We present two error estimation approaches for bounding or correcting the error in functional estimates such as lift or drag. Adjoint methods quantify the error in a particular output functional that results from residual errors in approximating the solution to the partial differential equation. Defect methods can be used to bound or reduce the error in the entire solution, with corresponding improvements to functional estimates. The approaches may be used separately or in combination to obtain highly accurate solutions with asymptotically sharp error bounds. The adjoint theory is extended to handle flows with shocks; numerical experiments confirm 4th order error estimates for a pressure integral of shocked quasi-1D Euler flow. Numerical results also demonstrate 4th order accuracy for the drag on a cusped lifting airfoil at subsonic conditions.

Introduction

Integrals of solutions to partial differential equations (PDEs) provide crucial feedback on system behavior in many areas of engineering and science. In many settings, integral functional values are the primary quantitative outputs of numerical simulations to PDEs. In the field of computational fluid dynamics, lift and drag are computed as surface integrals of pressure and shear forces. The desire for efficient computational algorithms that produce reliable and accurate lift and drag values has motivated a great deal of research during the last several decades. Integral functionals also arise in other aerospace areas such as the calculation of radar cross-sections in electromagnetics.

Modern numerical methods for PDEs make it possible to solve nonlinear systems with discontinuous solutions in complicated computational domains. Nonetheless, limited computational resources make it desirable to compute solutions to the minimum allowable accuracy. Supposing that the output of most interest is an integral functional, we arrive at two related challenges. For reliability, it is desirable to compute a bound on the remaining error in the functional. For efficiency, it is advantageous to compute the functional value to a higher order of accuracy than the overall solution on which it is based.

The present work describes two approaches to error bounding and error correction for functional estimates. Depending on the priorities of the engineer or scientist, an estimate of the leading term in the functional error may be used either to provide an asymptotically sharp error bound, or to remove the leading error term and obtain a superconvergent estimate. The first approach relies on the adjoint or dual PDE, whose solution describes the sensitivity of the functional of interest to residual errors in satisfying the original primal PDE. Smooth reconstructions of the primal and dual solutions are employed, so the method is equally applicable to finite difference, finite volume or finite element discretizations. The treatment of problems containing shocks requires careful consideration, as addressed in the present work. A second approach uses the reconstructed primal solution to drive a defect iteration that improves the accuracy of the underlying baseline solution. The resulting corrected solutions can be used to estimate the leading error term in the original functional estimate.

Adjoint sensitivities may also be employed as the basis for optimal adaptive meshing strategies that seek to maximize the accuracy of the functional estimate for a given computational cost. The issues of error bounding and adaptive error control have received particular attention in the finite element community, where the use of the adjoint PDE for error analysis was first investigated. The orthogonality properties of most finite element methods ensure that functional estimates are naturally su-
perconvergent. The present approach may be used to enhance the natural finite element superconvergence\(^2\).

The study of error convergence is particularly challenging if the true solution is unknown. To facilitate the study of functional accuracy for interesting physical systems and nontrivial computational domains, we formulate modified PDEs by postulating a solution and evaluating the source term that is required to make this the solution of the modified equations. If the postulated solution is close to a solution of the original PDEs, then the source term will be small and the modified problem will exercise the numerical method in a very similar manner to the true physics. In the present work, we describe modified Euler problems for two-dimensional flow in a duct, flow over a cylinder, and flow over a lifting Joukowski airfoil. These test cases have been invaluable for debugging error estimation algorithms.

Flows with shocks pose a major challenge to both adjoint calculations and adjoint error estimation. The correct formulation of the inviscid adjoint equations must account for linearized perturbations to the shock location. This approach reveals that the adjoint equations corresponding to the steady quasi-1D Euler equations require an interior boundary condition at the shock location\(^2\). Numerical results using either the “continuous” approach (approaching the analytical adjoint equations using numerical smoothing in place of the shock boundary condition) or the “discrete” approach (linearising and transposing the discrete flow equations) yield convergent results\(^2\). Ulbrich has recently developed the analytical formulation of the adjoint equations for unsteady 1D equations with scalar fluxes, such as Burgers equation\(^2\). In this case, numerical results\(^2\) indicate that the “discrete” adjoint approach does not necessarily yield convergent results, unless one uses numerical dissipation that leads to an increasing smoothing of the shock as the mesh is refined. It seems likely that there will be similar problems with the convergence of solutions to the steady adjoint Euler equations in two dimensions, although such convergence errors may be very small for weak shocks.

In addition to these difficulties in calculating adjoint solutions, there is the further problem for adjoint error estimation that any smooth reconstructed solution must necessarily have an \(O(1)\) local error near the shock. The residual error is therefore likely to increase without bound as the grid is refined. This behavior undermines the whole basis for adjoint methods, which assume small errors, allowing a linearized treatment for error estimation. Here, we describe a new approach that circumvents these difficulties by approximating the inviscid shock as the limiting structure of a viscous shock. Adjoint error estimates subsequently account for the error introduced by the nonzero viscosity and for the numerical error in approximating the viscous shock.

We begin by describing error bounding and correction alternatives using adjoint and defect methods. The approaches are then formulated for linear and nonlinear PDEs with inhomogeneous boundary conditions and bulk and boundary functionals. Additional theory is developed for the treatment of shocks and then numerical demonstrations are provided for smooth and shocked quasi-1D Euler flows, 2D duct flow, and flow over a lifting airfoil.

**Error Bounding and Correction**

Adjoint and defect methods based on smooth solution reconstructions are employed to bound and correct errors in estimates of integrals functionals. The basic methods and alternatives are now introduced in the simplest scenario of a linear differential equation with homogeneous boundary conditions and a bulk functional.

**Adjoint Methods**

Consider the linear differential equation

\[ Lu = f \]

subject to homogeneous boundary conditions on the domain \( \Omega \). Suppose we are interested in evaluating the linear functional \( (g, u) \), where \((\ldots)\) denotes an integral inner product on \( \Omega \). This functional may equivalently be evaluated in the dual form \((v, f)\), where \(v\) is the solution to the dual or adjoint PDE

\[ L^*v = g, \]

subject to homogeneous adjoint boundary conditions. The equivalence of the primal and dual functional representations follows from the definition of the adjoint operator

\[ (v, f) = (v, Lu) \equiv (L^*v, u) = (g, u). \]

The dual form of the functional indicates that the adjoint solution \(v\) represents the sensitivity of the functional to the primal source term \(f\).

Discrete approximate primal and dual solutions, \(U_h\) and \(V_h\), are computed on a mesh of average interval \(h\). Smooth reconstructions are then obtained

\[ u_h \equiv R_h U_h, \quad v_h \equiv R_h V_h, \]
where $R_h$ is a reconstruction operator (e.g. linear or cubic spline interpolation). The degree to which these functions do not satisfy the original PDEs can then be quantified by the primal and dual residual errors defined by

$$L u_h - f = L (u_h - u), \quad L^* v_h - g = L^*(v_h - v).$$

Assuming that the underlying physical solution is sufficiently smooth, the anticipated order of convergence for the functional estimate depends on:

- $n$, the order of the operator $L$,
- $p$, the order of the discrete solution,
- $r$, the order of the reconstruction.

Intuitively, the solution and residual errors are expected to satisfy

$$\|u_h - u\|, \|v_h - v\| = O\left(h^{\min(p,r)}\right) \quad (1)$$

$$\|Lu_h - f\|, \|L^* v_h - g\| = O\left(h^{\min(p,r-n)}\right),$$

where the $n$ differentiations required to evaluate the residual errors account for their reduced accuracy. In practice, these results may only hold in certain norms.

The error in the functional value based on the reconstructed primal solution may be expressed as

$$(g, u) - (g, u_h) = (g, u - u_h) = (L^* v, u - u_h) = (v, L(u - u_h)) = (v, f - Lu_h).$$

Introducing the reconstructed adjoint solution $v_h$

gives

$$(g, u) - (g, u_h) = (v_h, f - Lu_h) + (v - v_h, f - Lu_h).$$

The first term on the right hand side can be evaluated, since $f$, $u_h$ and $v_h$ are all known. The second term cannot be evaluated because $v$ is unknown. However, the discretization and reconstruction schemes can be chosen to ensure that the second term is $O(h^{\min(p,r)})$ smaller than the first. Therefore, the first term may be used as an error bound,

$$|(g, u) - (g, u_h)| \leq \|(v_h, f - Lu_h)\| + \|(v - v_h, f - Lu_h)\| = O\left(h^{\min(2,4) + \min(2,4 - 2)}\right) = O(h^4).$$

Alternatively, the first term can be moved to the left hand side to obtain a more accurate functional estimate

$$(g, u) - \left\{(g, u_h) + (v_h, f - Lu_h)\right\} = (v-v_h, f - Lu_h). \quad (3)$$

As a concrete example, consider a one-dimensional Poisson problem

$$L = L^* = \frac{d^2}{dx^2}, \quad f = x^3(1 - x)^3, \quad g = \sin \pi x$$

with homogeneous boundary conditions on $x \in [0,1]$. The problem is discretized using 2nd order finite differences and the solution is reconstructed using cubic spline interpolation ($n = 2$, $p = 2$, $r = 4$). Integrals are evaluated using 3-point Gauss quadrature.

From estimates (1), the reconstructed primal and dual solutions are $O(h^2)$. Also, the functional estimate $(g, u_h)$ has the same order of accuracy as the primal solution on which it is based. The remainder term in (2) and (3) is of order

$$|(v - v_h, f - Lu_h)| \leq O\left(h^{\min(2,4) + \min(2,4 - 2)}\right) = O(h^4).$$

Using adjoint error bounding, we expect a 2nd order functional estimate with an asymptotically sharp error bound that itself contains a 4th order error. Alternatively, using adjoint error correction, we expect a 4th order functional estimate. These two alternatives are illustrated by the numerical results in Figure 1a. Lines of slope $-2$ and $-4$ are drawn through the error values on the finest mesh to assist in determining the convergence rates. Note that the error bound is indistinguishable from the remaining error, as it is roughly $10^2$ times more accurate than the functional estimate on the coarsest mesh, increasing to roughly $10^3$ times more accurate on the finest mesh. Using adjoint error correction, rigorous a priori analysis of the errors in the primal and dual numerical solutions as well as the errors associated with the spline reconstruction confirms that the functional accuracy should in fact double from 2nd to 4th order.

Depending on the reconstruction method, it is possible that the inner product $(v_v - v_h, f - Lu_h)$ or equivalently $(g - L^* v_h, u - u_h)$ will exhibit a convergence rate that is faster than the product of the convergence rates of its components. This results from cancellation effects that have been observed and analyzed in the nonlinear case of smooth quasi-1D Euler flow.37
Defect Methods

As an alternative to adjoint methods, solution reconstruction may be used to drive a defect correction process. If the original numerical solution is obtained by solving the discrete problem

$$L_h u_h = T_h f,$$

where $T_h$ is an operator that transfers the continuous source term $f$ to discrete source terms associated with the each of the unknowns in $U_h$, then the defect correction iteration may be written as

$$L_h \Delta U_h = T_h (f - Lu_h),$$

$$u_{dh} = u_h + R_h \Delta U_h,$$

where $R_h$ is the linear reconstruction operator $^4$.$^5$. Note that this defect correction procedure differs from traditional defect correction approaches that evaluate $Lu_h$ using a higher order discrete operator $L_h'$ applied to the low order solution $U_h$ (instead of the differential operator $L$ applied to the reconstructed solution $u_h$). If the defect iteration is convergent, the final accuracy of the defect corrected approximate solution $u_{dh}$ is determined not by the low order discrete operator $L_h$ used to obtain the solution, but instead by the interpolation accuracy of the reconstruction method used to form $u_h$ and $u_{dh}$.

Using the reconstructed defect solution $u_{dh}$, the error in the original functional estimate may be represented

$$(g, u) - (g, u_h) = (g, u_{dh} - u_h) + (g, u - u_{dh}),$$

where the first term on the right hand side may be evaluated to provide an asymptotically sharp error bound

$$|(g, u) - (g, u_h)| \leq |(g, u_{dh} - u_h)| + |(g, u - u_{dh})|,$$

or subtracted to give a more accurate functional estimate

$$(g, u) - \{(g, u_h) + (g, u_{dh} - u_h)\} = (g, u - u_{dh}).$$

For the previously considered 1D Poisson problem, defect correction of the primal solution using cubic spline reconstruction yields 4th order solution errors and consequently a 4th order functional estimate. The behavior for error bounding and correction is illustrated in Figure 1b.

Combined Adjoint and Defect Methods

Combined approaches yield even sharper error estimates. The remaining error in (5) may be expressed
in the dual form
\[
(g, u) - (g, u_h) - (g, u_{d_h} - u_h) = (g, u - u_{d_h}) \\
= (L^*v, u - u_{d_h}) \\
= (v, L(u - u_{d_h})) \\
= (v, f - Lu_{d_h}).
\]

We introduce the reconstructed dual solution \(v_h\)
\[
(g, u) - (g, u_h) - (g, u_{d_h} - u_h) \\
= (v_h, f - Lu_{d_h}) + (v - v_h, f - Lu_{d_h}).
\]

and evaluate the first term on the right hand side to obtain either the asymptotically sharp error bound
\[
|(g, u) - (g, u_h) - (g, u_{d_h} - u_h)| \\
\leq |(v_h, f - Lu_{d_h})| + |(v - v_h, f - Lu_{d_h})|
\]
or the more accurate functional estimate
\[
(g, u) - \left\{ (g, u_h) + (g, u_{d_h} - u_h) + (v_h, f - Lu_{d_h}) \right\} \\
= (v - v_h, f - Lu_{d_h}) \\
= (g - L^*v_h, u - u_{d_h}). \quad (6)
\]

For the 1D Poisson problem, the order of the remainder term may be estimated as
\[
(g - L^*v_h, u - u_{d_h}) = O \left( h^{\min(2,4-2) + \min(4,4)} \right) \\
= O(h^5).
\]

Note that an estimate based on the alternative dual representation of the remainder in (6) would appear to be only \(O(h^3)\). Integration by parts to obtain the primal form shows that this estimate is overly pessimistic. Hence, in the numerical results of Figure 1c, we observe either a 4th order functional estimate with a sharp error bound that itself contains a 6th order error, or else a 6th order functional estimate without a computable bound.

**Linear Formulation**

**Adjoint Error Estimates**

We now extend the adjoint error estimation approach to problems with inhomogeneous boundary conditions and output functionals that contain boundary integrals\(^2\)\(^4\).

Let \(u\) be the solution of the linear differential equation
\[
Lu = f,
\]
in the domain \(\Omega\), subject to the linear boundary conditions
\[
Bu = e,
\]
on the boundary \(\partial \Omega\). In general, the number of boundary conditions described by the operator \(B\) may be different on different parts of the boundary (e.g. inflow and outflow sections for hyperbolic problems).

The output functional of interest is taken to be
\[
J = (g, u) + (h, Cu)_{\partial \Omega},
\]
where \((.,.)_{\partial \Omega}\) represents an integral inner product over the boundary \(\partial \Omega\). The boundary operator \(C\) may be algebraic (e.g. \(Cu \equiv u\)) or differential (e.g. \(Cu \equiv \frac{\partial u}{\partial n}\)). As with the boundary condition operator \(B\), the boundary functional operator \(C\) may have different numbers of components on different parts of the boundary. The corresponding components of \(h\) may be set to zero on those parts of the boundary where the functional does not have a boundary integral contribution.

The corresponding linear adjoint problem is
\[
L^*v = g,
\]
in \(\Omega\), subject to the boundary conditions
\[
B^*v = h,
\]
on the boundary \(\partial \Omega\). The fundamental identity defining \(L^*, B^*\) and the boundary operator \(C^*\) is
\[
(v, Lu) + (C^*v, Bu)_{\partial \Omega} = (L^*v, u) + (B^*v, Cu)_{\partial \Omega},
\]
for all \(u, v\). This identity is obtained using integration by parts and it implies that the primal functional operator \(C\) and the adjoint boundary condition operator \(B^*\) contain an equal number of components at any location on the boundary. The construction of the appropriate adjoint operators for the linearized Euler and Navier-Stokes equations is described elsewhere\(^2\)\(^-\)\(^3\)\(^0\).

Using the adjoint identity, the equivalent dual form of the output functional is
\[
J = (v, f) + (C^*v, e)_{\partial \Omega}.
\]

Given approximate reconstructed solutions \(u_h\) and \(v_h\), the error in the functional may be expressed
\[
(g, u) + (h, Cu)_{\partial \Omega} - (g, u_h) - (h, Cu_h)_{\partial \Omega} = \quad -(L^*v_h, u_h - u) - (B^*v_h, C(u_h - u))_{\partial \Omega} \\
+ (L^*v_h - g, u_h - u) + (B^*v_h - h, C(u_h - u))_{\partial \Omega} \\
= -(v_h, L(u_h - u)) - (C^*v_h, B(u_h - u))_{\partial \Omega} \\
+ (L^*(v_h - v), u_h - u) + (B^*(v_h - v), C(u_h - u))_{\partial \Omega} \\
= -(v_h, Lu_h - f) - (C^*v_h, Bu_h - e)_{\partial \Omega} \\
+ (v_h - v, L(u_h - u)) + (C^*(v_h - v), B(u_h - u))_{\partial \Omega}.
\]
In the final result, the first line comprises computable adjoint error estimates that describe the influence of the bulk and boundary residuals on the functional of interest. These terms may either be used to obtain a more accurate solution or to provide an asymptotically sharp bound on the error in the original functional estimate. The second line describes the higher order remaining error.

Defect Error Estimates

The linear defect iteration (4) can be generalized to inhomogeneous boundary conditions by ensuring that the reconstruction satisfies the analytical boundary conditions at the discrete mesh points located on the boundary.

Nonlinear Formulation

This section describes the extension of the linear theory to nonlinear operators and functionals\(^2\). It begins with some definitions and observations regarding the linearization of functions and operators.

Preliminaries

If \( u \) is a scalar variable and \( f(u) \) is a nonlinear scalar function, then a standard Taylor series expansion gives

\[
 f(u_2) = f(u_1) + f'(u_1) (u_2-u_1) + O((u_2-u_1)^2).
\]

Alternatively, an exact expression without remainder terms is obtained by starting from

\[
 \frac{d}{d\epsilon} f (u_1+\epsilon(u_2-u_1)) = f'(u_1+\epsilon(u_2-u_1)) (u_2-u_1),
\]

and then integrating from \( \theta=0 \) to \( \theta=1 \) to give

\[
 f(u_2) - f(u_1) = \int_0^1 f'(u_1+\epsilon(u_2-u_1)) \, d\epsilon,
\]

where

\[
 \int_0^1 f'(u_1+\epsilon(u_2-u_1)) \, d\epsilon.
\]

For the nonlinear operator \( N(u) \), the corresponding linearized operator \( L_u \) is defined formally by the Fréchet derivative

\[
 L_u \hat{u} \equiv \lim_{\epsilon \to 0} \frac{N(u + \epsilon \hat{u}) - N(u)}{\epsilon}.
\]

The subscript \( u \) denotes that \( L_u \) depends on the value of \( u \) around which \( N(u) \) is linearized. For example, if

\[
 N(u) = \frac{\partial}{\partial x} \left( \frac{1}{2} u^2 \right) - \nu \frac{\partial^2 u}{\partial x^2},
\]

then

\[
 L_u \hat{u} = \frac{\partial}{\partial x} (u \hat{u}) - \nu \frac{\partial^2 \hat{u}}{\partial x^2}.
\]

Starting from

\[
 \frac{d}{d\theta} \ N(u_1+\theta(u_2-u_1)) = L_{u_1+\theta(u_2-u_1)} (u_2-u_1)
\]

and integrating over \( \theta \) we obtain

\[
 N(u_2) - N(u_1) = \mathcal{T}_{(u_1,u_2)} (u_2-u_1),
\]

where

\[
 \mathcal{T}_{(u_1,u_2)} = \int_0^1 L_{u_1+\theta(u_2-u_1)} \, d\theta.
\]

Thus \( \mathcal{T}_{(u_1,u_2)} \) is the average linear operator over the “path” from \( u_1 \) to \( u_2 \).

Adjoint Error Estimates

Let \( u \) be the solution of the nonlinear differential equation

\[
 N(u) = 0
\]

in the domain \( \Omega \), subject to the nonlinear boundary conditions

\[
 D(u) = 0
\]

on the boundary \( \partial \Omega \).

The linear differential operators \( L_u \) and \( B_u \) are defined by the Fréchet derivatives of \( N \) and \( D \), respectively,

\[
 L_u \hat{u} \equiv \lim_{\epsilon \to 0} \frac{N(u + \epsilon \hat{u}) - N(u)}{\epsilon},
\]

\[
 B_u \hat{u} \equiv \lim_{\epsilon \to 0} \frac{D(u + \epsilon \hat{u}) - D(u)}{\epsilon}.
\]

It is assumed that the nonlinear functional of interest, \( J(u) \), has a Fréchet derivative of the form

\[
 \lim_{\epsilon \to 0} \frac{J(u + \epsilon \hat{u}) - J(u)}{\epsilon} = (g(u), \hat{u}) + (h, C_u \hat{u})_{\partial \Omega},
\]

where the operator \( C_u \) may be algebraic or differential.

The corresponding linear adjoint problem is

\[
 L_u^* v = g(u)
\]

in \( \Omega \), subject to the boundary conditions

\[
 B_u^* v = h
\]

on the boundary \( \partial \Omega \). The adjoint identity defining \( L_u^* \), \( B_u^* \) and the boundary operator \( C_u^* \) is

\[
 (v, L_u \hat{u}) + (C_u^* v, B_u \hat{u})_{\partial \Omega} = (L_u^* v, \hat{u}) + (B_u^* v, C_u \hat{u})_{\partial \Omega},
\]
for all $\tilde{u}, v$. This expression implies that $B^*_u$ has the
same number of components as $C(u)$ at any point on
the boundary.

We now consider approximate reconstructed pri-
mary and dual solutions $u_h$ and $v_h$. The error analysis
that follows makes use of the quantities

$$L^*_u v_h, \quad B^*_u v_h, \quad C^*_u v_h,$$

which are computable since the linear operators are
defined based on $u_h$ rather than $u$. The analysis also
requires averaged Fréchet derivatives defined by

$$L_{(u,u_h)} = \int_0^1 L|_{u+\theta(u_h-u)} \, d\theta,$$
$$B_{(u,u_h)} = \int_0^1 B|_{u+\theta(u_h-u)} \, d\theta,$$
$$C_{(u,u_h)} = \int_0^1 C|_{u+\theta(u_h-u)} \, d\theta,$$
$$\overline{g}(u,u_h) = \int_0^1 g(u+\theta(u_h-u)) \, d\theta,$$

so that

$$N(u_h) - N(u) = L_{(u,u_h)} (u_h - u),$$
$$D(u_h) - D(u) = B_{(u,u_h)} (u_h - u),$$
$$J(u_h) - J(u) = (\overline{g}(u,u_h), u_h - u) + (h, C_{(u,u_h)} (u_h - u))_{\partial \Omega}.$$

Adjoint error estimates may then be expressed

$$J(u_h) - J(u)$$
$$= (\overline{g}(u,u_h), u_h - u) + (h, C_{(u,u_h)} (u_h - u))_{\partial \Omega}$$
$$= (L^*_u v_h, u_h - u) + (B^*_u v_h, C_u (u_h - u))_{\partial \Omega}$$
$$- (L^*_u v_h - \overline{g}(u,u_h), u_h - u)$$
$$- (h, C_{(u,u_h)} (u_h - u))_{\partial \Omega}$$
$$+ (v_h, L_{(u,u_h)} (u_h - u))_{\partial \Omega}$$
$$= (v_h, L_{(u,u_h)} (u_h - u)) + (C^*_u v_h, B_{(u,u_h)} (u_h - u))_{\partial \Omega}$$
$$- (L^*_u v_h - \overline{g}(u,u_h), u_h - u)$$
$$- (h, C_{(u,u_h)} (u_h - u))_{\partial \Omega}$$
$$+ (v_h, L_{(u,u_h)} (u_h - u))_{\partial \Omega}$$
$$= (v_h, L_{(u,u_h)} (u_h - u)) + (C^*_u v_h, B_{(u,u_h)} (u_h - u))_{\partial \Omega}$$

$$= (v_h, N(u_h)) + (C^*_u v_h, D(u_h))_{\partial \Omega}$$
$$- (L^*_u v_h - \overline{g}(u,u_h), u_h - u)$$
$$- (h, C_{(u,u_h)} (u_h - u))_{\partial \Omega}$$
$$+ (v_h, L_{(u,u_h)} (u_h - u))_{\partial \Omega}$$
$$+ (C^*_u v_h, (B_{(u,u_h)} - \overline{B}_{(u,u_h)}) (u_h - u))_{\partial \Omega}.$$
Adjoint Methods for Shocked Flows

Non-oscillatory shock-capturing schemes have revolutionized the calculation of transonic flows, providing one-point shock structures. Unfortunately, sharp shocks introduce fundamental difficulties when attempting to use linearization approaches to evaluate the sensitivities of functionals to solution errors. In fact, a convergent nonlinear discretization may have linear sensitivities that do not converge \(^2\).

One solution to this problem is to approach it from the perspective of well-resolved viscous shocks. Let \(u_\varepsilon\) be the solution of the “viscous” quasi-1D Euler equations

\[
\frac{\partial}{\partial x} \left( A \rho q_\varepsilon \begin{pmatrix} \frac{\varepsilon}{\rho} \\ \frac{\varepsilon}{\rho} \end{pmatrix} \right) + A \frac{\partial}{\partial x} \left( \begin{pmatrix} p \\ 0 \end{pmatrix} \right) = A \varepsilon \frac{\partial^2}{\partial x^2} \left( \begin{pmatrix} \rho \\ q_\varepsilon \end{pmatrix} \right),
\]

where \(A(x)\) is the duct area. This may be written symbolically as

\[
N(u_\varepsilon) = \varepsilon S(u_\varepsilon). \tag{7}
\]

In the limit \(\varepsilon \to 0\), \(u_\varepsilon\) will converge to the discontinuous inviscid solution \(u\) at every point except at the shock point. If \(u_{\varepsilon,h}\) is an approximation to \(u_\varepsilon\), then the error in the computed value of the functional \(J(u)\) may be split into two parts

\[
J(u) - J(u_{\varepsilon,h}) = J(u) - J(u_\varepsilon) + (J(u_\varepsilon) - J(u_{\varepsilon,h})).
\]

The first part is the error due to the viscosity. A matched inner and outer asymptotic analysis reveals that for functionals such as the integrated pressure,

\[
J(u_\varepsilon) = J(u) + a \varepsilon + O(\varepsilon^2),
\]

for some constant \(a\). Accordingly,

\[
J(u) - J(u_\varepsilon) = -\varepsilon \frac{d}{d \varepsilon} J(u_\varepsilon) + O(\varepsilon^2),
\]

where the quantity

\[
\frac{d}{d \varepsilon} J(u_\varepsilon) = \left( g(u_\varepsilon), \frac{du_\varepsilon}{d \varepsilon} \right)
\]

may be evaluated by the adjoint approach since by definition, the gradient with respect to \(\varepsilon\) is based on infinitesimal perturbations to the viscous solution. Differentiating (7) with respect to \(\varepsilon\) gives

\[
L_{u_\varepsilon} \frac{du_\varepsilon}{d \varepsilon} = S(u_\varepsilon),
\]

where \(L_{u_\varepsilon}\) is the Fréchet derivative of the nonlinear operator \(N - \varepsilon S\). Hence,

\[
\left( g(u_\varepsilon), \frac{du_\varepsilon}{d \varepsilon} \right) = (v_\varepsilon, S(u_\varepsilon)),
\]

assuming that the viscous adjoint solution \(v_\varepsilon\) exactly satisfies the inviscid boundary conditions. If \(v_{\varepsilon,h}\) is an approximation to the viscous adjoint \(v_\varepsilon\), then \(\varepsilon(v_{\varepsilon,h}, S(u_{\varepsilon,h}))\) is an approximation to the functional error due to the viscosity.

The second part of the error in (8) is due to the approximation of the solution to the viscous equation. With a well-resolved shock, it is possible to ensure that \(u_\varepsilon - u_{\varepsilon,h}\) is small, so that the resulting functional error may be approximated by the usual adjoint estimate \((v_{\varepsilon,h}, N(u_{\varepsilon,h}) - \varepsilon S(u_{\varepsilon,h}))\). Adding the two correction terms gives the combined adjoint error estimate

\[
(v_{\varepsilon,h}, N(u_{\varepsilon,h}) - \varepsilon S(u_{\varepsilon,h})) + \varepsilon(v_{\varepsilon,h}, S(u_{\varepsilon,h})) = (v_{\varepsilon,h}, N(u_{\varepsilon,h}))).
\]

It is quite striking that the final result simplifies to the standard adjoint error approximation using the inviscid operator \(N\) but the “viscous” approximate solutions \(u_{\varepsilon,h}\) and \(v_{\varepsilon,h}\). Since the viscous operator is not applied to the reconstructed solutions, the treatment of shocked flows imposes no additional accuracy requirements on the reconstruction scheme.

We conjecture that a similar treatment may be used for contact discontinuities. In that setting, the smoothing introduced by viscosity \(\varepsilon\) leads to a functional error which is \(O(\sqrt{\varepsilon})\) to leading order. Hence, the final form of the adjoint correction will not have quite such a pleasingly simple form.

One-dimensional Results

Subsonic quasi-1D flow

We first consider subsonic quasi-1D Euler flow in a converging-diverging nozzle

\[
A(x) = \begin{cases} 
2, & -1 \leq x \leq -\frac{1}{2}, \\
2 - \sin^2[\pi(x + \frac{1}{2})], & -\frac{1}{2} < x < \frac{1}{2}, \\
2, & \frac{1}{2} \leq x \leq 1, 
\end{cases}
\]

with a functional that is the integral of pressure. The flow is fully determined by specifying stagnation enthalpy \((H = 4)\) and stagnation pressure \((p_0 = 2)\) at the inlet and pressure \((p = 1.9)\) at the exit. The numerical solution of Figure 2a is computed using a 2nd order finite volume scheme and reconstructed
The performance of adjoint error bounding and correction is illustrated in Figure 2b. The bound is sharp, containing an $O(h^4)$ error compared to the $O(h^2)$ accuracy of the functional estimate. By subtracting the leading error term, we obtain an $O(h^4)$ functional estimate. Note that the temporary excursion of the base error from the overall trend is caused by a change in the sign of the error.

It is surprising that very similar error estimates are obtained using piecewise linear reconstruction. Linear interpolation provides $O(h^2)$ solution accuracy but only $O(h)$ residuals (as a result of differentiating once). Hence, the corrected functional estimate is expected to be only $O(h^3)$. However, numerical experiments reveal that the functional accuracy is actually $O(h^4)$, as seen in Figure 2c. This unexpected accuracy results from a cancellation effect between the leading order terms in the adjoint solution and the flow residual.

Returning to cubic spline reconstruction, the combined use of defect and adjoint error correction is illustrated in Figure 2d. The 2nd order base error is bounded by the defect error estimate, or alternatively, it is corrected to obtain 4th order accuracy. Adjoint methods are then used to obtain a sharp bound on the 4th order functional estimate, or alternatively, to obtain a 7th order functional estimate. The primal solution is $O(h^4)$ and the adjoint residual is $O(h^2)$ so we expect $O(h^6)$ accuracy. The higher observed rate of convergence may be related to the choice of geometry or it may result from a cancella-
tion effect. The 7th order accuracy is also observed for a related asymmetrical geometry.

**Shocked quasi-1D flow**

We now consider the integral of pressure for shocked flow in an expanding duct. The geometry is defined by the quintic polynomial $A(x)$ that yields $A'(x) = A''(x) = 0$ at $x = 0$, 1 with $A(0) = 0.95$ and $A(1) = 1.05$. Uniform inlet and outlet sections of length 0.1 are appended to this smooth expansion. The flow and adjoint solutions are both obtained using 2nd order finite volume schemes. Hence, the errors in the functional resulting from viscosity and from the discretization error are both 2nd order.

Adjoint error correction is implemented using two adaptive meshing approaches: grid redistribution and grid refinement. Using grid redistribution, grid points are moved to better resolve regions with high gradients and/or second derivatives. Using grid refinement, extra grid points are added by subdividing cells to better resolve the gradients in the shock region. In this implementation, both methods used a smoothed indicator function based on the pressure gradient and the local cell size. Care was taken to ensure that the additional numerical smoothing in the discretization of the inviscid flux terms remains 2nd order accurate even when there are jumps in the grid spacing. The viscous coefficient is defined by $\varepsilon = N^{-2}$, where $N$ is the number of grid points. The effect of the grid adaptation is to smear the shock across an increasing number of grid points as $N$ increases.

Evaluating the combined adjoint error estimates for viscous modeling error and numerical residual error, we obtain either a sharp bound on the 2nd order base error or a 4th order functional estimate as seen in Figure 3. These results were obtained using cubic spline reconstruction, but virtually indistinguishable results were obtained using linear interpolation.

**Two-dimensional Implementation**

**Discretization**

The two-dimensional Euler equations are discretized using a 2nd order accurate cell-centered finite volume scheme with dummy cells to enforce boundary conditions. The solution is marched to a steady state using multigrid with Runge–Kutta smoothing\textsuperscript{34, 35}. Numerical dissipation scaled by the spectral radius of the flux Jacobian is based on 4th differences of the vector of conserved variables $u = (\rho, \rho q_x, \rho q_y, \rho E)^T$.

**Boundary Conditions**

Correct implementation of the boundary conditions is important to the order of accuracy of the functional estimates. We now briefly describe the form of the flow and adjoint boundary conditions, using boundary normals which point out of the computational domain.

For the flow equations, there is one incoming characteristic at the wall and the corresponding physical boundary conditions is

$$ q_n = q_x n_x + q_y n_y = 0. $$

All conserved variables are linearly extrapolated to the dummy cells inside the wall so as to enforce zero normal velocity with 2nd order accuracy.

At an inflow boundary, three physical boundary conditions and one numerical boundary condition must be specified. This is accomplished by using a Newton iteration to enforce

$$ R \equiv \left( \begin{array}{c} H_{\infty} - \bar{H} \\ s_{\infty} - \bar{s} \\ \bar{q}_t - \bar{q}_t \\ \Delta p + \bar{p} \bar{c} \Delta q_n \end{array} \right) = 0 $$

at the inflow boundary, where a bar denotes an average at the boundary of the values in the adjacent interior cell and exterior dummy cell, and $\Delta$ denotes a difference across the boundary of the values in the same two cells. The first three equations represent specification of the stagnation enthalpy, entropy and tangential velocity. For a modified Euler problem, $\bar{q}_t$ is obtained from the known analytical solution. For the duct, the equation for entropy is replaced by stagnation pressure, and $\bar{q}_t = 0$. The fourth equation is a characteristic boundary condition on the outgoing characteristic.

At an outlet boundary, a Newton iteration is used to enforce one physical boundary condition and three numerical boundary conditions

$$ R \equiv \left( \begin{array}{c} \bar{c}^2 \Delta \rho - \Delta \rho \\ \Delta q_t \\ \Delta p + \bar{p} \bar{c} \Delta q_n \\ p_{\bar{f}} - \bar{p} \end{array} \right) = 0. $$

The first three equations represent characteristic boundary conditions on the three outgoing characteristics and the fourth equation sets the exit pressure based on a far field model. For the duct, the exit pressure is uniform and for the airfoil, it is based on the known solution to the modified Euler equations.
Figure 3. Shocked quasi-1D flow. Mach number distribution on a sequence of meshes with adaptive resolution of the shock provided by a) grid redistribution or c) grid refinement. Adjoint error bounding and correction using cubic spline reconstruction and b) grid redistribution or d) grid refinement. Here, $N$ is the number of grid points and the superimposed lines have slopes $-2$ and $-4$.

The adjoint boundary conditions are defined so as to remove the dependence of the augmented linearized functional on perturbations to the flow variables\cite{28,29}.

For the adjoint equations, the flow of information along characteristics is reversed. At the wall, there is one outgoing flow characteristic and hence one adjoint boundary condition. The specific boundary condition depends on the choice of integral functional. If the linearized form of the nonlinear functional is $(h, \frac{\partial \mu}{\partial u} \tilde{u})_{\partial \Omega}$, corresponding to a weighted integral of the surface pressure perturbation, then the adjoint boundary condition has the form\cite{28,29}

$$v_2 n_x + v_3 n_y = h,$$

which is enforced at the wall with 2nd order accuracy.

At inlet and outlet boundary conditions, the linearized augmented functional contains an expression of the form\cite{28,29}

$$v^T A_n \tilde{u},$$

where $A_n$ is the flux Jacobian in the coordinate system normal to the boundary. For convenience, the boundary term may be written in the equivalent characteristic form

$$\psi^T \Lambda \tilde{\Omega}.$$

Here, the characteristic adjoint and flow variables are

$$\psi = T^T v, \quad \tilde{\Omega} = T^{-1} \tilde{u},$$

$A$ is the diagonal matrix of eigenvalues of $A_n$, and $T$ is the matrix of right eigenvectors of $A_n$. This characteristic form may be partitioned into incoming
and outgoing adjoint and flow components to give

\[ \psi^T_{\text{out}} \Lambda_{\text{in}} \tilde{\Omega}_{\text{in}} + \psi^T_{\text{in}} \Lambda_{\text{out}} \tilde{\Omega}_{\text{out}}, \]

where the number of incoming flow and outgoing adjoint components is identical. Likewise, there are the same number of incoming adjoint and outgoing flow components.

Outgoing adjoint characteristic components \( \psi_{\text{out}} \) are linearly extrapolated to the boundary of the domain. The incoming characteristic flow perturbations \( \tilde{\Omega}_{\text{in}} \) are expressed in terms of the unknown outgoing perturbations \( \tilde{\Omega}_{\text{out}} \) by invoking the flow boundary condition \( R = 0 \). The effect of perturbations to incoming and outgoing characteristic variables on \( R \) is described by

\[ D_{\text{in}} \tilde{\Omega}_{\text{in}} + D_{\text{out}} \tilde{\Omega}_{\text{out}} = \delta R \]

where \( (D_{\text{in}}|D_{\text{out}}) = \frac{\partial R}{\partial u} T \).

Perturbations to the incoming characteristic variables may then be expressed

\[ \tilde{\Omega}_{\text{in}} = -D_{\text{in}}^{-1} D_{\text{out}} \tilde{\Omega}_{\text{out}}. \]

After eliminating \( \tilde{\Omega}_{\text{in}} \), the boundary term (9) becomes

\[ (\psi^T_{\text{in}} \Lambda_{\text{out}} - \psi^T_{\text{out}} \Lambda_{\text{in}} D_{\text{in}}^{-1} D_{\text{out}}) \tilde{\Omega}_{\text{out}}. \]

Ensuring that this is zero for any \( \tilde{\Omega}_{\text{out}} \) yields the adjoint boundary condition

\[ \psi_{\text{in}} = \Lambda_{\text{out}}^{-1} (D_{\text{in}}^{-1} D_{\text{out}}) \Lambda_{\text{in}} \psi_{\text{out}}. \]

**Reconstruction**

For the two-dimensional Euler equations, the discrete solution is computed at the cell centers of a structured quadrilateral mesh. The solution is averaged to the grid nodes prior to reconstruction so that the mesh and the solution are defined at the same locations. The analytical wall and far field boundary conditions are then enforced at the mesh points prior to reconstruction. The wall boundary condition makes use of the exact wall normals to enforce flow tangency. This boundary fix makes it unnecessary to evaluate the boundary contribution to the adjoint error estimate because the leading term in the boundary residual is shifted into the interior of the domain.

The approximate solutions \( u_h \) and \( v_h \) are then formed using bi-cubic spline interpolation for each component. Not-a-knot boundary conditions are employed except in cases where one of the computational coordinates is periodic. The coordinate data is also splined, so that the solutions and coordinates, \( u_h, v_h, x_h, y_h \), are all defined parametrically as functions of the two spline coordinates \( \xi, \eta \). Derivatives of each component of \( u_h \) can then be evaluated by solving

\[
\begin{pmatrix}
\frac{\partial u_h}{\partial \xi} \\
\frac{\partial u_h}{\partial \eta}
\end{pmatrix} = \begin{pmatrix}
\frac{\partial x_h}{\partial \xi} & \frac{\partial y_h}{\partial \xi} \\
\frac{\partial x_h}{\partial \eta} & \frac{\partial y_h}{\partial \eta}
\end{pmatrix} \begin{pmatrix}
\frac{\partial u_h}{\partial x} \\
\frac{\partial u_h}{\partial y}
\end{pmatrix}.
\]

The error correction integral is evaluated in \((\xi, \eta)\) coordinates using \(3 \times 3\) Gauss quadrature on each cell.

The boundary fix procedure is also useful for reconstructed solutions that are used to drive a defect iteration. The defect transfer operator \( T_h \) that defines the source term at each cell center is based on the average value of the source term over the computational cell as evaluated using \(3 \times 3\) Gauss quadrature.

Note that the residuals that drive the defect iteration are based on a discrete solution defined at the grid nodes. The process of averaging from the cell centers to the grid nodes may be interpreted as part of the overall 2nd order accurate discretization procedure. The defect iteration produces a solution at the cell centers that becomes 4th order accurate only after the discretization process is completed by again averaging to the grid nodes. This interesting property simplifies the issue of moving solution data to the nodes.

When using defect or adjoint methods alone, the approaches described above suffice to provide 4th order accuracy. However, when attempting to achieve 6th order accuracy, there are additional sources of error that must be considered. After defect correction, the present scheme defines a reconstructed flow solution that is 4th order accurate and an adjoint solution that is 2nd order with a splined geometry that is 4th order accurate. One source of remaining error is the boundary residual contribution to the adjoint correction (which is not necessary for 4th order accuracy when using the boundary fix described above). Another source of error is the evaluation of boundary integrals on the approximate geometry. There is also an error in the bulk adjoint correction term resulting from the neglect of the slivers that exist between the splined and true geometries. However, these contributions should be \(O(h^6)\) since the total neglected area is \(O(h^4)\) and the residual integrated over this area is \(O(h^2)\). A careful investigation of each source of error is currently underway.
Modified Euler equations

2D Duct. The flow field is defined to be the exact quasi-1D flow solution with a vertical velocity component that varies linearly from the upper to lower walls so as to satisfy flow tangency

\[ q_y = q_x \frac{dx}{dy}. \]

Here, \( a(x) = \frac{1}{2} A(x) \) is the half-height of the duct and \( y = 0 \) is an axis of symmetry. The constructed solution \( u_m \) is substituted into the 2D Euler operator \( N \) to obtain a source term to drive the modified Euler equations

\[ f_m = N(u_m). \]

Derivatives of the flow quantities may be obtained using standard differential relations between the flow quantities and the duct variation.

Subsonic Cylinder. The velocity field is defined to correspond to incompressible flow around a cylinder. Using standard complex potential flow methods, the geometry is defined by \(|w| = 1\) in the complex \( w = u + iv \) plane, and the velocity field is based on the complex potential

\[ \Phi = q_0 (w + w^{-1}) \]

where \( q_0 \) is the real free stream velocity magnitude. The Cartesian velocity components \( q_u \) and \( q_v \) are obtained from

\[ q_u - iq_v = \frac{d\Phi}{dw} \]

with derivatives

\[ \frac{\partial q_u}{\partial u} = -\frac{\partial q_v}{\partial v} = R \left\{ \frac{d^2 \Phi}{dw^2} \right\}, \]

\[ \frac{\partial q_v}{\partial u} = \frac{\partial q_u}{\partial v} = -I \left\{ \frac{d^2 \Phi}{dw^2} \right\}. \]

Given this definition of the velocity, the pressure and density, and their derivatives, are then defined by specifying uniform stagnation enthalpy \( H \) and entropy \( s \) throughout the flow field.

Subsonic Lifting Airfoil. The velocity field over a subsonic lifting Joukowski airfoil is again specified to correspond to incompressible flow, and is obtained by constructing a complex potential using conformal mapping. Starting from the unit cylinder \(|w| = 1\) in the \( w = u + iv \) plane, we first map to a shifted scaled cylinder in the \( z = x + iy \) plane centered at

\[ \gamma = \varepsilon_x - i \varepsilon_y, \quad \varepsilon_x, \varepsilon_y > 0, \]

with radius \( R = |1+\gamma| \). The mapping from \( w \) to \( z \) is

\[ z = -\gamma + Re^{i\alpha}w, \]

and the inverse mapping is

\[ w = R^{-1} e^{-i\alpha} (z + \gamma), \]

where \( \alpha \) is the angle of attack. The cylinder in the \( z \) plane is then mapped to a Joukowski airfoil in the \( c = a + ib \) plane using

\[ c = \frac{1}{2} (z + z^{-1}) \]

with inverse mapping

\[ z = c + \sqrt{c^2 - 1}. \]

The geometry mapping derivatives are given by

\[ \frac{dz}{dw} = Re^{i\alpha}, \quad \frac{dw}{dz} = R^{-1} e^{-i\alpha}, \]

and

\[ \frac{dc}{dz} = \frac{1}{2} (1 - z^{-2}), \quad \frac{dz}{dc} = 1 + \frac{c}{\sqrt{c^2 - 1}}. \]

Care must be taken to define the branch cut for the square root to lie inside the airfoil geometry.

The trailing edge of the airfoil is at \( c = 1 \), which corresponds to \( z = 1 \) and

\[ w = e^{-i(\alpha + \beta)}, \quad \tan \beta = \frac{\varepsilon_y}{1 + \varepsilon_x}. \]

The complex potential in the \( w \)-plane is

\[ \Phi = q_0 (w + w^{-1}) + i \Gamma \log w, \]

with \( q_0 \) being real. The Cartesian velocity components, \( q_a \) and \( q_b \), in the \( c \)-plane are then

\[ q_a - iq_b = \frac{d\Phi}{dc} = \frac{d\Phi}{dw} \frac{dw}{dz} = \frac{dc}{dz} \frac{dw}{dz}. \quad (10) \]

Asymptotically, as \( c \to \infty \), \( q_a - iq_b \to 2R^{-1} e^{-i\alpha} q_0 \), so a freestream speed \( q_\infty \) at angle of attack \( \alpha \) requires

\[ q_0 = \frac{1}{2} R q_\infty. \]

There is a critical point in the Joukowski mapping at the cusped trailing edge, where \( \frac{dc}{dz} = 0 \) at \( c = 1 \). Examining the expression for complex velocity (10), the Kutta condition requires that \( \frac{dc}{dz} = 0 \) at the cusp. This corresponds to placing a stagnation point in the \( w \) plane at \( w = e^{-i(\alpha + \beta)} \). The corresponding vortex strength leading to smooth flow at the trailing edge is

\[ \Gamma = 2q_0 \sin(\alpha + \beta). \]

The velocity expression (10) is indeterminate at the cusped trailing edge, but the velocity at this point can be found using l’Hospital’s rule

\[ q_a - iq_b = \left( 2q_0 w^{-3} - i \Gamma w^{-2} \right) \left( \frac{dw}{dz} \right)^2, \]
with \( w = e^{-i(\alpha + \beta)} \). The flow derivatives are obtained from

\[
\frac{d^2 \Phi}{dc^2} = \frac{d^2 \Phi}{dw^2} \left( \frac{dw}{dz} \frac{dz}{dc} \right)^2 + \frac{d\Phi}{dw} \frac{dw}{dz} \frac{d^2 z}{dc^2},
\]

with

\[
\frac{\partial q_a}{\partial a} = -\frac{\partial q_b}{\partial b} = R \left\{ \frac{d^2 \Phi}{dc^2} \right\},
\]

\[
\frac{\partial q_b}{\partial a} = \frac{\partial q_a}{\partial a} = -I \left\{ \frac{d^2 \Phi}{dc^2} \right\}.
\]

The pressure and density are again obtained by specifying uniform stagnation enthalpy and entropy throughout the flow field.

### Two-dimensional Results

#### Subsonic flow in a duct

We now consider adjoint and defect methods for subsonic Euler flow in a smooth 2D duct. We consider the drag functional, which should be identically zero for this problem. In developing the implementation, we found it very helpful to work on a test case where the solution is known in addition to the functional value. In a subsequent section, we describe a modified Euler problem for 2D duct geometries that has a known analytical solution. For the present studies, we return to the unmodified Euler equations and rescale the geometry used for the quasi-1D test case (8) to be ten times longer. The same inlet and outlet conditions are used, with the additional restriction that the flow is uniform at the inlet (\( q_y = 0 \)).

The equations are discretized using a 2nd order accurate finite volume scheme. Reconstruction is performed using bi-cubic splining with not-a-knot boundary conditions. Boundary integrals are evaluated using 3-point Gauss quadrature and bulk integrals are evaluated using 3×3 Gauss quadrature. Figure 4a depicts a sample computational mesh, computed pressure contours, and residual contours obtained by substituting the reconstructed solution into the first component of the Euler equations.

The baseline drag estimate is \( O(h^3) \) for this problem, as illustrated in Figure 4b. Adjoint methods provide either a sharp bound that is in error by \( O(h^3) \), or else an \( O(h^5) \) functional estimate. The numerical discretization provides \( O(h^2) \) primal and dual solutions and cubic spline reconstruction provides a residual with the same order of accuracy. Hence we expect at least 2nd order functional accuracy before correction and 4th order accuracy after correction. In the present setting, we observe an additional order of accuracy in each case. These results are reproducible on ducts with different throat constrictions or asymmetric shape changes.

Figure 4c illustrates that linear reconstruction provides nearly identical performance. Unlike in the quasi-1D case, a theoretical justification for this behavior is not currently available. We are not yet convinced of the generality of this result, as the performance of linear interpolation does not hold up on the airfoil test case to be discussed later. Nonetheless, linear reconstruction is very attractive from a practical viewpoint so it merits consideration until definitive conclusions are reached regarding its viability.

A combination of defect and adjoint methods are presented for this 2D duct flow in Figure 4d. Defect methods provide an error estimate that is used either to provide a sharp bound on the 3rd order baseline error or subtracted to obtain a 4th order functional estimate. Adjoint methods then provide a bound on the 4th order defect estimate or else produce a 5th order functional estimate. Note that the functional accuracy is improved by roughly an order of magnitude relative to the 5th order functional estimates obtained in Figure 4b. In theory, the primal solution after defect correction should be \( O(h^4) \) and the adjoint residual should be \( O(h^2) \) so we expect \( O(h^6) \) functional accuracy using the combined approach. Further work is required to investigate the remaining sources of error that prevent 6th order functional convergence. A fundamental difficulty is that the reconstructed solution is defined on a splined geometry that is only 4th order accurate.

#### Subsonic lifting flow over an airfoil

Our final test case examines the drag for lifting flow over a Joukowski airfoil with free stream Mach number \( M_\infty = 0.5 \) and angle of attack \( \alpha = 3^\circ \). For this geometry, we construct a modified Euler problem with a known analytical solution. Constant entropy and stagnation enthalpy conditions are combined with a velocity field derived from the potential flow solution for the same geometry. The computational domain is truncated at approximately 27 chords, where the far field boundary conditions are based on the exact solution to the modified Euler problem. The exact drag is non-zero for the modified solution owing to the effects of the small forcing terms in the modified equation. The reconstruction scheme uses periodic cubic splines around the airfoil including on the wall boundary.

A sample computational mesh and corresponding pressure contours are depicted in Figures 5a and 5b.
This problem is more challenging than the smooth 2D duct, since it contains a geometric singularity at the cusped trailing edge. In Figure 5c, we observe a base error in the drag that is $O(h^{2.5})$. Using adjoint error bounding we obtain an asymptotically sharp bound. Using adjoint error correction, we obtain 4th order accuracy in the functional estimate.

Conclusions

We have described adjoint and defect methods for obtaining sharp estimates of the error in integral functionals of PDE solutions. This approach has been demonstrated for the drag on a lifting airfoil in subsonic flow. Using 2nd order discretizations for the flow and adjoint systems and cubic spline solution reconstruction, we obtain either an asymptotically sharp bound on the error in the functional, or else a corrected functional estimate with 4th order accuracy. Adjoint error estimation methods have also been extended to treat shocked flows, using a two step correction process to account for modeling and discretization errors. Again, 4th order error estimates are obtained.

A modified equation approach is employed to provide test cases on interesting geometries with known analytical solutions. At truncated computational boundaries, the solution to the modified equation may be used to provide an exact far field model. The issue of far field model accuracy is conceptually distinct from the sources of error treated in this paper. Further studies are required to determine the impact of approximate far field models on the performance of the methods presented here. It may be interest-
The present bounding and correction methods can be extended to unstructured computational meshes by changing to an unstructured reconstruction scheme\textsuperscript{18}. A discrete version of the present approach has been employed successfully on unstructured meshes\textsuperscript{6,7}, where the error estimates are used to drive an adaptive meshing algorithm. The use of individual cell or element error contributions to drive adaptive error control methods is often based on a “localization” of the error contribution via the triangle inequality\textsuperscript{21}. Localization introduces a safety margin by reducing the sharpness of the bound (to the degree that it eliminates cancellation effects between elements with errors of opposite sign).

The combined use of adjoint and defect methods to attempt 6th order error estimates using 2nd order numerics and 4th order reconstruction is currently underway. These same ingredients have been used successfully for smooth quasi-1D Euler flow, even when the exact geometry is replaced by a splined representation.

**Acknowledgments**

This work was funded by NASA/Ames Cooperative Agreement No. NCC 2-5431.

**References**


