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Towards a Hybrid Adjoint Approach for Arbitrarily Complex Partial Differential Equations

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Adjoint methods are widely used in various areas of computational science to efficiently obtain sensitivities of functionals which result from the solution of partial differential equations (PDEs). In addition, adjoint methods have been used in other settings including error estimation, uncertainty quantification and inverse problem formulations. When deriving the adjoint equations, there are two main approaches one can follow: the discrete and the continuous methods, which differ principally in the order of the linearization and discretization steps. The discrete adjoint method starts from the discretized form of the partial differential equation, which is then linearized. On the other hand, the continuous method linearizes the continuous governing equations first and then discretizes the resulting problem. Each of these approaches is found to have advantages and disadvantages over the other. In this paper we consider a hybrid approach between these two methods that aims to combine the better qualities of both: reducing the time spent on the mathematical derivation while also lowering the computational requirements of the discrete method and increasing the overall quality of the adjoint solution.

I. Nomenclature

Subscript and Superscript Definition

$()_i$	= Value at inlet
$()_e$	= Value at exit
$()_{k,l}$	= Cell identifiers
$()_s$	= Value at shock
$()_{s^-}$	= Value just before shock
$()_{s^-}$	= Value just after shock
$()_C$	= Variable treated in continuous manner
$()_D$	= Variable treated in discrete manner
$()_E$	= Term from Euler governing equations
$()_{E,E}$	= Term from Euler governing equations present in Euler adjoint equations
$()_{E,\lambda}$	= Term from Euler governing equations present in combustion model adjoint equations
$()_E$	= Term from Euler governing equations
$()_H$	= Variable treated in hybrid manner
$()_\lambda$	= Term related to combustion model governing equations

Variable Definition

j	= Integrand in continuous functional
h	= Height of duct

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m = Mass flow
p = Pressure
p^* = Pressure constant for non-differentiable cost function
p_0 = Stagnation pressure
q = Specific heat release
t = Time
x = Spatial coordinate
C = Constant in exponential source term
F = Direct problem flux vector
G = Adjoint problem flux vector
H = Stagnation enthalpy
$L()$ = Linearized problem operator
$L^*()$ = Adjoint linearized problem operator
M = Mach number
N = Number of cells on grid
P = Pressure source term vector
Q = Combustion source term vector
R = Gas constant
T = Static temperature
T_0 = Stagnation temperature
T^* = Initiation temperature constant for Heaviside source term
U = Flow variables
$\mathcal{B}$ = Boundary conditions
$\mathcal{G}$ = Governing equations
$\mathcal{J}$ = Objective function
$\mathcal{L}$ = Lagrangian
$\mathcal{N}$ = Flow equations
$\mathcal{R}$ = Residual equations
$\mathcal{V}$ = General adjoint variable
α = System parameters under which perturbation to objective function is considered
β = Switching variable to select discrete ($\beta = 0$) or continuous ($\beta = 1$) objective function
γ = Ratio of specific heats
ϵ = Energy flow variable
λ = Combustion flow variable
μ = Hybrid adjoint variable from enforcing discrete governing equations
ν = Hybrid adjoint variable from enforcing continuous governing equations
ρ = Density
ϕ = Continuous adjoint variable
ψ = Discrete adjoint variable
ω = Combustion source term
Γ = Boundary surface
Λ = Reaction progress variable, $0 \leq \Lambda \leq 1$
Ψ = Discrete adjoint variable in error estimation
Ω = Domain

Mathematical Notation

$()'$ = Perturbed value
$\widehat{()}$ = Numerical flux
$\widetilde{()}$ = Roe flux
$()^T$ = Transpose
$\mathcal{H}$ = Heaviside function
$\delta()$ = Continuous perturbation
$\Delta()$ = Discrete perturbation
$\{\delta, \Delta\}()$ = Hybrid perturbation

$\frac{\partial()}{\partial()}$ = Continuous Jacobian
$\frac{\mathfrak{D}()}{\mathfrak{D}()}$ = Discrete Jacobian

II. Introduction

The adjoint method was first developed for aerodynamic shape optimization applications through the use of control theory by Jameson[1] in the late 1980s and early 1990s using ideas adapted from more general work by Lions[2] 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,[3] goal-oriented numerical error estimation and mesh adaptation,[4,5] sensitivity analysis, and uncertainty quantification.[6]

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 equation is derived from the analytical form of the PDE and is then discretized to obtain a discrete representation of the adjoint equations. 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.

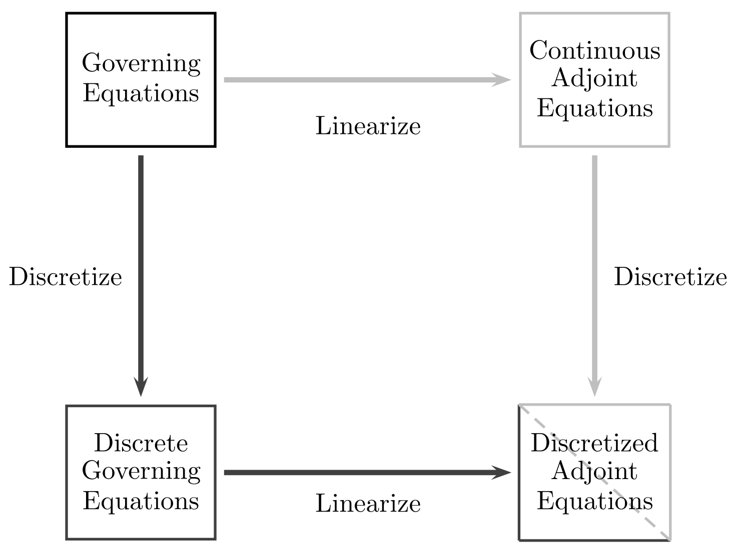


Figure 1. General scheme for deriving discrete and continuous adjoints

The discrete method can employ algorithmic Automatic Differentiation,[7] either via source code transformation, e.g. using TAPENADE,[8] or operator overloading, e.g. using ADOL-C,[9] 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 should also be noted that it is 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.[10] 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 an 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 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. It is also worth mentioning that, 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.

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

	Discrete	Continuous
Ease of development[7,10,11]	+	−
Compatibility of numerical gradients with the discretized PDE[7,10,11]	+	−
Compatibility of numerical gradients with the continuous PDE[11]	−	+
Surface formulation for gradients[12]	−	+
Ability to handle arbitrary functionals)[7]	+	−
Ability to handle non-differentiability)[7,11,13]	+	−
Computational cost (CPU usage and storage)[7,10,11]	−	+
Flexibility in solution[10,11,14]	−	+

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 paper we introduce a hybrid approach that combines these two methods by enforcing part of the governing equations continuously and part discretely. The choice between which terms will be enforced discretely and continuously is intended to be made so that non-differentiable or highly complex functions will be removed from the continuous part of the formulation, and so as to reduce the mathematical development time usually associated with the continuous adjoint. The general hybrid scheme is shown in Figure 2.

In summary, the intent of this paper is to lay down the foundation for the derivation of adjoint equations for *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, multi-phase 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.

Section III provides an introduction to the adjoint method, both discrete and continuous. Section IV discusses our approach to the combination of continuous and discrete methods into a *hybrid* method. The remaining sections describe an application to quasi one-dimensional flow with a simple combustion model and the results we have obtained with the method so far.

III. Introduction to Adjoint Methods

Adjoint equations can most conveniently be 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 and Pierce[11] and Belegundu and Arora,[15] they can also be interpreted as representing the sensitivity of the

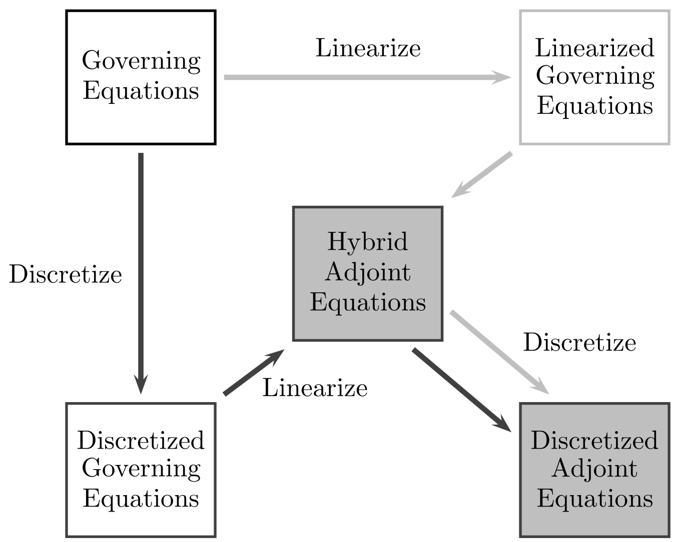


Figure 2. General scheme for deriving hybrid adjoint

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 can be used to compute the sensitivities of $\mathcal{J}$ to changes in all of the parameters that define the problem at any point in the domain without additional computations. In contrast, though finite-difference or complex-step methods[16] 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 with respect to each parameter in the domain and, in the case of finite differencing, these methods can be potentially less accurate.

There are two main approaches used to derive the adjoint equations: the Primal-Dual Equivalence Theorem and an optimization framework using Lagrange multipliers.[11,15] In this paper we consider the latter method, and present the discrete, continuous and then hybrid derivations in an identical context. To demonstrate the basic method we will consider the model problem of the objective function:

$$\mathcal{J}(U, \alpha) \quad \text{on } \Omega \text{ or } \Gamma, \tag{1}$$

defined on the domain or boundary shown in Figure 3, and subject to the contraints:

$$\mathcal{G}(U, \alpha) = 0 \quad \text{on } \Omega \text{ and } \Gamma, \tag{2}$$

where the constraints are the governing equations, including both the flow equations, $\mathcal{N} = 0$ on Ω, and boundary conditions, $\mathcal{B} = 0$ on Γ.

The derivation process follows these steps:

1. Introduce a Lagrangian, $\mathcal{L}$, to enforce the governing equations in the objective function via a set of Lagrange multipliers:

$$\mathcal{L} = \mathcal{J} + \mathcal{V}^T \mathcal{G}, \tag{3}$$

where $\mathcal{V}$ are the Lagrange multipliers, which we will later denote as the adjoint variable (or variables), and we note that as $\mathcal{G} = 0$, $\mathcal{L} \equiv \mathcal{J}$ for any value of $\mathcal{V}$.

2. Write down the perturbation of the Lagrangian, $\delta\mathcal{L}$, relative to a small change in some parameter α (which may induce perturbations in the flow, domain and boundary):

$$\delta\mathcal{L} = \delta\mathcal{J} + \mathcal{V}^T \delta\mathcal{G}, \tag{4}$$

noting that we have constrained $\mathcal{V}$ such that it does not depend on α.

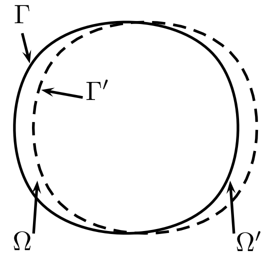


Figure 3. Unperturbed and perturbed domain and boundary surface

3. Expand and mathematically manipulate the terms in $\delta\mathcal{L}$ so as to group those dependent on the flow perturbation, δU. Neglecting domain or surface perturbations:

$$\begin{aligned} \delta\mathcal{L} &= \frac{\partial\mathcal{J}}{\partial\alpha}\delta\alpha + \frac{\partial\mathcal{J}}{\partial U}\delta U + \mathcal{V}^T\left(\frac{\partial\mathcal{G}}{\partial\alpha}\delta\alpha + \frac{\partial\mathcal{G}}{\partial U}\delta U\right) \\ &= \left(\frac{\partial\mathcal{J}}{\partial\alpha} + \mathcal{V}^T\frac{\partial\mathcal{G}}{\partial\alpha}\right)\delta\alpha + \left(\frac{\partial\mathcal{J}}{\partial U} + \mathcal{V}^T\frac{\partial\mathcal{G}}{\partial U}\right)\delta U. \end{aligned} \tag{5}$$

4. Identify the Lagrange multipliers as the adjoint variables and introduce constraints on these variables, including an adjoint equation and boundary conditions, such that any explicit dependence of $\delta\mathcal{L}$ on δU is removed. Here we note that through definition of the adjoint equation:

$$\frac{\partial\mathcal{J}}{\partial U} + \mathcal{V}^T\frac{\partial\mathcal{G}}{\partial U} = 0, \tag{6}$$

the perturbation to the Lagrangian can then be written:

$$\delta\mathcal{L} = \left(\frac{\partial\mathcal{J}}{\partial\alpha} + \mathcal{V}^T\frac{\partial\mathcal{G}}{\partial\alpha}\right)\delta\alpha. \tag{7}$$

5. Equate $\delta\mathcal{L}$ to the perturbation to the objective function, $\delta\mathcal{J}$, allowing us to easily find, once the adjoint problem has been solved, the sensitivities of $\mathcal{J}$ relative to any system parameter, i.e.:

$$\frac{d\mathcal{J}}{d\alpha} = \frac{\delta\mathcal{J}}{\delta\alpha} = \frac{\partial\mathcal{J}}{\partial\alpha} + \mathcal{V}^T\frac{\partial\mathcal{G}}{\partial\alpha}. \tag{8}$$

For the case where there is no explicit dependence of $\mathcal{J}$ on α we can write this as the simple inner product:

$$\frac{\delta\mathcal{J}}{\delta\alpha} = \mathcal{V}^T\frac{\partial\mathcal{G}}{\partial\alpha}. \tag{9}$$

A. 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, $\mathcal{R}_k$, i.e. $\mathcal{G} = \{\mathcal{R}_k\} = 0$. We note that these residuals include the boundary conditions from the primal solution. This gives the Lagrangian:

$$\mathcal{L} = \mathcal{J}_D + \sum_{k=1}^{N}\psi_k^T\mathcal{R}_k, \tag{10}$$

and the perturbation:

$$\Delta\mathcal{L} = \Delta\mathcal{J}_D + \sum_{k=1}^{N}\psi_k^T\Delta\mathcal{R}_k. \tag{11}$$

The terms on the right hand side can then be linearized and expanded as:

$$\Delta \mathcal{J}_D = \sum_{l=1}^{N} \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_l} \Delta U_l + \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha} \Delta\alpha, \tag{12}$$

and:

$$\Delta \mathcal{R}_k = \sum_{l=1}^{N} \frac{\mathfrak{D}\mathcal{R}_k}{\mathfrak{D}U_l} \Delta U_l + \frac{\mathfrak{D}\mathcal{R}_k}{\mathfrak{D}\alpha} \Delta\alpha = 0, \tag{13}$$

which gives, after rearrangement:

$$\Delta \mathcal{L} = \sum_{k=1}^{N} \psi_k^T \frac{\mathfrak{D}\mathcal{R}_k}{\mathfrak{D}\alpha} \Delta\alpha + \sum_{k=1}^{N} \left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N} \psi_l^T \frac{\mathfrak{D}\mathcal{R}_l}{\mathfrak{D}U_k} \right) \Delta U_k + \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha} \Delta\alpha. \tag{14}$$

Then finally we may define the adjoint equation as:

$$\sum_{l=1}^{N} \left(\frac{\mathfrak{D}\mathcal{R}_l}{\mathfrak{D}U_k} \right)^T \psi_l = - \left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} \right)^T, \tag{15}$$

allowing us to write:

$$\Delta \mathcal{J}_D = \Delta \mathcal{L} = \sum_{k=1}^{N} \psi_k^T \frac{\mathfrak{D}\mathcal{R}_k}{\mathfrak{D}\alpha} \Delta\alpha + \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha} \Delta\alpha, \tag{16}$$

or, in terms purely of the sensitivity to α:

$$\frac{d\mathcal{J}_D}{d\alpha} = \sum_{k=1}^{N} \psi_k^T \frac{\mathfrak{D}\mathcal{R}_k}{\mathfrak{D}\alpha} + \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha}, \tag{17}$$

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

B. Continuous Adjoint Approach

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

$$\mathcal{L} = \mathcal{J}_C - \int_\Omega \phi^T \mathcal{N} d\Omega - \int_\Gamma \phi^T \mathcal{B} d\Gamma, \tag{18}$$

where the continuous objective function $\mathcal{J}_C$ can be defined over either the entire domain or just the boundary, i.e.:

$$\mathcal{J}_C = \int_\Omega j d\Omega \quad \text{or} \quad \mathcal{J}_C = \int_\Gamma j d\Gamma. \tag{19}$$

Also, we note that the sign of the terms introduced to enforce the constraints is negative. This ensures that after the mathematical derivation steps, the final continuous adjoint variables are of the same sign as the discrete adjoint variables.

The perturbation to the Lagrangian now becomes:

$$\delta \mathcal{L} = (\mathcal{J}_C' - \mathcal{J}_C) - \left(\int_{\Omega'} \phi^T \mathcal{N}' d\Omega - \int_\Omega \phi^T \mathcal{N} d\Omega \right) - \left(\int_{\Gamma'} \phi^T \mathcal{B}' d\Gamma - \int_\Gamma \phi^T \mathcal{B} d\Gamma \right), \tag{20}$$

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 to manipulate and rearrange terms such that the direct dependence of this quantity on the flow perturbations δU is removed, whilst retaining those terms dependent on perturbations to α and/or the domain and boundary surface. As these remaining terms are either known or easily calculated quantities the perturbation to the objective function 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.

IV. 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. The only approaches that we are aware of, such as Lozano and Ponsin's, have used continuous adjoint variables in a discrete adjoint framework to calculate sensitivities.[14] The method discussed in this paper attempts to build a more general hybrid representation.

In our approach, we will split the governing equations into those that will be incorporated continuously and those that will be incorporated 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 will be those that will not change when minor adjustments are made to the flow equations, such as altering the source terms, and that are easily differentiable (e.g. the Euler equations for a perfect gas or even the laminar Navier-Stokes equations). The terms that will be treated discretely will include those that are not easily differentiable, 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 of 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 and allowing the reuse of existing code.

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

$$\mathcal{J}_H = \beta \mathcal{J}_C + (1-\beta)\mathcal{J}_D, \tag{21}$$

where β can be set to 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, though we do not to intend to combine them as a weighted sum.

The Lagrangian now becomes:

$$\mathcal{L} = \beta \mathcal{J}_C + (1-\beta)\mathcal{J}_D - \int_\Omega \nu^T \mathcal{N}_C d\Omega - \int_\Gamma \nu^T \mathcal{B}_C d\Gamma + \sum_{k=1}^{N} \mu_k^T \mathcal{R}_{D,k}, \tag{22}$$

and its perturbation can be written as

$$\begin{aligned} \{\delta, \Delta\}\mathcal{L} \quad = \quad & \beta\left(\mathcal{J}_C' - \mathcal{J}_C\right) + (1-\beta)\Delta\mathcal{J}_D \\ & - \left(\int_{\Omega'} \nu^T \mathcal{N}_C' d\Omega - \int_\Omega \nu^T \mathcal{N}_C d\Omega\right) - \left(\int_{\Gamma'} \nu^T \mathcal{B}_C' d\Gamma - \int_\Gamma \nu^T \mathcal{B}_C d\Gamma\right) \\ & + \sum_{k=1}^{N} \mu_k^T \Delta\mathcal{R}_{D,k}. \end{aligned} \tag{23}$$

The next steps in this derivation mirror those introduced previously for the discrete and continuous parts, mathematically manipulating the equation so as to remove the explicit dependence of the perturbation on the discrete and continuous flow perturbations, ΔU and δU, respectively, and in so doing generating the adjoint equation and boundary conditions for ν and μ. When deriving and calculating the hybrid adjoint for a specific problem, two important choices will need to be made. The first deals with the selection of which governing equations will be treated discretely and 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.

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

A. Primal problem

1. Definition

We consider quasi one-dimensional Euler flow (smooth or shocked) in the duct $x \in [x_i, x_e]$ with height $h(x)$ as shown in Figure 4. Additionally, inspired by Powers,[17] we include a simple combustion model, introducing the reaction progress variable Λ and the additional flow variable $\lambda = \rho\Lambda$.

Figure 4. Quasi one-dimensional duct

The analytical governing equations are given as:

$$\mathcal{N} \equiv \frac{d}{dx}(hF) - \frac{dh}{dx}P - hQ = 0, \quad x \in [x_i, x_e], \tag{24}$$

where:

$$U = \begin{pmatrix} \rho \\ m \\ \epsilon \\ \lambda \end{pmatrix}, \quad F = \begin{pmatrix} m \\ \frac{m^2}{\rho} + p \\ mH \\ m\Lambda \end{pmatrix}, \quad P = \begin{pmatrix} 0 \\ p \\ 0 \\ 0 \end{pmatrix}, \quad Q = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \omega \end{pmatrix}, \tag{25}$$

$$H = \frac{\epsilon + p}{\rho}, \tag{26}$$

$$p = (\gamma - 1)(\epsilon - \frac{m^2}{2\rho} + \lambda q), \tag{27}$$

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

$$T = \frac{p}{\rho R}. \tag{28}$$

We shall consider purely supersonic flow in the numerical experiments of this paper, and due to the hyperbolic nature of the governing equation, apply boundary conditions based on characteristics, thus defining all conditions at the inlet, and none at the exit.

We consider two possible forms for the combustion source term ω:

1. A differentiable, exponential form: $\omega = \rho(1 - \Lambda)e^{-C/RT}$
2. 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:

1. A differentiable form, the 'lift' over the duct: $\mathcal{J} = \int_{x_i}^{x_e} p dx$
2. A non-differentiable form, the magnitude of a pressure difference: $\mathcal{J} = \int_{x_i}^{x_e} |p - p^*| \, dx$

Note, 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.

2. Solution strategy

The steady-state problem can be solved by discretizing and then iterating the following equation until the variation in U between each time-step is sufficiently small:

$$h\frac{\partial U}{\partial t} = -\frac{\partial}{\partial x}\left(hF\right) + \frac{dh}{dx}P + hQ. \tag{29}$$

In this case, to make use of existing methods we first split this equation into a set of coupled equations, one for the Euler variables:

$$h\frac{\partial U_E}{\partial t} = -\frac{\partial}{\partial x}\left(hF_E\right) + \frac{dh}{dx}P_E, \tag{30}$$

where:

$$F_E = \begin{pmatrix} m \\ \frac{m^2}{\rho} + p \\ mH \end{pmatrix}, \quad P_E = \begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix}, \tag{31}$$

and the other for the combustion variable:

$$h\frac{\partial U_\lambda}{\partial t} = -\frac{\partial}{\partial x}\left(hF_\lambda\right) + hQ_\lambda. \tag{32}$$

where:

$$F_\lambda = \left(m\Lambda\right), \quad Q_\lambda = \left(\omega\right), \tag{33}$$

and will solve these by treating them to be uncoupled within each iteration.

Applying a finite volume method for the cell k we can then obtain:

$$h_k\frac{\Delta U_{E,k}}{\Delta t}\Delta x + \mathcal{R}_{E,k} = 0, \tag{34}$$

and:

$$h_k\frac{\Delta U_{\lambda,k}}{\Delta t}\Delta x + \mathcal{R}_{\lambda,k} = 0, \tag{35}$$

where the numerical residuals are given by:

$$\mathcal{R}_{E,k} = \widehat{hF}_{E,k+\frac{1}{2}} - \widehat{hF}_{E,k-\frac{1}{2}} - \Delta h_k P_{E,k}, \tag{36}$$

and:

$$\mathcal{R}_{\lambda,k} = \widehat{hF}_{\lambda,k+\frac{1}{2}} - \widehat{hF}_{\lambda,k-\frac{1}{2}} - h_k Q_{\lambda,k}\Delta x, \tag{37}$$

and also the numerical fluxes for the Euler variables are given via the Roe scheme:

$$\widehat{hF}_{E,k+\frac{1}{2}} = \frac{1}{2}\left(hF_{E,k+1} + hF_{E,k}\right) - \frac{1}{2}\left|\widetilde{\frac{\partial F_E}{\partial U_E}}\right|_{k+\frac{1}{2}}\left(hU_{E,k+1} - hU_{E,k}\right), \tag{38}$$

and those for the combustion variable are given by a simple upwinding scheme:

$$\widehat{hF}_{\lambda,k+\frac{1}{2}} = \frac{1}{2}\left(hF_{\lambda,k+1} + hF_{\lambda,k}\right) - \frac{1}{2}\left|\frac{\partial F_\lambda}{\partial U_\lambda}\right|_{k+\frac{1}{2}}\left(hU_{\lambda,k+1} - hU_{\lambda,k}\right). \tag{39}$$

In this paper we discretize the domain into a uniform mesh of cells of width Δx and wrap each iteration within a fourth-order Runge-Kutta step. Since we consider only supersonic flow, the left-hand boundary conditions are Dirichlet and the right-hand uses extrapolation from within the domain to find the outgoing flux.

B. Discrete adjoint method

1. Definition

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

$$\sum_{l=1}^{N} \left(\frac{\mathfrak{D}\mathcal{R}_l}{\mathfrak{D}U_k} \right)^T \psi_l = -\left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} \right)^T, \tag{40}$$

and the perturbation to the objective function:

$$\Delta\mathcal{J}_D = \sum_{k=1}^{N} \psi_k^T \frac{\mathfrak{D}\mathcal{R}_k}{\mathfrak{D}\alpha}\Delta\alpha + \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha}\Delta\alpha, \tag{41}$$

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

2. Solution strategy

The required Jacobians are found by applying automatic differentiation via the software tool ADOL-C,[9] and then the following equation is solved directly using the forward Euler method until the variation in ψ between each time-step was sufficiently small. This is equivalent to solving the linear system iteratively.

$$\frac{\Delta\psi_k}{\Delta t}\Delta x = -\sum_{l=1}^{N} \left(\frac{\mathfrak{D}\mathcal{R}_l}{\mathfrak{D}U_k} \right)^T \psi_l - \left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} \right)^T, \tag{42}$$

where we note that the Δx term is required because the Jacobians are obtained from applying ADOL-C to a finite volume method.

C. Continuous adjoint method

1. Definition

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 and Pierce,[18] we state that the adjoint equation is:

$$L^*(\phi) - \left(\frac{\partial j}{\partial U} \right)^T = 0, \quad x \in [x_i, x_e], \tag{43}$$

where:

$$L^*(\phi) = -h \left(\frac{\partial F}{\partial U} \right)^T \frac{d\phi}{dx} - \left(\frac{dh}{dx} \left(\frac{\partial P}{\partial U} \right)^T + h \left(\frac{\partial Q}{\partial U} \right)^T \right) \phi, \tag{44}$$

with the boundary conditions:

$$\left[h\phi^T \frac{\partial F}{\partial U}\delta U \right]_{x_i}^{x_e} = 0, \tag{45}$$

giving the perturbation to the objective function:

$$\delta\mathcal{J}_C = \int_{x_i}^{x_e} \phi^T \frac{\partial\mathcal{N}}{\partial\alpha}\delta\alpha dx + \int_{x_i}^{x_e} \frac{\partial j}{\partial\alpha}\delta\alpha dx. \tag{46}$$

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:

$$\mathcal{J}_C = \int_{x_i}^{x_s} j dx + \int_{x_s}^{x_e} j dx, \tag{47}$$

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

$$h_s\phi_s^T \left[\frac{dF}{dx} \right]_{x_{s-}}^{x_{s+}} = -\left[j \right]_{x_{s-}}^{x_{s+}}. \tag{48}$$

2. Solution strategy

Similar to the direct problem, the steady-state problem can be solved by discretizing and then iterating the following equation until the variation in the adjoint variables, ϕ, between each time-step is sufficiently small:

$$h\frac{\partial \phi}{\partial t} + L^{*}\left(\phi\right) - \left(\frac{\partial j}{\partial U}\right)^{T} = 0, \tag{49}$$

and we again make use of existing methods by first splitting this equation into a set of coupled equations, one for the Euler adjoint variables, and another for the combustion adjoint variable. However, care should be given to the explicit coupling existing between the two sets of equations. For the Euler part we have:

$$h\frac{\partial \phi}{\partial t} + L^{*}_{E}\left(\phi\right) - \left(\frac{\partial j}{\partial U}\right)^{T} = 0, \tag{50}$$

where:

$$L^{*}_{E}\left(\phi\right) = -h\left(\frac{\partial F}{\partial U_E}\right)^{T}\frac{d\phi}{dx} - \left(\frac{dh}{dx}\left(\frac{\partial P}{\partial U_E}\right)^{T} + h\left(\frac{\partial Q}{\partial U_E}\right)^{T}\right)\phi, \tag{51}$$

and for the combustion part:

$$h\frac{\partial \phi}{\partial t} + L^{*}_{\lambda}\left(\phi\right) - \left(\frac{\partial j}{\partial U}\right)^{T} = 0, \tag{52}$$

where:

$$L^{*}_{\lambda}\left(\phi\right) = -h\left(\frac{\partial F}{\partial U_\lambda}\right)^{T}\frac{d\phi}{dx} - \left(\frac{dh}{dx}\left(\frac{\partial P}{\partial U_\lambda}\right)^{T} + h\left(\frac{\partial Q}{\partial U_\lambda}\right)^{T}\right)\phi. \tag{53}$$

Applying a finite volume method for the cell k, and noting that this flow is no longer conservative, we can then obtain:

$$\begin{aligned}&\frac{\Delta\phi_{E,k}}{\Delta t}\Delta x - h_{k+\frac{1}{2}}\widehat{G}_{E,k,k+\frac{1}{2}} + h_{k-\frac{1}{2}}\widehat{G}_{E,k,k-\frac{1}{2}} - h_k\left(\frac{\partial F_\lambda}{\partial U_E}\right)^{T}_{k}\Delta\phi_{\lambda,k}\\ &-\left(\frac{dh}{dx}\left(\frac{\partial P}{\partial U_E}\right)^{T} + h\left(\frac{\partial Q}{\partial U_E}\right)^{T}\right)_{k}\phi_k\Delta x - \left(\frac{\partial j}{\partial U_E}\right)^{T}_{k}\Delta x = 0,\end{aligned} \tag{54}$$

and:

$$\begin{aligned}&\frac{\Delta\phi_{\lambda,k}}{\Delta t}\Delta x - h_{k+\frac{1}{2}}\widehat{G}_{\lambda,k,k+\frac{1}{2}} + h_{k-\frac{1}{2}}\widehat{G}_{\lambda,k,k-\frac{1}{2}} - h_k\left(\frac{\partial F_E}{\partial U_\lambda}\right)^{T}_{k}\Delta\phi_{E,k}\\ &-\left(\frac{dh}{dx}\left(\frac{\partial P}{\partial U_\lambda}\right)^{T} + h\left(\frac{\partial Q}{\partial U_\lambda}\right)^{T}\right)_{k}\phi_k\Delta x - \left(\frac{\partial j}{\partial U_\lambda}\right)^{T}_{k}\Delta x = 0,\end{aligned} \tag{55}$$

where the numerical fluxes for the Euler adjoint variables are given via a method based on the Roe scheme:[19]

$$\widehat{G}_{E,k,k+\frac{1}{2}} = \frac{1}{2}\left(\frac{\partial F_E}{\partial U_E}\right)^{T}_{k}\left(\phi_{k+1}+\phi_k\right) + \frac{1}{2}\left|\widetilde{\left(\frac{\partial F_E}{\partial U_E}\right)}^{T}_{k+\frac{1}{2}}\right|\left(\phi_{k+1}-\phi_k\right), \tag{56}$$

and those for the combustion adjoint variable are given by a simple upwinding scheme:

$$\widehat{G}_{\lambda,k,k+\frac{1}{2}} = \frac{1}{2}\left(\frac{\partial F_\lambda}{\partial U_\lambda}\right)^{T}_{k}\left(\phi_{k+1}+\phi_k\right) + \frac{1}{2}\left|\left(\frac{\partial F_\lambda}{\partial U_\lambda}\right)^{T}_{k+\frac{1}{2}}\right|\left(\phi_{k+1}-\phi_k\right). \tag{57}$$

Each complete iteration is again wrapped within a fourth-order Runge-Kutta step. Since we consider only supersonic flow and are solving for the adjoint variables, whose characteristics are all incoming at the exit, the right-hand boundary conditions are Dirichlet, and set so that $\phi = 0$, and the left-hand uses extrapolation from within the domain to find the outgoing flux.

D. Hybrid adjoint method

1. Derivation

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 to discretely enforce the residual for the solution of the combustion model, $\mathcal{R}_{\lambda,k}$, i.e. $\mathcal{G} = \{\{\mathcal{N}_E, \mathcal{B}_E\}_C, \{\mathcal{R}_{\lambda,k}\}_D\}$.

We note that 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:

$$\mathcal{B}_E = [hF_E]_{x_{s^-}}^{x_{s^+}} = 0, \tag{58}$$

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:

$$\begin{aligned} \mathcal{L} \;=\;& \beta\left(\int_{x_i}^{x_s} j dx + \int_{x_s}^{x_e} j dx\right) + (1-\beta)\mathcal{J}_D \\ & - \int_{x_i}^{x_s} \nu^T \mathcal{N}_E dx - \int_{x_s}^{x_e} \nu^T \mathcal{N}_E dx - \nu_s^T \left[hF_E\right]_{x_{s^-}}^{x_{s^+}} + \sum_{k=1}^{N} \mu_k^T \mathcal{R}_{\lambda,k}, \end{aligned} \tag{59}$$

and its perturbation:

$$\begin{aligned} \{\delta,\Delta\}\mathcal{L} \;=\;& \beta\left(\int_{x_i}^{x_s} \delta j dx + \int_{x_s}^{x_e} \delta j dx - [j]_{x_{s^-}}^{x_{s^+}}\right) + (1-\beta)\Delta\mathcal{J}_D \\ & - \int_{x_i}^{x_s} \nu^T \delta\mathcal{N}_E dx - \int_{x_s}^{x_e} \nu^T \delta\mathcal{N}_E dx - \nu_s^T \delta\left([hF_E]_{x_{s^-}}^{x_{s^+}}\right) + \sum_{k=1}^{N} \mu_k^T \Delta\mathcal{R}_{\lambda,k}. \end{aligned} \tag{60}$$

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

$$\delta j = \frac{\partial j}{\partial U}\delta U + \frac{\partial j}{\partial \alpha}\delta\alpha, \tag{61}$$

$$\Delta\mathcal{J}_D = \sum_{k=1}^{N} \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k}\Delta U_k + \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha}\Delta\alpha, \tag{62}$$

$$\delta\mathcal{N}_E = L_E(\delta U) - \frac{\partial \mathcal{N}_E}{\partial \alpha}\delta\alpha = 0, \tag{63}$$

where:

$$L_E(\delta U) = \frac{d}{dx}\left(h\left(\frac{\partial F_E}{\partial U}\delta U\right)\right) - \frac{dh}{dx}\left(\frac{\partial P_E}{\partial U}\delta U\right), \tag{64}$$

$$\Delta\mathcal{R}_{D,k} = \sum_{l=1}^{N} \frac{\mathfrak{D}\mathcal{R}_{D,k}}{\mathfrak{D}U_l}\Delta U_l + \frac{\mathfrak{D}\mathcal{R}_{D,k}}{\mathfrak{D}\alpha}\Delta\alpha = 0, \tag{65}$$

and:

$$\delta\left([hF_E]_{x_{s^-}}^{x_{s^+}}\right) = h_s\left[\frac{\partial F_E}{\partial U}\delta U\right]_{x_{s^-}}^{x_{s^+}} - h_s\left[\frac{dF_E}{dx}\right]_{x_{s^-}}^{x_{s^+}}\delta x_s. \tag{66}$$

Incorporating these into Equation (60) and performing integration by parts on the continuous terms, followed by rearrangement, we obtain:

$$
\begin{aligned}
\{\delta,\Delta\}\mathcal{L} \quad = \quad & \int_{x_i}^{x_s} \nu^T \frac{\partial \mathcal{N}_E}{\partial \alpha}\delta\alpha dx + \int_{x_s}^{x_e} \nu^T \frac{\partial \mathcal{N}_E}{\partial \alpha}\delta\alpha dx + \sum_{k=1}^{N} \mu_k^T \frac{\mathfrak{D}\mathcal{R}_{\lambda,k}}{\mathfrak{D}\alpha}\Delta\alpha \\
& + \beta\left(\int_{x_i}^{x_s} \frac{\partial j}{\partial \alpha}\delta\alpha dx + \int_{x_s}^{x_e} \frac{\partial j}{\partial \alpha}\delta\alpha dx\right) + (1-\beta)\frac{\mathfrak{D}\mathcal{R}_{\lambda,k}}{\mathfrak{D}\alpha}\Delta\alpha \\
& - \int_{x_i}^{x_s}\left(L_E^*(\nu) - \beta\left(\frac{\partial j}{\partial U}\right)^T\right)^T \delta U dx - \int_{x_s}^{x_e}\left(L_E^*(\nu) - \beta\left(\frac{\partial j}{\partial U}\right)^T\right)^T \delta U dx \\
& + \sum_{k=1}^{N}\left((1-\beta)\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N}\mu_l^T \frac{\mathfrak{D}\mathcal{R}_{\lambda,l}}{\mathfrak{D}U_k}\right)\Delta U_k \\
& - \left(h_s \nu_s^T \left[\frac{dF_E}{dx}\right]_{x_{s-}}^{x_{s+}} + [j]_{x_{s-}}^{x_{s+}}\right)\delta x_s \\
& - h_s\left(\nu_s^T - \nu^T(x_{s+})\right)\left(\frac{\partial F_E}{\partial U}\delta U\right)\bigg|_{x_{s-}} + h_s\left(\nu_s^T - \nu^T(x_{s-})\right)\left(\frac{\partial F_E}{\partial U}\delta U\right)\bigg|_{x_{s+}} \\
& - \left[h\nu^T \frac{\partial F_E}{\partial U}\delta U\right]_{x_i}^{x_e},
\end{aligned}
\tag{67}
$$

where:

$$
L_E^*(\nu) = -h\left(\frac{\partial F_E}{\partial U}\right)^T \frac{d\nu}{dx} - \frac{dh}{dx}\left(\frac{\partial P_E}{\partial U}\right)^T \nu. \tag{68}
$$

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 last three lines leads to:

$$
\nu_s = \nu, \tag{69}
$$

the external boundary condition:

$$
\left[h\nu^T \frac{\partial F_E}{\partial U}\delta U\right]_{x_i}^{x_e} = 0, \tag{70}
$$

and the internal shock boundary condition:

$$
\nu_2(x_s) = \left(\frac{dh_s}{dx}\right)^{-1} \frac{[j]_{x_{s-}}^{x_{s+}}}{[p]_{x_{s-}}^{x_{s+}}}. \tag{71}
$$

The final step is then to define the hybrid adjoint equation:

$$
\int_{x_i}^{x_e}\left(L_E^*(\nu) - \beta\left(\frac{\partial j}{\partial U}\right)^T\right)^T \delta U dx = \sum_{k=1}^{N}\left((1-\beta)\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N}\mu_l^T \frac{\mathfrak{D}\mathcal{R}_{D,l}}{\mathfrak{D}U_k}\right)\Delta U_k, \tag{72}
$$

and thus the perturbation to the objective function can be written:

$$
\begin{aligned}
\{\delta,\Delta\}\mathcal{J}_H = \{\delta,\Delta\}\mathcal{L} \quad = \quad & \int_{x_i}^{x_s} \nu^T \frac{\partial \mathcal{N}_E}{\partial \alpha}\delta\alpha dx + \sum_{k=1}^{N}\mu_k^T \frac{\mathfrak{D}\mathcal{R}_{\lambda,k}}{\mathfrak{D}\alpha}\Delta\alpha \\
& + \beta\int_{x_i}^{x_s}\frac{\partial j}{\partial \alpha}\delta\alpha dx + \beta\int_{x_s}^{x_e}\frac{\partial j}{\partial \alpha}\delta\alpha dx + (1-\beta)\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}\alpha}\Delta\alpha.
\end{aligned}
\tag{73}
$$

However, it can be seen that Equation (72) 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:

$$
\sum_{k=1}^{N}\int_k \left(L_E^*(\nu) - \beta\left(\frac{\partial j}{\partial U}\right)^T\right)^T \delta U dx = \sum_{k=1}^{N}\left((1-\beta)\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N}\mu_l^T \frac{\mathfrak{D}\mathcal{R}_{D,l}}{\mathfrak{D}U_k}\right)\Delta U_k, \tag{74}
$$

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

$$\int_k \left(L_E^*(\nu) - \beta \left(\frac{\partial j}{\partial U} \right)^T \right)^T \delta U dx = \left((1-\beta) \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N} \mu_l^T \frac{\mathfrak{D}\mathcal{R}_{D,l}}{\mathfrak{D}U_k} \right) \Delta U_k. \tag{75}$$

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:

$$\left(\int_k \left(L_E^*(\nu) - \beta \left(\frac{\partial j}{\partial U} \right)^T \right)^T dx \right) \delta U_k = \left((1-\beta) \frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} + \sum_{l=1}^{N} \mu_l^T \frac{\mathfrak{D}\mathcal{R}_{D,l}}{\mathfrak{D}U_k} \right) \Delta U_k. \tag{76}$$

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:

$$\int_k \left(L_E^*(\nu) - \beta \left(\frac{\partial j}{\partial U} \right)^T \right) dx = (1-\beta) \left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} \right)^T + \sum_{l=1}^{N} \left(\frac{\mathfrak{D}\mathcal{R}_{D,l}}{\mathfrak{D}U_k} \right)^T \mu_l, \quad x \in [x_i, x_e]. \tag{77}$$

2. Solution strategy

Similar to the continuous method, the steady-state problem can be solved by discretizing and then iterating the following equation, noting that the hybrid equation is already presented in a semi-discretized format, until the variation in the adjoint variables $\{\nu, \mu\}$ between each time-step is sufficiently small:

$$h_k \frac{\Delta\{\nu,\mu\}_k}{\Delta t} + \int_k \left(L_E^*(\nu) - \beta \left(\frac{\partial j}{\partial U} \right)^T \right) dx = (1-\beta) \left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_k} \right)^T + \sum_{l=1}^{N} \left(\frac{\mathfrak{D}\mathcal{R}_{D,l}}{\mathfrak{D}U_k} \right)^T \mu_l. \tag{78}$$

We again intend to make use of existing methods by first splitting this equation into a set of coupled equations, one for the Euler adjoint variables, and another for the combustion adjoint variable. However, we must again be careful due to the explicit coupling between the two sets of equations. For the Euler part we have:

$$h_k \frac{\Delta \nu_k}{\Delta t} + \int_k \left(L_{E,E}^*(\nu) - \beta \left(\frac{\partial j}{\partial U_E} \right)^T \right) dx = (1-\beta) \left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_{E,k}} \right)^T + \sum_{l=1}^{N} \left(\frac{\mathfrak{D}\mathcal{R}_{D,l}}{\mathfrak{D}U_{E,k}} \right)^T \mu_l, \tag{79}$$

where:

$$L_{E,E}^*(\nu) = -h \left(\frac{\partial F_E}{\partial U_E} \right)^T \frac{d\nu}{dx} - \frac{dh}{dx} \left(\frac{\partial P_E}{\partial U_E} \right)^T \nu, \tag{80}$$

and for the combustion part:

$$h_k \frac{\Delta \mu_k}{\Delta t} + \int_k \left(L_{E,\lambda}^*(\nu) - \beta \left(\frac{\partial j}{\partial U_\lambda} \right)^T \right) dx = (1-\beta) \left(\frac{\mathfrak{D}\mathcal{J}_D}{\mathfrak{D}U_{\lambda,k}} \right)^T + \sum_{l=1}^{N} \left(\frac{\mathfrak{D}\mathcal{R}_{D,l}}{\mathfrak{D}U_{\lambda,k}} \right)^T \mu_l, \tag{81}$$

where:

$$L_{E,\lambda}^*(\nu) = -h \left(\frac{\partial F_E}{\partial U} \right)^T \frac{d\nu}{dx} - \frac{dh}{dx} \left(\frac{\partial P_E}{\partial U} \right)^T \nu. \tag{82}$$

Identifying the integral as the equivalent of applying a finite volume method to the cell k, we can then obtain:

$$\begin{aligned} \frac{\Delta \nu_k}{\Delta t} \Delta x - h_{k+\frac{1}{2}} \widehat{G}_{E,k,k+\frac{1}{2}} - h_{k-\frac{1}{2}} \widehat{G}_{E,k,k-\frac{1}{2}} - \frac{dh_k}{dx} \left(\frac{\partial P_E}{\partial U_E} \right)_k^T \nu_k \Delta x - \beta \left(\frac{\partial j}{\partial U_E} \right)_k^T \Delta x \\ = (1-\beta) \left(\frac{\mathfrak{D}\bar{\jmath}}{\mathfrak{D}U_E} \right)_k^T + \left(\frac{\mathfrak{D}\mathcal{R}_D}{\mathfrak{D}U_E} \right)_k^T \mu_k, \end{aligned} \tag{83}$$

and:

$$\frac{\Delta\mu_k}{\Delta t}\Delta x - h_k\left(\frac{\partial F_E}{\partial U_\lambda}\right)_k^T \Delta\nu_k - \frac{dh_k}{dx}\left(\frac{\partial P_E}{\partial U_\lambda}\right)_k^T \nu_k\Delta x - \beta\left(\frac{\partial j}{\partial U_\lambda}\right)_k^T \Delta x = (1-\beta)\left(\frac{\mathfrak{D}\bar{j}}{\mathfrak{D}U_\lambda}\right)_k^T + \left(\frac{\mathfrak{D}\mathcal{R}_D}{\mathfrak{D}U_\lambda}\right)_k^T \mu_k, \tag{84}$$

where the numerical fluxes for the Euler adjoint variables are again given via a method based on the Roe scheme:

$$\widehat{G}_{E,k,k+\frac{1}{2}} = \frac{1}{2}\left(\frac{\partial F_E}{\partial U_E}\right)_k^T (\nu_{k+1}+\nu_k) + \frac{1}{2}\left|\widetilde{\left(\frac{\partial F_E}{\partial U_E}\right)}_{k+\frac{1}{2}}^T\right|(\nu_{k+1}-\nu_k). \tag{85}$$

Each complete iteration is again wrapped within a fourth-order Runge-Kutta step. Since we consider only supersonic flow and are solving for the adjoint variables, the right-hand boundary conditions are Dirichlet, and set so that $\nu = 0$, and the left-hand uses extrapolation from within the domain to find the outgoing flux. Note that we do not enforce boundary conditions on μ.

VI. Results

A. Theoretical Analysis

Careful analysis of the numerical implementation of the three different adjoint methods used in this paper highlights certain key differences between the approaches:

1. The primal problem was solved by first decoupling the Euler and combustion variable parts of the governing equations. Considering the general upwind formulation for the numerical flux:

$$\widehat{hF}_{k+\frac{1}{2}} = \frac{1}{2}(hF_{k+1}+hF_k) - \frac{1}{2}\left|\frac{\partial F}{\partial U}\right|_{k+\frac{1}{2}}(hU_{k+1}-hU_k), \tag{86}$$

For the fully coupled system this would expand to give:

$$\begin{pmatrix}\widehat{hF}_E\\ \widehat{hF}_\lambda\end{pmatrix}_{k+\frac{1}{2}} = \frac{1}{2}\left(\begin{pmatrix}hF_E\\ hF_\lambda\end{pmatrix}_{k+1} + \begin{pmatrix}hF_E\\ hF_\lambda\end{pmatrix}_k\right) - \frac{1}{2}\begin{vmatrix}\frac{\partial F_E}{\partial U_E} & \frac{\partial F_E}{\partial U_\lambda}\\ \frac{\partial F_\lambda}{\partial U_E} & \frac{\partial F_\lambda}{\partial U_\lambda}\end{vmatrix}_{k+\frac{1}{2}}\left(\begin{pmatrix}hU_E\\ hU_\lambda\end{pmatrix}_{k+1} - \begin{pmatrix}hU_E\\ hU_\lambda\end{pmatrix}_k\right), \tag{87}$$

but for the uncoupled approach, gathering the two uncoupled equations into one, we have:

$$\begin{pmatrix}\widehat{hF}_E\\ \widehat{hF}_\lambda\end{pmatrix}_{k+\frac{1}{2}} = \frac{1}{2}\left(\begin{pmatrix}hF_E\\ hF_\lambda\end{pmatrix}_{k+1} + \begin{pmatrix}hF_E\\ hF_\lambda\end{pmatrix}_k\right) - \frac{1}{2}\begin{vmatrix}\frac{\partial F_E}{\partial U_E} & 0\\ 0 & \frac{\partial F_\lambda}{\partial U_\lambda}\end{vmatrix}_{k+\frac{1}{2}}\left(\begin{pmatrix}hU_E\\ hU_\lambda\end{pmatrix}_{k+1} - \begin{pmatrix}hU_E\\ hU_\lambda\end{pmatrix}_k\right) \tag{88}$$

where it can be seen that the cross terms in the artificial dissipation in Equation (87) are absent.

This difference is expected to affect the discrete adjoint, which depends explicitly on the form of the flow residuals, and also parts of the hybrid adjoint. However, assuming that the methods are consistent and the same flow solution is obtained, the continuous adjoint should be unaffected.

2. The Jacobian, $\frac{\mathfrak{D}()}{\mathfrak{D}()}$, at any point in the discrete adjoint equation is a derivative of some quantity at that point relative to parameters defined at every other point throughout the domain. In contrast, in the continuous adjoint the Jacobian, $\frac{\partial()}{\partial()}$, at any point is a derivative of the quantity at that point with respect to parameters only at that same point. This immediately implies that the Jacobians in the discrete formulation are much larger than for the continuous, though the actual stencil used in the flow residual calculation is likely to mean the Jacobian matrix will mostly contain zeros. As it includes both discrete and continuous Jacobians, the hybrid approach lies somewhere between the discrete and continuous in terms of the memory requirements that would be needed to store these terms.

3. When applying automatic differentiation to find the discrete Jacobians, additional terms that give the sensitivity of the artificial dissipation of the Roe and upwinding schemes to the flow variables will be automatically included. For example, considering the following numerical flux:

$$\widehat{hF}_{E,k+\frac{1}{2}} = \frac{1}{2}\left(hF_{E,k+1} + hF_{E,k}\right) - \frac{1}{2}\left|\frac{\partial \widetilde{F_E}}{\partial U_E}\right|_{k+\frac{1}{2}} \left(hU_{E,k+1} - hU_{E,k}\right), \tag{89}$$

we can see that taking derivatives with respect to $U_{E,k}$ will introduce the Hessian term:

$$-\frac{1}{2}\left(\frac{\mathfrak{D}}{\mathfrak{D}U_{E,k}}\left|\frac{\partial \widetilde{F_E}}{\partial U_E}\right|_{k+\frac{1}{2}}\right)\left(hU_{E,k+1} - hU_{E,k}\right). \tag{90}$$

Though we expect this to be small, a cumbersome term-by-term expansion of the numerical methods used to solve the continuous, discrete and hybrid adjoints in this case reveals that the only difference between them is due to such terms. The continuous has no such terms, and the hybrid has fewer than the discrete since in that case these only appear in the fluxes of the Euler adjoint variables.

4. The derivation of the hybrid reveals two important points. The first is that the terms treated continuously do not involve the combustion source term ω, and the second is that it is possible to deal with a purely discrete objective function in the definition of the adjoint equation. The implications of both of these are that once the continuous part has been derived once, it will not be altered by modifications to the source term, and that it will be valid for non-differentiable source and objective functions. Additionally, it implies that at least part of any code developed for the continuous adjoint can be reused.

B. Numerical Analysis

1. Flow conditions

The test case used to investigate the characteristics of the hybrid adjoint method is a compression-expansion nozzle, as used by Giles and Pierce.[18] The nozzle area (height) is given by:

$$h(x) = \begin{cases} 2 & \text{for } x \leq -\frac{1}{2} \text{ or } x \geq -\frac{1}{2} \\ 1 + sin^2(\pi x) & \text{for } -\frac{1}{2} < x < \frac{1}{2} \end{cases}, \tag{91}$$

and is shown in Figure 5.

The flow conditions and mesh used in this paper are:

- Inlet Mach number, $M_i = 4.0$
- Inlet stagnation enthalpy, $H_i = 4.0$
- Inlet stagnation pressure, $p_{0i} = 2.0$
- CFL number $= 0.5$
- Number of mesh cells $= 100$
- Exponential source term constant, $C = 0.1$

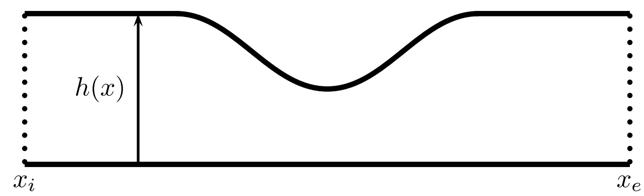


Figure 5. Compression-expansion nozzle

- Gas constant, $R = 1.0$
- Ratio of specific heats, $\gamma = 1.4$
- Heaviside source term constant, $b = 1.0$
- Specific heat release, $q = 1.0$
- Heaviside initiation temperature, $T^* = 0.3$
- Absolute value functional pressure constant, $p^* = 0.03$

Figures 6 and 7 show the pressure and progress variables for the flow solutions with the exponential and Heaviside source terms, respectively. Of note, the step nature of the Heaviside source function can be seen in Figure 7b), where the combustion progress variable remains constant until the duct height has changed sufficiently to cause the temperature to rise above T^*.

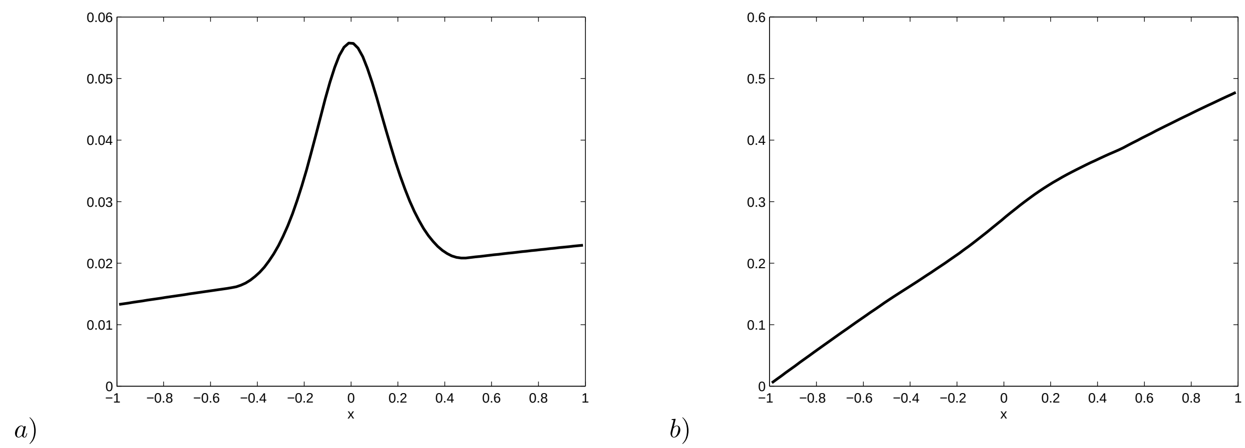
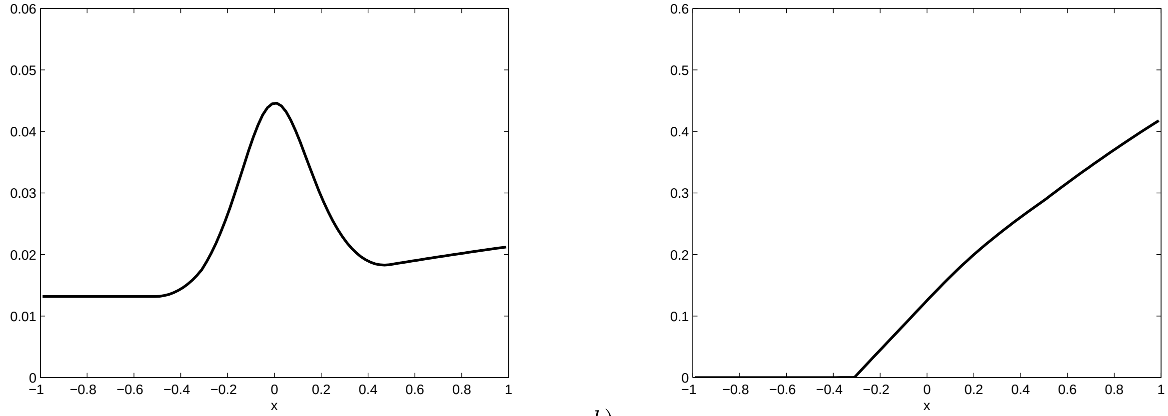


Figure 6. Flow solution with exponential combustion source term: a) pressure, b) combustion progress variable

2. Adjoint variables

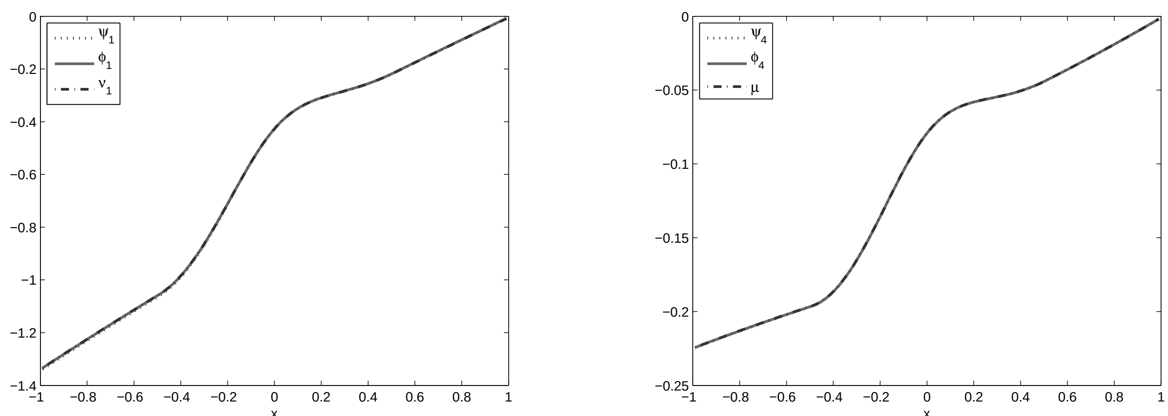
The first and fourth adjoint variables (related to the density and combustion variable parts of the flow, respectively) computed by the discrete, continuous and hybrid approaches are shown in the following graphs for the cases: exponential source term and integral of pressure functional (Figure 8), Heaviside source term and integral of pressure functional (Figure 9), and exponential source term and absolute value functional (Figure 10). In all three, close agreement is seen between the adjoint variables produced by the different methods.



a) *b)*

Figure 7. Flow solution with Heaviside combustion source term: a) pressure, b) combustion progress variable

Additionally, Figures 9 and 10 show cases in which there are difficulties with applying the continuous adjoint due to non-differentiability in the source function and objective function, respectively. In these cases we compare just the discrete and hybrid variables, demonstrating that the hybrid adjoint can be used in situations that could be problematic for the continuous method.



a) *b)*

Figure 8. Adjoint variables (discrete (ψ), continuous (ϕ) and hybrid (ν & μ)) for the exponential combustion source term and the integral of pressure functional: a) first variable, b) fourth variable

3. Difference in adjoint variables

Figure 11 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, and Figures 12 and 13 show the difference between the hybrid and discrete for the Heaviside source term and integral of pressure functional, and the exponential source term and absolute value functional, respectively. This shows, in general, closer agreement between the hybrid and continuous approaches where the continuous exists (Figure 11). It is also possible to see that this difference fluctuates most where the duct height changes most rapidly ($x = \pm 0.25$).

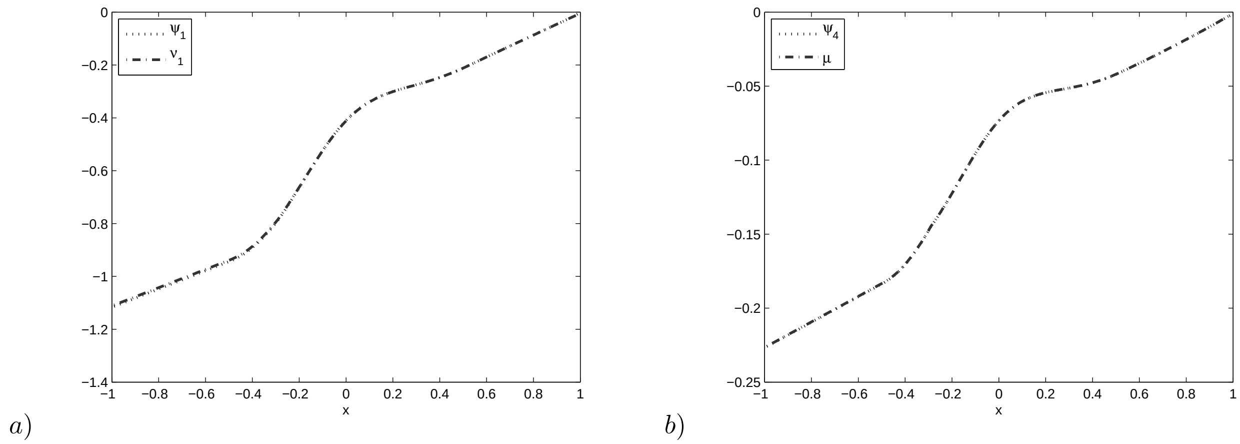


Figure 9. Adjoint variables (discrete (ψ) and hybrid (ν & μ)) for the Heaviside combustion source term and the integral of pressure functional: a) first variable, b) fourth variable

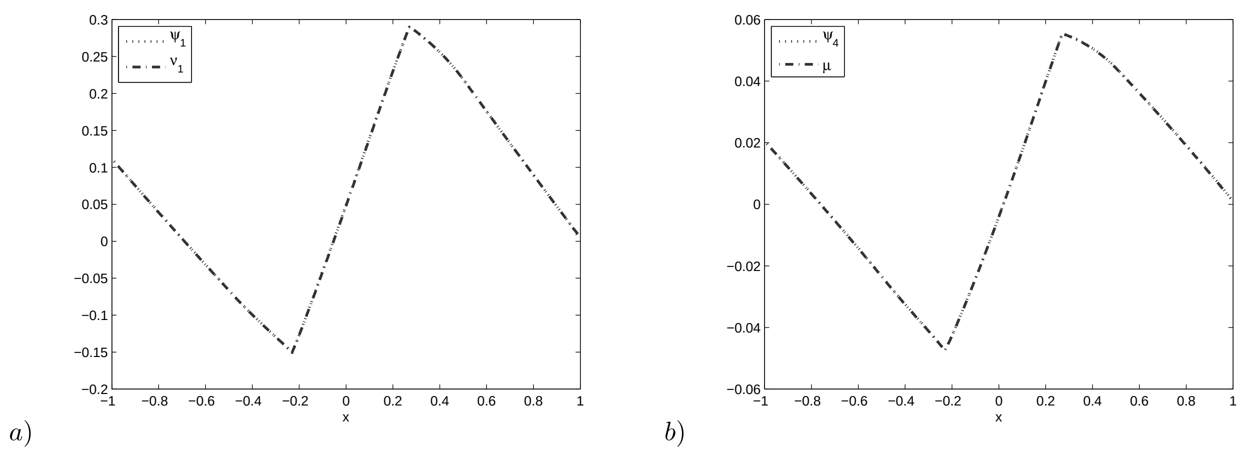
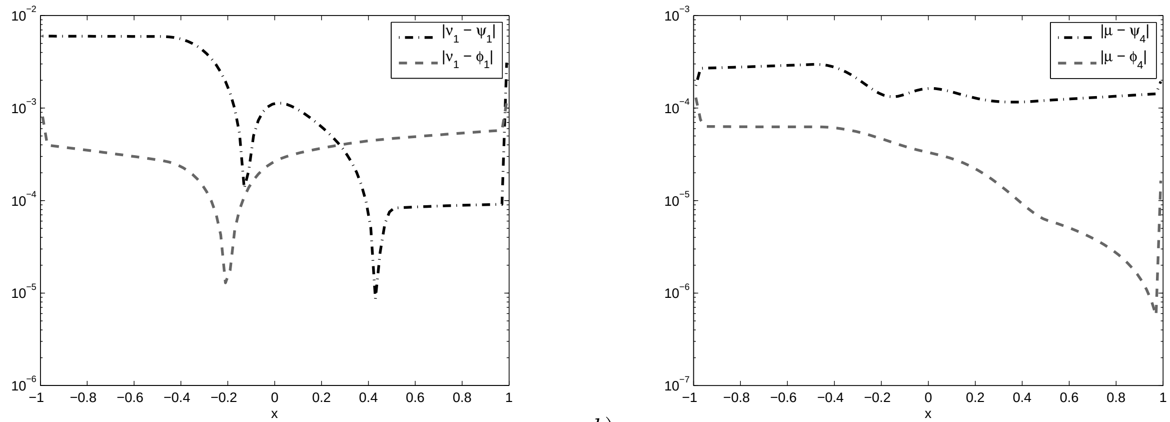
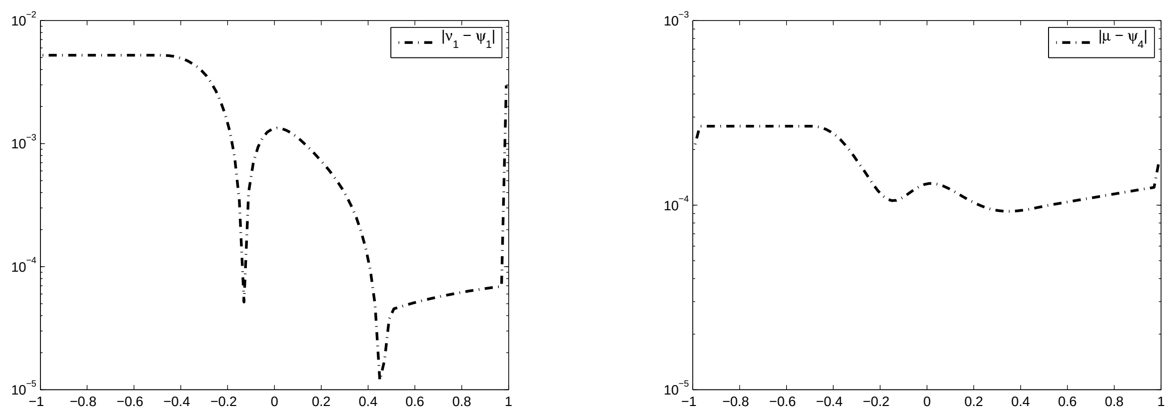


Figure 10. Adjoint variables (discrete (ψ) and hybrid (ν & μ)) for the exponential combustion source term and the absolute value functional: a) first variable, b) fourth variable



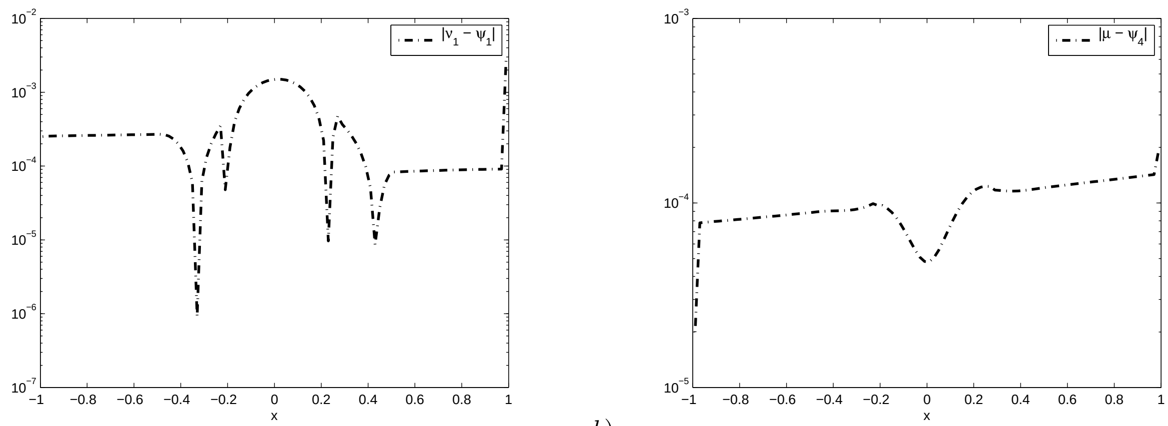
a) *b*)

Figure 11. Size of difference in adjoint variables (the hybrid and discrete ($|\{\nu, \mu\} - \psi|$), and the hybrid and continuous ($|\{\nu, \mu\} - \phi|$)) for the exponential combustion source term and integral of pressure functional: a) first variable, b) fourth variable



a) *b*)

Figure 12. Size of difference in adjoint variables (the hybrid and discrete ($|\{\nu, \mu\} - \psi|$) for the Heaviside combustion source term and the integral of pressure functional: a) first variable, b) fourth variable



a) *b)*

Figure 13. Size of difference in adjoint variables (the hybrid and discrete ($|\{\nu,\mu\} - \psi|$) for the exponential combustion source term and the absolute value functional: a) first variable, b) fourth variable

4. Sensitivity

The perturbation of the objective function, $\mathcal{J}$, relative to a change in the inlet Mach number can be written, substituting α for M_i, neglecting any explicit dependence of the functional on M_i and only including the $\mathcal{R}$ and $\mathcal{N}$ at locations that explicitly depend on this, as:

- Discrete approach:

$$\Delta\mathcal{J}_D = \psi_i^T \frac{\mathfrak{D}\mathcal{R}_i}{\mathfrak{D}M_i}\frac{\Delta M_i}{\Delta x} \tag{92}$$

- Continuous approach:

$$\delta\mathcal{J}_C = \phi_i^T \frac{\partial\mathcal{N}_i}{\partial M_i}\delta M_i \tag{93}$$

- Hybrid approach:

$$\{\delta,\Delta\}\mathcal{J}_H = \nu_i^T \frac{\partial\mathcal{N}_{E,i}}{\partial M_i}\delta M_i + \mu_i^T \frac{\mathfrak{D}\mathcal{R}_{\lambda,i}}{\mathfrak{D}M_i}\frac{\Delta M_i}{\Delta x} \tag{94}$$

The formulae for the sensitivities, with $\delta M_i \approx \Delta M_i$, can then be written:

- Discrete approach:

$$\frac{d\mathcal{J}_D}{dM_i} = \psi_i^T \frac{\mathfrak{D}}{\mathfrak{D}M_i}\frac{\mathcal{R}_i}{\Delta x} \tag{95}$$

- Continuous approach:

$$\frac{d\mathcal{J}_C}{dM_i} = \phi_i^T \frac{\partial\mathcal{N}_i}{\partial M_i} \tag{96}$$

- Hybrid approach:

$$\frac{d\mathcal{J}_H}{dM_i} = \nu_i^T \frac{\partial\mathcal{N}_{E,i}}{\partial M_i} + \mu_i^T \frac{\mathfrak{D}}{\mathfrak{D}M_i}\frac{\mathcal{R}_{\lambda,i}}{\Delta x} \tag{97}$$

where we note that as $\Delta x \to 0$, we expect $\frac{\mathcal{R}}{\Delta x} \to \mathcal{N}$ and the equations to become identical.

Figure 14 shows the variation of the sensitivity to the inlet Mach number over a range of Mach numbers calculated by finite differencing and all three adjoint methods for all four combinations of source and objective function considered in this paper. It can be seen that for all the cases considered, the four methods give very good agreement, which is expected since the adjoint variables shown previously in Figures 8, 9 and 10 demonstrated very good agreement over the domain, including at the inlet. It also should be noted that combinations b), c) and d) include non-differentiable terms, and thus again confirm the applicability of the hybrid to cases that could be problematic for the continuous adjoint.

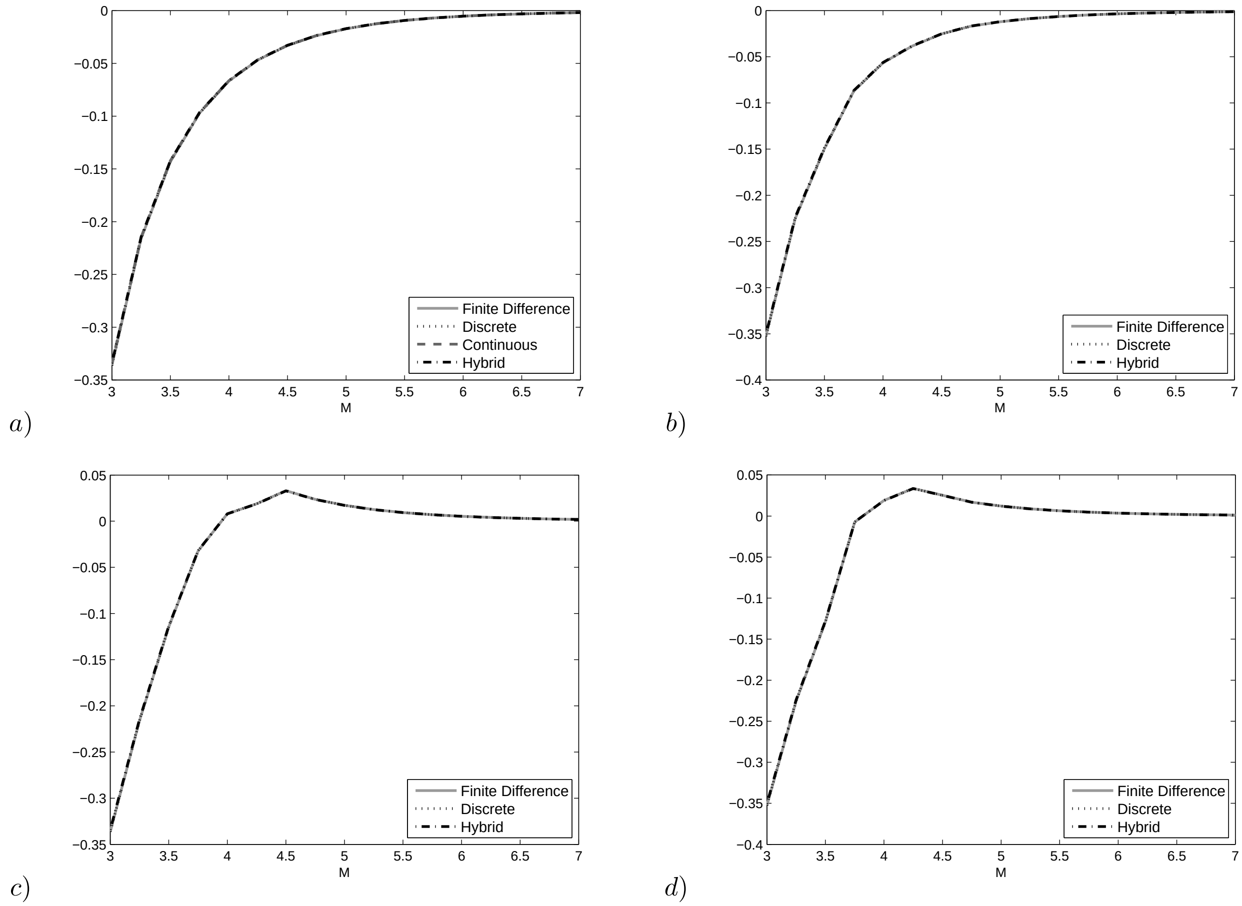


Figure 14. Sensitivity of functional to incoming Mach number along Mach regime: a) exponential source term and integral of pressure functional, b) Heaviside source term and integral of pressure functional, c) exponential source term and absolute value functional, d) Heaviside source term and non-differentiable functional

5. 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 15. From Figures 15a,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 15c, 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 seen that replacing the absolute value integrand of the functional with a smooth and differentiable approximation produced very similar results, and thus it can be concluded that the non-differentiability of the cost function is not the cause of the non-smooth convergence rate. Instead, it appears that this specific form of the functional is highly sensitive to the error in the flow solution, especially on a coarse grid.

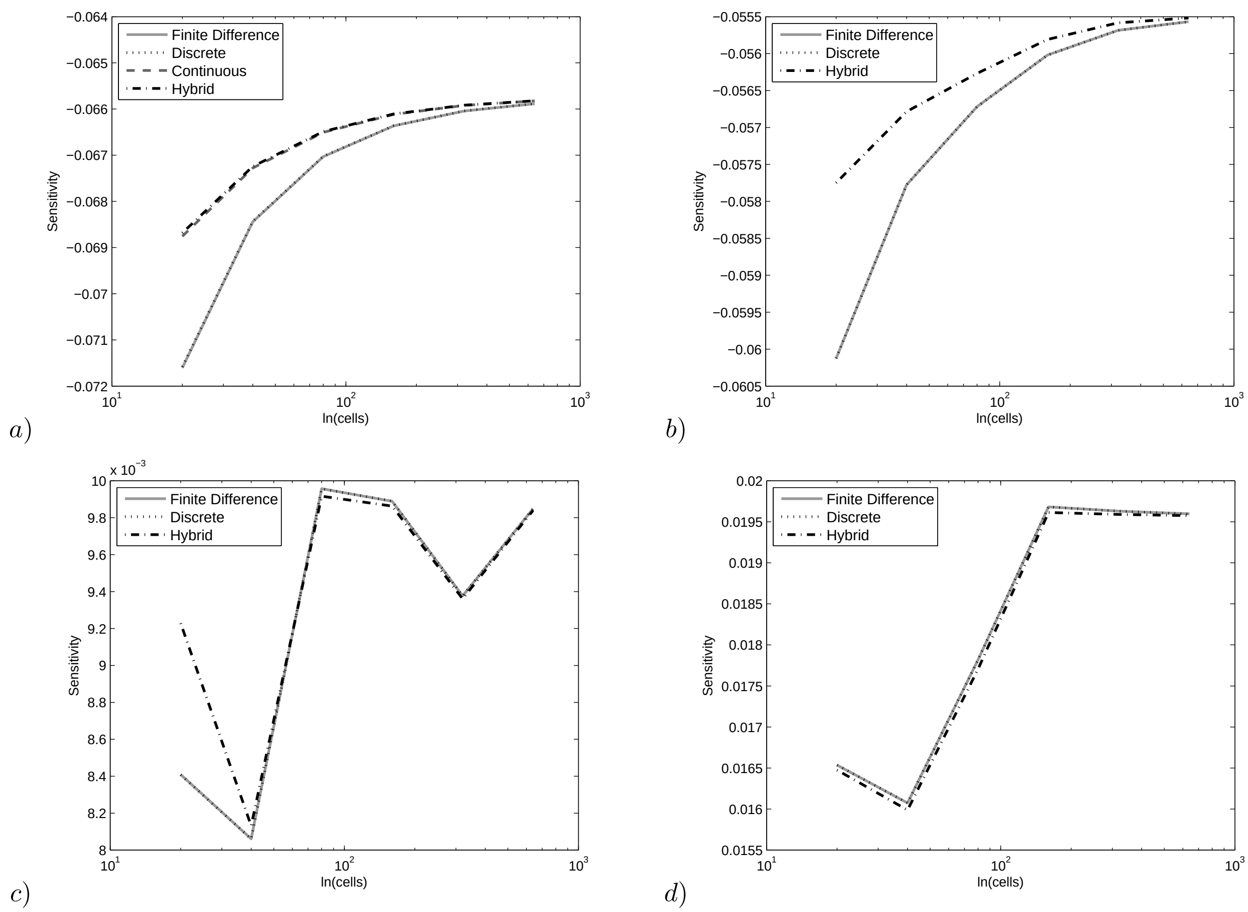


Figure 15. Sensitivity of functional to incoming Mach number at different grid refinement levels: a) exponential source term and integral of pressure functional, b) Heaviside source term and integral of pressure functional, c) exponential source term and non-differentiable functional, d) Heaviside source term and absolute value functional

VII. 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 seen to better match 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 the 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 2 updates Table 1 from the introduction, summarizing the relative advantages and disadvantages of the hybrid approach in comparison with the standard methods. Here a ± 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.

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

	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	−	+	**±**

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 while the set of equations for turbulence scalars will be treated discretely.

While 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.

Acknowledgments

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