In this work, the utility of the adjoint equations in error estimation of functional outputs and goal oriented mesh adaptation is investigated with specific emphasis towards application to high speed flows with strong shocks. Continuous and discrete adjoint formulations are developed for the compressible Euler equations and the accuracy and robustness of the implementation is assessed by evaluating adjoint-computed sensitivities. The two-grid approach of Venditti and Darmofal\(^1\) - where the flow and adjoint solutions on a baseline mesh are processed to estimate the functional on a finer mesh - is used for error estimation and goal oriented mesh adaptation. Using a carefully designed set of test cases for the Quasi one dimensional Euler equations, it is shown that discrete adjoints can be used to estimate the fine grid functional more accurately, whereas continuous adjoints are marginally better at estimating the analytical value of the functional when the flow and adjoint solutions are well resolved. These observations appear to be true in multi-dimensional inviscid flows, but the distinction is not as clear. The discrete adjoint is shown to be robust when applied to goal oriented mesh adaptation in a flow with multiple strong shocks, and hence offers promise as a viable strategy to control the numerical error in Hypersonic flow applications.

**Nomenclature**

- \(f\) Functional
- \(U\) Flow solution
- \(\Psi\) Adjoint solution
- \(R\) Flow residual
- \(R^\Psi\) Adjoint residual
- \(E_{\text{Real}}\) Real error (\(f_{\text{exact}} - f_H\))
- \(E_{\text{Relative}}\) Relative error (\(f_h - f_H\))
- \(\epsilon_{cc}\) Computable error estimate

**Subscript**

- \(H\) Baseline (or coarse grid)
- \(h\) Uniformly refined grid

**Abbreviations**

- \(C\) Continuous Adjoint
- \(D\) Discrete Adjoint

**I. Introduction**

Accurate determination of functionals (integrals such as lift, drag, thrust, range etc.) involving flowfield quantities is typically a major objective of any engineering flow computation. In computing such functionals, it is important to quantify the error due to numerical discretization if confidence is to be placed in the predictions. With practical utility in mind, this has to be achieved without prior knowledge of analytical solutions. The availability of such an estimate of the numerical error will be a vastly powerful tool in formal solution verification of computational simulations.
Further, if such simulations are to be meaningfully used in validations or predictions of complex real world problems, it is critical to ensure that the numerical error does not obscure modeling errors. In this work, specific attention is devoted to the issue of accurate quantification and robust management of numerical error in high speed flows. The authors consider this to be a critical first step in achieving their ultimate objective of developing a robust and automatic (to the fullest extent possible) strategy to control the error in multi-physics simulations of Scramjet propulsion.

Approaches to quantifying numerical error in the context of Finite Elements have been pursued for the past two decades, primarily with the objective of providing a indicator of the local contribution to the functional error. Aposteriori estimation techniques that are applicable to Finite Volume based discretizations is, however, relatively recent. Pierce and Giles presented a framework using which super convergent functional estimates were demonstrated by adding a correction term based on the adjoint (or a dual) of the original governing equations. In this procedure, the correction term involves evaluations of the residual of the governing equations in their continuous form via an appropriately reconstructed high order interpolation of the computed solution. A novelty of this methodology is its generic nature and applicability to finite element/volume/difference based discretizations. Venditti and Darmofal proposed an algebraic equivalent of the Pierce and Giles approach. This approach also utilizes the adjoint equations and the functional error on the baseline mesh is improved by computing an estimate of the functional on a refined mesh. Further, information from the adjoint solution has been shown to be useful in efficiently adapting the baseline mesh to better approximate the functional of interest. In the present work, the approach of Venditti and Darmofal will be pursued because of its robust behavior.

While these error estimation strategies have been utilized in applications involving subsonic and transonic flow, they do not appear to have been widely used in problems involving strong shocks which will be the focus of the present work.

II. The adjoint formulation for the compressible Euler equations

To explore and compare the utility of discrete and continuous adjoints in error estimation and mesh adaptation, both formalisms have been implemented within an unstructured grid compressible Navier–Stokes solver. In this section, some detail will be provided on the derivation and implementation of discrete and continuous adjoint equations. Further information on the theoretical aspects of continuous and discrete adjoints can be seen from . The adjoint procedure is an efficient method to compute the variation of a functional $f$ and hence is useful in computing sensitivities that can be used in error estimation, optimal design, uncertainty quantification, etc. From the viewpoint of implementation and application, either of the following approaches can be pursued: in the discrete approach, the adjoint equations are directly derived from the discretized governing equations, whereas in the continuous approach, the adjoint equations are derived from the flow equations and subsequently discretized.

A. Discrete adjoint formulation

Although the primary focus of this work concerns error estimation, adjoint equations can most conveniently be introduced in the context of evaluation of functional variation. Let $R(U, \alpha) = 0$ represent the governing equations in a domain $\Omega$ that are to be solved for flow variables $U$ in the presence of one or more flow/geometric parameters $\alpha$. We are interested in a functional $f(U, \alpha)$ and, for purposes of illustration, its variation with respect to parameters $\alpha$. When solved numerically on a mesh $\Omega_H$, a discretized form of the governing equations $R_H(U_H, \alpha)$ is used to compute a discrete functional $f_H(U_H)$. The variation of this discrete functional to some change in the parameters $\delta \alpha$ is

$$\delta f_H = \left( \frac{\partial f_H}{\partial \alpha} + \frac{\partial f_H}{\partial U_H} \frac{\partial U_H}{\partial \alpha} \right) \delta \alpha. \quad (1)$$

This variation can be evaluated if $\frac{\partial R_H}{\partial \alpha}$ is known, and this can be determined, for instance, by linearizing the governing equations $R_H(U_H, \alpha)$

$$\frac{\partial R_H}{\partial \alpha} + \frac{\partial R_H}{\partial U_H} \frac{\partial U_H}{\partial \alpha} = 0. \quad (2)$$

The above equation must be solved iteratively and the computational effort is comparable to solving the governing equation $R_H = 0$. Since eqn. 2 has to be solved for every component $\alpha_i$, this direct approach will be expensive if a large number of parameters $\alpha$ are present. In order to circumvent this computational expense, the adjoint approach is useful; by introducing the adjoint variable $\Psi$ as a Lagrange multiplier, we can write

$$\delta f_H = \left( \frac{\partial f_H}{\partial \alpha} + \frac{\partial f_H}{\partial U_H} \frac{\partial U_H}{\partial \alpha} + \Psi^T \left[ \frac{\partial R_H}{\partial \alpha} + \frac{\partial R_H}{\partial U_H} \frac{\partial U_H}{\partial \alpha} \right] \right) \delta \alpha,$$

$$= \left( \frac{\partial f_H}{\partial \alpha} + \Psi^T \frac{\partial R_H}{\partial \alpha} \right) \delta \alpha, \quad (3)$$

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provided
\[
\left[ \frac{\partial R_H}{\partial U_H} \right]^T \Psi_H = - \left[ \frac{\partial f_H}{\partial U_H} \right]^T.
\] (4)

Equation 4 is called the discrete adjoint equation because its derivation proceeds directly from the discretized form of the governing equations. Note that unlike eqn. 2, eqn. 4 does not contain derivatives with respect to \( \alpha \). This means that, irrespective of the dimension of \( \alpha \), we have to solve just one adjoint equation; the full gradient is then obtained from eqn. 3 which only requires dot products and is hence computationally inexpensive. With this approach, the expense of computing the full gradient is roughly equal to two flow solutions.

1. Implementation of the discrete adjoint equations

The discrete adjoint approach requires computation of derivatives like eqn. 4. In the discrete adjoint approach, we have to solve just one adjoint equation; the full gradient is then obtained from eqn. 3 which only requires dot products and is hence computationally inexpensive. With this approach, the expense of computing the full gradient is roughly equal to two flow solutions.

1. Implementation of the discrete adjoint equations

The discrete adjoint approach requires computation of derivatives like \((\partial f_H / \partial U_H)^T, (\partial f_H / \partial \alpha)^T, (\partial R_H / \partial \alpha)^T \Psi\) and \((\partial R_H / \partial U_H)^T \Psi\). While it is possible to perform such differentiation by hand for relatively simple governing equations, it is convenient to make use of Automatic Differentiation (AD) tools\(^{13}\) to perform this task. AD tools automate the process of applying the chain rule of differentiation to existing computer programs to generate a new program that computes required derivatives. In this work, the software suite ADOL-C\(^{14}\) has been used for differentiation of relevant routines written in C++. ADOL-C uses operator overloading to implement the chain rule; and the independent, dependent and any intermediate real variables that affect the derivative computation are re-declared to be of a special type adouble. The independent and dependent variables are marked using a specific syntax, the section of the code that has to be differentiated is also marked, and the code is then compiled using a standard C++ compiler and linked to the ADOL-C library. In order to improve efficiency, and compute the adjoint terms like \((\partial R_H / \partial U_H)^T \Psi\), the reverse mode\(^{13}\) of AD is used. Once the required derivatives and matrix vector products in eqn. 4 are obtained, iterative solution is performed.

B. Continuous adjoint formulation

In contrast to discrete adjoints, the continuous adjoint equations are derived from the continuous form of the linearized governing equations. In the following derivation, special care is given to the derivation of the functional variation in the presence of flow discontinuities. Assume that the governing equations are formulated on a fluid domain \( \Omega \), enclosed by boundaries divided into an inlet \( S_{in} \), outlet \( S_{out} \), and solid wall boundaries \( S_{wall} \). The objective is to compute the variation of a functional \( f \) with respect to changes in some flow or geometric parameters. It is important to note that in the continuous adjoint formulation for the Euler equations, \( f(p, \vec{n}_S) \) has to be a function of the pressure \( p \). Note that \( \vec{n}_S \) is the inward pointing normal to the surface \( S \).

In the presence of strong flow discontinuities \( \Sigma \) in the flow that touch the surface \( S \) and \( x_b = \Sigma \cap S \), the total variation (due to geometrical or flow changes) of \( f \) is

\[
\delta f = \int_S \left[ \frac{\partial f}{\partial p} \delta p + \vec{t} \cdot \delta g \left( \frac{\partial f}{\partial \vec{n}_S} \right) - \kappa \left( f + \frac{\partial f}{\partial \vec{n}_S} \vec{n}_S \right) \right] \delta S \, ds
+ \int_{S_{in} \cup \cup S_{out}} \frac{\partial f}{\partial p} \delta p \, ds - \left[ f \right]_{x_b} \delta \vec{n}_S \cdot \vec{t}_\Sigma \, ds(x_b),
\] (5)

where \([f]_{x_b}\) is the jump of \( f \) across the discontinuity at point \( x_b \), vectors \( \vec{n}_S \) and \( \vec{t}_\Sigma \) stand for the normal and tangential unit vectors to the shock discontinuity \( \Sigma \), and \( \kappa \) is the surface curvature. Finally \( \delta p \) and \( \delta S \) could be computed by using the linearized state.

In the presence of shocks, the linearized sensitivity of the model needs to take into account the perturbations of the solution and perturbations of the location of the shock. In this case, \( \delta U \) stands for the infinitesimal change in the state on both sides of the discontinuity and results from the solution of the linearized Euler equations, whereas \( \delta S \) describes the infinitesimal normal deformation of the discontinuity and it results from a linearization of the Rankine-Hugoniot conditions. The linearized form is

\[
\vec{\nabla} \cdot \left( \vec{A} \delta U \right) = 0, \quad \text{in } \Omega \setminus \Sigma,
\delta \vec{n}_S = - \delta S \partial_n \vec{v} \cdot \vec{n}_S + (\partial g \delta S) \vec{v} \cdot \vec{t}_S, \quad \text{on } S_{wall} \setminus x_b,
(\delta W)^{\Sigma}_+ = \delta W_{in}, \quad \text{on } S_{in},
(\delta W)^{\Sigma}_+ = 0, \quad \text{on } S_{out},
\left[ \vec{A} \left( \delta S \partial_n U + \delta U \right) \right]_{\Sigma} \cdot \vec{n}_S + \left[ \vec{F} \right]_{\Sigma} \cdot \delta \vec{n}_S = 0 \quad \text{on } \Sigma,
\]

with \((\delta W)^{\Sigma}_+\) representing the incoming characteristics and \( \partial \vec{F} / \partial U = \vec{A} \) is the flux Jacobian matrix. In order to
Before using adjoints in error estimation, it is desirable to verify the accuracy and robustness of the implementation by the adjoint variables. Then, the result is integrated over the domain (taking into consideration, the discontinuities), and finally the result is added to eqn. 5. Upon identifying the corresponding terms in that final expression with the adjoint equations, the variation of the functional can be written as:

$$
\delta f = \int_S \left[ \frac{\partial f}{\partial \rho} \frac{\partial \rho}{\partial n} + \nabla \cdot \bf{F} \right] \delta \rho \, dS
$$

where $\kappa$ is the surface curvature, $\varphi = (\psi_2, \psi_3)$ and $\vartheta = \rho \psi_1 + \rho \nabla \cdot \varphi + \rho H \psi_4$. Using (7) and (8) we are able to compute any variation of $f$ due to a geometrical or inlet flow change, even when the computation of $f$ includes a shock discontinuity impinging on the surface of integration $S$. Note that the importance of some of these terms depends on the actual flow condition and, in particular, on the relative angle of impingement of the discontinuity on the surface $S$.

For the results in the present work, discontinuities are not explicitly treated as mentioned above and this derivation is given for completeness and to suggest the potential flexibilities offered in the continuous adjoint formulation to handle discontinuities in a formal manner. Within the context of actual flow discretizations, discontinuities are represented by regions of high gradients. Therefore, the importance of all terms must be carefully assessed.

1. **Discretization of the continuous adjoint equations**

The adjoint equations have been discretized with a standard cell-center-based finite volume formulation, obtained by applying the integral formulation of the adjoint equations to a control volume $\Omega_j$ and performing an integration around the outer boundary of this control volume. Using a time marching strategy, and starting with the weak formulation of the adjoint equations, the following semi-discrete formulation can be obtained:

$$
|\Omega_j| \frac{d\Psi_j}{dt} = \int_{\Gamma_j} \Psi \cdot \bf{n} \, dS = \sum_{k=1}^{m_j} f_{jk} \cdot \nabla \cdot U_{jn} S_{jk} = \sum_{k=1}^{m_j} f_{jk} S_{jk},
$$

where $\nabla$ is the transposed Euler flux Jacobian evaluated at the cell $j$, $\Gamma_j$ is the boundary of $\Omega_j$, $|\Omega_j|$ is the area of $\Omega_j$ and, for every neighbor cell $k$ of $j$, $\nabla \cdot U_{jn}$ is the outward unit vector normal to the common face and $S_{jk}$ is its length, $f_{jk}$ is the numerical flux vector at the said face, $\Psi_j$ is the value of $\Psi$ at the cell $j$ (it has been assumed that $\Psi_j$ is equal to its volume average over $\Omega_j$), and $m_j$ is the number of neighbors of the cell $j$.

An upwind scheme based upon Roe’s flux difference splitting scheme has been developed for the adjoint equations. In this case, the aim is to use upwind type formulae to evaluate $\nabla \cdot \bf{n} \Psi$. Taking into account that $A^T = - (P^T)^{-1} A P^T$, where $A^T = \bar{A}^T \cdot \bf{n}$ is the projected Jacobian matrix, $\Lambda$ is diagonal matrix of eigenvalues and $P$ is the corresponding eigenvector matrix, the upwind flux is computed as

$$
f_{jk}^{upw} = \frac{1}{2} \left( \bar{A}^T \cdot \bf{n}_{jk} (\Psi_j + \Psi_k) - |A^T_{jk}|(\Psi_k - \Psi_j) \right) = \frac{1}{2} \left( \bar{A}^T \cdot (\Psi_j + \Psi_k) + (P^T)^{-1} \Lambda |P^T| \delta \Psi \right),
$$

where $|A^T_{jk}| = - (P^T)^{-1} |\Lambda| P^T$, the subindex $jk$ denotes an average value in the interface. Note that $f_{jk}^{upw} \neq f_{kj}^{upw}$. A second order scheme is obtained by a reconstruction (with slope limiters) of the adjoint variables about the common face between the cells.

C. **Verification and behavior of adjoint implementation**

Before using adjoints in error estimation, it is desirable to verify the accuracy and robustness of the implementation in problems involving strong shocks. This is especially important because linearized perturbation of the flow solution
Figure 1. Geometry for oblique shock problem

Figure 2. Adjoint density for oblique shock problem
Figure 3. Sensitivities (derivative of post shock pressure with respect to freestream Mach number) predicted by discrete and continuous adjoints for the oblique shock problem

near discontinuities can become questionable as mentioned in the previous section. However, it is not clear whether this would necessarily warrant an explicit treatment of the continuous adjoint solution near shocks. Also, it has been previously shown that discrete adjoints are inconsistent with the continuous partial differential equation near shocks\textsuperscript{15}. However, in practice, flow discontinuities appear as high gradient regions in the numerical solution, and hence, the behavior of the adjoint solution needs to be carefully studied.

To evaluate the adjoint solutions, a problem\textsuperscript{14} of two dimensional inviscid supersonic flow (at a Mach number of 4) over a 25\textdegree wedge as shown in fig. 1 will be considered. The objective function is taken to be the integral of pressure on the lower wall (over a region that includes 10 cell faces) and its sensitivity with respect to the freestream Mach number will be considered. The flow solution is computed using a second order accurate Least squares slope reconstruction (on a grid composed of triangles) with a minmod limiter. Adjoint solutions computed using various approaches are shown in fig. 2. The adjoint solution for a supersonic flow essentially represents a backward propagation of the characteristics of the flow Jacobian (clear evidence of this is seen in the three characteristics that are visible before the shock. The seemingly minor differences between the three adjoint solutions turn out to be very important for the computation of flow gradients. The gradient computed by the discrete adjoint was confirmed to match the discrete sensitivities to within 0.01\% (discrete sensitivities can be verified by using a complex step method\textsuperscript{16} or via sufficiently accurate finite differencing). However, the difference between the discrete and analytical gradients (analytical gradients can be obtained by linearizing the oblique shock relations) was found to be 12\%. The continuous adjoint solution with minmod limiting of the reconstruction of the adjoint solution was found to give sensitivities that are within 4\% of the analytical sensitivity. Utilizing the flexibility offered by the continuous adjoint formulation, a central difference implementation with fourth order dissipation for the adjoint equations yielded a gradient that was within 0.2\% of the analytical sensitivity. Figure 3 shows the comparison over a broader range of Mach numbers, and further reveals the discrepancy of discrete sensitivities with analytical sensitivities. It has to be mentioned that the apparent noise in the discrete sensitivity reduces with increasing resolution of the domain of the functional.

To understand more clearly the differences between the discrete and continuous adjoints, it is perhaps useful to derive compatible expressions. Consider two versions of the adjoint: the classical discrete adjoint and a new discrete adjoint which mimics the behavior of the continuous adjoint equations:

- In the classical discrete adjoint approach, a modified version of the governing equation including a dissipation $D$ is fulfilled, and the following Lagrangian can be built\textsuperscript{1}: $\mathcal{L}(U, \alpha) = f(U) + \Psi^D(R(U, \alpha) + D(U))$.

- On the other hand, using ideas inspired in the continuous adjoint problem, one can define the Lagrangian as $\mathcal{L}(U, \alpha) = f(U) + \Psi^C(R(U, \alpha) + C)$, where $C$ includes high-order terms of the discretization of the adjoint equations as in the continuous adjoint procedure.

The variation of the objective function $f$ in these approaches is, therefore:

\[
\delta f = \frac{\partial f}{\partial U} \delta U + \frac{\partial f}{\partial \alpha} \delta \alpha + \Psi^D \left( \frac{\partial R}{\partial U} + \frac{\partial D}{\partial U} \right) \delta U + \Psi^D \left( \frac{\partial R}{\partial \alpha} \right) \delta \alpha, \tag{11}
\]

\[
\delta f = \frac{\partial f}{\partial U} \delta U + \frac{\partial f}{\partial \alpha} \delta \alpha + \Psi^C \left( \frac{\partial R}{\partial U} \right) \delta U + \Psi^C \left( \frac{\partial R}{\partial \alpha} \right) \delta \alpha. \tag{12}
\]

\textsuperscript{1}To verify the adjoint solutions in a Quasi one dimensional Euler problem, a comparison with an analytical adjoint is shown in the Appendix

\textsuperscript{11}Matrix transposes are ignored in the following discussion to aid in clarity

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These expressions for the sensitivities hold if $\Psi^D$ and $\Psi^C$ satisfy the following adjoint equations:

$$
\frac{\partial f}{\partial U} = -\Psi^D \left[ \frac{\partial R}{\partial U} + \frac{\partial D}{\partial U} \right], \quad \frac{\partial f}{\partial \Psi} = -\Psi^C \frac{\partial R}{\partial \Psi},
$$

allowing for the classical discrete adjoint to be written as:

$$
\Psi^D = \frac{\partial f}{\partial U} \left[ \frac{\partial R}{\partial U} \right]^{-1} - \Psi^D \frac{\partial D}{\partial U} \left[ \frac{\partial R}{\partial U} \right]^{-1}.
$$

As a final step, the difference between the discrete adjoint which mimics the continuous adjoint behavior and the classical discrete adjoint can be written as:

$$
\Psi^C = \Psi^D \left[ \frac{\partial D}{\partial U} \left[ \frac{\partial R}{\partial U} \right]^{-1} + I \right],
$$

where $\frac{\partial D}{\partial U} \left[ \frac{\partial R}{\partial U} \right]^{-1}$ can be considered to be smoother of the “continuous” adjoint solution. In a situation involving strong shocks, we hypothesize that this operator produces a strong damping in high frequencies of the continuous adjoint beyond a critical wave number. In other words, the high frequency numerics of the continuous adjoint solution are limited due to the dispersion produced by $\frac{\partial D}{\partial U} \left[ \frac{\partial R}{\partial U} \right]^{-1}$. Preliminary results reported by the authors elsewhere\(^1\) suggests that the major component of this noise is introduced at the scale of the local cell size.

In summary, the discrete and continuous adjoint implementations appear to give sensitivities consistent with the discrete and continuous variations of the functional and these were confirmed to be robust for a wide range of test problems involving strong shocks.

### III. Error estimation for functionals using adjoint equations

In the following discussion, the basis for the two-grid error estimation\(^1\) in integral outputs (functionals) will be reviewed. A more rigorous treatment is provided in\(^18\). Consider a baseline (or coarse) grid $\Omega_I$ and a fine grid $\Omega_h$ which can be obtained, for instance, by isotropically refining the baseline mesh. The goal of this approach is to obtain an accurate estimate of some functional $\Psi$ which can be obtained, for instance, by isotropically refining the baseline mesh. The goal of this approach is to obtain an accurate estimate of some functional $\Psi$ which can be obtained, for instance, by isotropically refining the baseline mesh. The target functional, in this case, is the performance of interest (e.g., lift, drag, etc.), which is written as:

$$
\Psi = \int_{\Omega} f(U) \, d\Omega,
$$

where $f(U)$ is an arbitrary function of the solution $U$. The functional $\Psi$ can be approximated by evaluating it on the discrete grids $\Omega_I$ and $\Omega_h$:

$$
\Psi_I \approx \frac{1}{|\Omega_I|} \sum_{i=1}^{N_I} f(U_i), \quad \Psi_h \approx \frac{1}{|\Omega_h|} \sum_{i=1}^{N_h} f(U_i),
$$

where $N_I$ and $N_h$ are the number of grid points in $\Omega_I$ and $\Omega_h$, respectively.

The difference between the functional evaluated on the coarse and fine grids, $\delta \Psi = \Psi_h - \Psi_I$, is an estimate of the functional error:

$$
\delta \Psi = \frac{1}{|\Omega_h|} \sum_{i=1}^{N_h} \left( f(U_i) - \frac{1}{|\Omega_I|} \sum_{i=1}^{N_I} f(U_i) \right).
$$

Using this estimate, the error in the functional $\Psi$ can be approximated as:

$$
|\delta \Psi| \approx |\delta U| \left( \frac{\partial f}{\partial U} \right)_{U_h} |\Psi_h|.
$$

where $\left( \partial f / \partial U \right)_{U_h}$ is the sensitivity of $f$ with respect to $U$ evaluated at the fine grid solution $U_h$.

The sensitivity of the functional $\Psi$ can be approximated using the discrete adjoint equation:

$$
\Psi^D \left[ \frac{\partial R}{\partial U} \right]^{-1},
$$

where $\Psi^D$ is the discrete adjoint of the functional $\Psi$, and $\left[ \frac{\partial R}{\partial U} \right]^{-1}$ is the inverse of the residual operator.

The error in the functional can then be approximated as:

$$
|\delta \Psi| \approx \left\| \Psi^D \left[ \frac{\partial R}{\partial U} \right]^{-1} \left( U_h - U_I \right) \right\|.
$$

In this equation, the first two terms can be evaluated by post-processing the coarse grid flow and adjoint solutions while the third term is not computable. For the error estimation to be accurate, it would be desirable for $|\epsilon_{rc}|$ to be
small relative to $|\epsilon_{cc}|$. A possible way of achieving this could be to target the reduction of $|R_h^W(I_h^H \Psi_H)|$ via mesh adaptation.

Primarily because the definition of the adjoint residual in eqn.19 is the same as the definition of the discrete adjoint equation (eqn. 4), one could argue that the discrete adjoint equations might be naturally well suited for purposes of the aforementioned error estimation strategy. Further, the discrete adjoint formulation is indeed an approximate adjoint of the modified partial differential equation that includes the numerical error. However, one can expect discrete and continuous adjoint solutions to approach each other with increasing resolution, and hence, this raises the question whether continuous adjoints can also be applied within the above framework. Further, as seen in the previous section, continuous adjoints contain information about the original continuous partial differential equation, and hence, it is important to evaluate whether any additional benefits can be gained by using them.

IV. Numerical Results

In this section, the utility and effectiveness of continuous and discrete adjoints in error estimation and goal-oriented mesh adaptation will be investigated. Specific attention is given to quantitative evaluation of the accuracy of the bi-grid strategy in the presence of shocks.

1. Quasi one dimensional Euler equations

As a first set of test cases, the solution of steady Euler equations for a quasi one dimensional nozzle will be considered. The area of the diverging nozzle is taken to be a linear function of the streamwise coordinate $x$ and is given by: $A(x) = 1.0512 + 0.07x$, with $x = [0...10]$. Spatial discretization is performed using a cell centered scheme on a uniformly spaced mesh. The inflow Mach number is set at 1.5 and the ratio of the inlet to the outlet pressure is specified as 2.5. This induces a shock near $x \approx 4.7$ as shown in fig. 4. Three different functionals are defined, each involving the integral of pressure, but with the following integration domains:

- Patch 1 : $[2.8...4.0]$ (Smooth profile in the domain of dependence of functional and the integration domain)
- Patch 2 : $[4.0...5.2]$ (Discontinuous profile in the domain of dependence and the integration domain)
- Patch 3 : $[5.2...6.4]$ (Discontinuous profile in the domain of dependence, smooth profile in the integration domain)

A second order slope limited MUSCL scheme is used for solution reconstruction in the flow solver as well as for interpolation of the flow and adjoint solutions from the coarse mesh onto the fine mesh. To assess the accuracy of the error estimation procedure, the process is repeated on successively refined meshes. Figure 5 shows the functional for Patch 2 as computed on the baseline grid ($f_H$) and the functional with error estimation (using continuous (C) and discrete (D) adjoints) as detailed in the previous section. The analytical value of the functional as well as the discrete functional value computed on a mesh that is twice as fine ($f_h$) is shown for reference. It is apparent from this figure that the discrete adjoint based error estimation approximates the fine grid functional well while the continuous adjoint based error estimate appears to be particularly poor on low resolution meshes. Figure 6 compares the error estimate with the relative error (defined as $|f_h - f_H|$) and the real error ($|f_{exact} - f_H|$). The discrete adjoint approximates the relative error consistently better than the continuous adjoint, whereas the latter is marginally better at estimating the real error on finely resolved meshes. Notice that the convergence of both error estimates is approximately second order. Figure 7 further quantifies the error estimation. Of particular interest is the fact that the discrete adjoint based estimation is consistently within $5\%$ of the relative error.

For the other patches, the error convergence approaches 4th order (fig. 8). Even though the domain of dependence of the functional in patch 3 contains the shock, the improved convergence property is possibly due to the fact that the interpolation operator is more accurate in transferring the coarse grid functional to the fine grid (because of the smoothness of the integrand in the region of integration). Figures 10 and 11 further confirm that the error estimation for Patch 1 (essentially a smooth continuous problem) is highly accurate.

2. Two dimensional Euler equations

The shock-reflection problem as shown in fig. 12 is studied next in the context of error estimation and mesh adaptation. The incoming flow at a Mach number of 5 passes over a $6^\circ$ wedge resulting in an oblique shock that reflects from the top wall. The original mesh is composed of roughly equilateral triangles of side 0.001 units. The flow solution is formally second order accurate with a Least squares based reconstruction that is limited using a standard minmod limiter. The functional of interest covers the foot of the shock reflection on the upper wall of the computational domain. To serve as indicators for mesh adaptation, the following strategies (these have previously been recommended in Refs. 1, 5) were used as local indicators in cell $i$:

1. $I_j = |\epsilon_{cc}|_j = |(I_h^H \Psi_H)^T R_h(U_h^H)|_j$,
2. $I_j = |\epsilon_{ce}|_j \approx |R_h^W(I_h^H \Psi_H)^T(U_Q - U_L)|_j$,
3. $I_j = |\epsilon_{ce}|_j + |\epsilon_{re}|_j$.
Figure 4. Sample flow solution in diverging nozzle test case (100 cells over entire domain)

Figure 5. Functional evaluation and correction in diverging nozzle (Patch 2)

Figure 6. Difference between error estimate and real, relative error for diverging nozzle (Patch 2)
(a) Error Estimate/Relative Error

(b) Error Estimate/Real Error

Figure 7. Error estimate as a fraction of real, relative error for diverging nozzle (Patch 2)

(a) Patch 1

(b) Patch 3

Figure 8. Difference between error estimate and relative error for diverging nozzle

(a) Patch 1

(b) Patch 3

Figure 9. Difference between error estimate and real error for diverging nozzle
Figure 10. Error estimate as a fraction of relative error for diverging nozzle

Figure 11. Error estimate as a fraction of real error for diverging nozzle

Figure 12. Geometry for shock-reflection problem
Figure 13. Mesh and Mach number contours for shock reflection problem

Figure 14. Functional with error estimate for shock reflection problem
Figure 15. Geometry for idealized Hyshot problem. Red line denotes domain of integration of functional

Figure 16. Pressure contours before and after adaptation for idealized Hyshot simulation

Figure 17. Goal oriented mesh adaptation and error estimation for idealized Hyshot
where, $U_Q$ is a quadratic interpolation of the coarse grid solution onto the fine mesh and $U_L$ is the original linear reconstruction. In the present work, all three approaches were attempted, but for the range of problems that were evaluated, with minimal differences were found between them. For the results presented in this work, the third strategy will be used. Once the error indicators are constructed, cells that yield an error indicator beyond a threshold value are flagged for isotropic mesh adaptation. Figures 13-14 show the performance of the discrete and continuous adjoint based mesh adaptation strategies when the error threshold is set at 2% of the discrete adjoint based error estimate for the baseline (unadapted) mesh. Figure 13 shows the mesh clustering near the shock. While such an adaptation can be achieved using standard strategies such as the gradient based adaptation, the benefit brought in by the goal oriented adaptation strategy is evident from the fact that a) Adaptation is only performed in the domain of dependence of the functional (the mesh near the reflected shock to the right of the functional domain is unadapted), and b) Adaptation is performed in the area where the functional is defined (and thus would help reduce integration errors). The functional error estimate as computed by the discrete adjoint is seen to converge robustly to the analytical value, whereas the continuous adjoint based estimation/ adaptation is comparatively oscillatory. It has to be mentioned that further refinement and a wider range of tests are required before concrete judgments can be made. Further, it has to be borne in mind that there is a high degree of flexibility in choosing numerical schemes to discretize the continuous adjoint equations, whereas the discrete adjoint has none.

As a final test, an idealized version of the Hyshot-II Scramjet test will be studied. The geometry as shown in fig.15 replicates the isolator, combustor and nozzle of the test vehicle. The inflow to the isolator is approximately at Mach 2.7 and a shock train is generated by a blunt lip at the entrance to the lower wall of the isolator. In these simulations, no fuel is injected, and thus the results correspond to the cold flow side of the measurements. The objective function is chosen to be the thrust generated by the lower wall of the nozzle and a discrete adjoint based mesh adaptation strategy is used. Figure 16 shows the increased resolution of flow features after 5 levels of mesh adaptation. A close inspection of the adapted meshes revealed a clustering of mesh cells near the foot of the shocks. Figure 17 confirms the convergence of the functional and the error estimate.

V. Conclusions and Future work

Continuous and discrete adjoint formulations were developed for the compressible Euler equations and their utility in computing functional sensitivities, error estimation and goal oriented mesh adaptation was investigated for flows with strong shocks. Even without an explicit treatment of the adjoint solution near shocks, continuous adjoints were seen to give accurate sensitivities, while the discrete adjoint was confirmed to provide sensitivities consistent with complex step and finite difference methods. When used within the framework of a bi-grid error estimation technique, it was shown that discrete adjoints are capable of estimating the relative error between the fine and coarse meshes more accurately, whereas continuous adjoints appear to be marginally better at estimating the true error in the limit of well converged flow and adjoint solutions. The robustness of the discrete adjoint in goal oriented mesh adaptation suggests this approach to be a promising candidate for quantification and management of numerical errors in Hypersonic flows.

Presently, the methodology is being applied to a wider range of problems involving compressible laminar flows. Ultimately, it is expected that the present formulation will be extended to turbulent (RANS) flows with supersonic combustion. Further work will be required to incorporate anisotropic adaptation, development of sensors to estimate the strength of local adaptation and to obtain rigorous upper bounds for the error estimation.

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References

Appendix : Validation/Verification of Adjoints for Quasi 1D Euler equations

Figure 18 compares the numerically computed continuous and discrete adjoint solutions with the analytical adjoint solution for a converging-diverging quasi one dimensional nozzle with a nozzle shape give by \( A(x) = 1 + \sin(\pi x)^2 \) for \( |x| < 0.5 \) and \( A(x) = 2 \) otherwise. The throat is in a sonic condition and the pressure ratio between the exit and the inlet is 0.8, causing a shock in the diverging portion of the nozzle. The objective function is the integral of pressure over the entire length of the nozzle. Note that because of the sonic condition at the throat, the analytical adjoint solution contains a logarithmic singularity.