{D}U_1} \end{pmatrix} \delta U_i = 0, \tag{4.28}$$

and

$$\begin{pmatrix} h_e \nu_e^T & \mu_N^T \end{pmatrix} \begin{pmatrix} \left.\dfrac{\partial F_E}{\partial U}\right|_e \\ -\dfrac{\mathfrak{D}\widehat{hF}_{\lambda_N}}{\mathfrak{D}U_N} \end{pmatrix} \delta U_e = 0, \tag{4.29}$$

where we have used the assumption that $\delta U_i \approx \Delta U_1$ and $\delta U_e \approx \Delta U_N$. This leaves the hybrid adjoint equation

$$\int_{x_i}^{x_e} \left(L_E^*(\nu) - \beta \left(\frac{\partial j}{\partial U} \right)^T \right)^T \delta U dx = \sum_{k=1}^{N} \left((1-\beta) \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N} \mu_l^T \frac{\mathfrak{D}\mathcal{R}_{\lambda_l}}{\mathfrak{D}U_k}^* \right) \Delta U_k, \tag{4.30}$$

where

$$\frac{\mathfrak{D}\mathcal{R}_{\lambda_l}}{\mathfrak{D}U_k}^* = \begin{cases} \dfrac{\mathfrak{D}\mathcal{R}_{\lambda_1}}{\mathfrak{D}U_1} + \dfrac{\mathfrak{D}\widehat{hF}_{\lambda_1}}{\mathfrak{D}U_1} & \text{if } l = k = 1 \\ \dfrac{\mathfrak{D}\mathcal{R}_{\lambda_N}}{\mathfrak{D}U_N} - \dfrac{\mathfrak{D}\widehat{hF}_{\lambda_N}}{\mathfrak{D}U_N} & \text{if } l = k = N \\ \dfrac{\mathfrak{D}\mathcal{R}_{\lambda_l}}{\mathfrak{D}U_k} & \text{otherwise,} \end{cases} \tag{4.31}$$

and thus the perturbation to the objective function can be written

$$\begin{aligned} \{\delta, \Delta\}\mathcal{J}_H = \{\delta, \Delta\}\mathcal{L} \quad = \quad & \int_{x_i}^{x_s} \nu^T \frac{\partial \mathcal{N}_E}{\partial \alpha} \delta\alpha dx + \sum_{k=1}^{N} \mu_k^T \frac{\mathfrak{D}\mathcal{R}_{\lambda_k}}{\mathfrak{D}\alpha} \Delta\alpha \\ & + \beta \int_{x_i}^{x_s} \frac{\partial j}{\partial \alpha} \delta\alpha dx + \beta \int_{x_s}^{x_e} \frac{\partial j}{\partial \alpha} \delta\alpha dx + (1-\beta) \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha} \Delta\alpha. \end{aligned} \tag{4.32}$$

However, it can be seen that Eq. (4.30) still retains a dependency on the flow perturbation through δU and ΔU. To remove this we first write the integral over the domain as a sum of the integrals over each cell:

$$\sum_{k=1}^{N} \int_k \left(L_E^*(\nu) - \beta \left(\frac{\partial j}{\partial U} \right)^T \right)^T \delta U dx = \sum_{k=1}^{N} \left((1-\beta) \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N} \mu_l^T \frac{\mathfrak{D}\mathcal{R}_{\lambda_l}}{\mathfrak{D}U_k}^* \right) \Delta U_k, \tag{4.33}$$

and then impose the condition that, as well as being true over the whole domain, this is also true over each cell, allowing us to drop the leading summation signs

$$\int_k \left(L_E^*(\nu) - \beta \left(\frac{\partial j}{\partial U} \right)^T \right)^T \delta U dx = \left((1-\beta) \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N} \mu_l^T \frac{\mathfrak{D}\mathcal{R}_{\lambda_l}}{\mathfrak{D}U_k}^* \right) \Delta U_k. \tag{4.34}$$

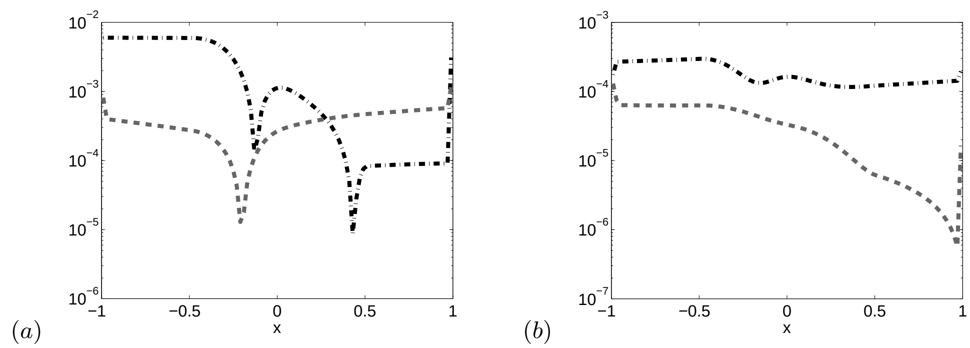

FIGURE 3. Size of difference in adjoint variables (dot-dashed line: the hybrid and discrete ($|\{\nu,\mu\}-\psi|$); dashed line: the hybrid and continuous ($|\{\nu,\mu\}-\phi|$)) for the exponential combustion source term and integral of pressure functional: (a) first variable, (b) fourth variable

We also now assume that the flow perturbation is in general small, and thus only varies gradually over the domain. This means that as the cell width decreases, it can be treated as constant within each cell, allowing us to factor δU out of the integral

$$\left(\int_k \left(L_E^*(\nu) - \beta\left(\frac{\partial j}{\partial U}\right)^T\right)^T dx\right)\delta U_k = \left((1-\beta)\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N}\mu_l^T \frac{\mathfrak{D}\mathcal{R}_{\lambda_l}}{\mathfrak{D}U_k}^*\right)\Delta U_k. \tag{4.35}$$

Finally, asserting that $\delta U_k \to \Delta U_k$ as $\Delta x \to 0$, we factor out the flow perturbation and arrive at the final hybrid adjoint equation:

$$\int_k \left(L_E^*(\nu) - \beta\left(\frac{\partial j}{\partial U}\right)^T\right) dx = (1-\beta)\left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k}\right)^T + \sum_{l=1}^{N}\left(\frac{\mathfrak{D}\mathcal{R}_{\lambda_l}}{\mathfrak{D}U_k}^*\right)^T \mu_l, \quad x\in[x_i,x_e]. \tag{4.36}$$

5. Results

5.0.1. *Difference in adjoint variables*

Figure 3 shows the difference between the hybrid and discrete, and hybrid and continuous variables for the first and fourth adjoint variables for the exponential source term and integral of pressure functional. This shows, in general, closer agreement between the hybrid and continuous approaches where the continuous exists. Also, this difference fluctuates most where the duct height changes most rapidly ($x=\pm 0.25$).

5.0.2. *Grid convergence*

Using the formulae for the sensitivity of the objective function to the inlet Mach number, a grid refinement study of all four combinations of source and objective functions is shown in Figure 4. From Figures 4(a), (b), it can be seen that the finite difference and discrete adjoint compare very well, as do the hybrid and continuous adjoint methods. However, the latter two methods appear to give a better approximation to the fine grid sensitivity on the coarser meshes.

In Figures 4(c), (d), which consider the absolute value functional, the computed sensitivities do not reach a steady value in a monotonic fashion as the grid is refined, though the three methods agree well with each other. On further investigation, it was concluded

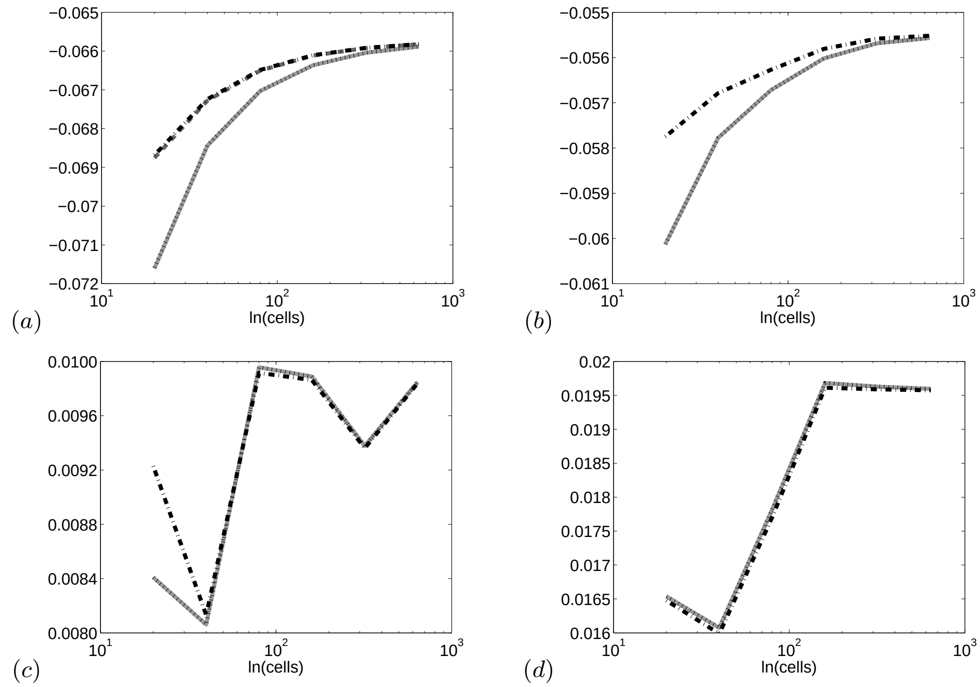

FIGURE 4. Sensitivity of functional to incoming Mach number at different grid refinement levels using finite difference (solid line), discrete adjoint (dotted line), continuous adjoint (dashed line) and hybrid adjoint (dot-dashed line): (a) exponential source term and integral of pressure functional, (b) Heaviside source term and integral of pressure functional, (c) exponential source term and non-differentiable functional, (d) Heaviside source term and absolute value functional

that the non-differentiability of the cost function is not the cause of the non-smooth convergence rate. Instead, this specific form of the functional appears to be highly sensitive to the error in the flow solution, especially on a coarse grid.

6. Conclusions and future work

The concept of a hybrid adjoint which combines the properties of a discrete adjoint and a continuous adjoint has been introduced and the theory has been applied to the quasi one-dimensional compressible flow with a simple model of combustion. Numerical experiments indicate that the hybrid adjoint approach can be used to estimate the sensitivity, showing generally good agreement with finite differencing, discrete adjoints and continuous adjoints. It is also better matches the continuous adjoint result where available, but, perhaps most importantly, can be applied to problems where the development and application of the continuous method would be difficult. In terms of ease of development, the initial hybrid derivation is of a similar level of complexity as that of the continuous adjoint, but, once derived, can easily be applied to more complex problems with minimal mathematical development.

Table 6 updates Table 1 from the introduction, summarizing the relative advantages and disadvantages of the hybrid approach in comparison with standard methods. Here a $\pm$ sign indicates where the hybrid is seen to lie between the advantages and disadvantages of the discrete and continuous, and a ? indicates that further investigation is required.

	Discrete	Continuous	**Hybrid**
Ease of development	+	−	**±**
Compatibility of numerical gradients to the discretized PDE	+	−	**?**
Compatibility of numerical gradients to the continuous PDE	−	+	**?**
Surface formulation for gradients	−	+	**?**
Ability to handle arbitrary functionals	+	−	**+**
Ability to handle non-differentiability	+	−	**+**
Computational cost (CPU usage and storage)	−	+	**?**
Flexibility in solution	−	+	**±**

TABLE 2. Simple comparison between the discrete, continuous and hybrid adjoint approaches

Having developed the general hybrid adjoint approach, and applied it to a simple test case of supersonic quasi one-dimensional flow with a simple combustion model, the next steps in this research are to extend the development and application to more complex problems. Though the treatment of discontinuities in the flow solution has been been addressed, numerical experiments have not been conducted. Such an exercise will be undertaken in the near future. Furthermore, we are currently focusing on the application to two- and three-dimensional problems of interest in aerospace engineering. With the demonstrated flexibility of handling arbitrary expressions in the governing equations (using discrete representations), the method can be naturally extended to treat Reynolds Averaged Navier–Stokes-based turbulence models. In such a situation, the conservation equations of mass, momentum and energy will be handled continuously, whereas the set of equations for turbulence scalars will be treated discretely.

Although the approach holds promise in combining the best properties of continuous and discrete adjoint methods, some of the aforementioned exercises will confirm the viability of the hybrid adjoint approach as a useful tool in several areas of computational science.

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