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Adjoint Recovery of Superconvergent Functionals from PDE Approximations*

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Abstract. Motivated by applications in computational fluid dynamics, a method is presented for obtaining estimates of integral functionals, such as lift or drag, that have twice the order of accuracy of the computed flow solution on which they are based. This is achieved through error analysis that uses an adjoint PDE to relate the local errors in approximating the flow solution to the corresponding global errors in the functional of interest. Numerical evaluation of the local residual error together with an approximate solution to the adjoint equations may thus be combined to produce a correction for the computed functional value that yields the desired improvement in accuracy. Numerical results are presented for the Poisson equation in one and two dimensions and for the nonlinear quasi-one-dimensional Euler equations. The theory is equally applicable to nonlinear equations in complex multi-dimensional domains and holds great promise for use in a range of engineering disciplines in which a few integral quantities are a key output of numerical approximations.

Key words. PDEs, adjoint equations, error analysis, superconvergence

AMS subject classifications. 65G99, 76N15

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1. Introduction.

In aeronautical applications of computational fluid dynamics (CFD), engineers desire very accurate predictions of the lift and drag, which are defined by integrals over the entire surface of the wing or aircraft being considered [27]. They are also interested in the details of the flow field in general, but to a lesser degree of accuracy since the main purpose is to understand the qualitative nature of the flow (e.g., is there a strong shock producing an extensive flow separation?) in order to make design changes that will improve the lift or drag. Other areas of CFD analysis also have a particular interest in a few key integral quantities, such as total production of nitrous oxides in combustion modeling or the net seepage of a pollutant into an aquifer when modeling soil contamination.

Integral quantities are important in other disciplines as well. In electrochemical simulations of the behavior of sensors, the quantity of interest is the total current flowing into an electrode [1]. In electromagnetics, radar cross-section calculations are concerned with the scattered field emanating from an aircraft. The amplitude of the

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wave propagating in a particular direction can be evaluated by a convolution integral over a closed surface surrounding the aircraft [9, 26]. Similar convolution integrals are used in the analysis of multiport electromagnetic devices such as microwave ovens and EMR body scanners to evaluate radiation, transmission, and reflection coefficients that characterize the behavior of the device.

In structural mechanics, one is sometimes concerned with the total force or moment exerted on a surface [29], but more often the quantities of most concern are point quantities such as the maximum stress or temperature. Because integral quantities can be approximated with much greater accuracy, Babuška and Miller [3] developed a technique using an auxiliary function to represent a point quantity by an equivalent integral. The same technique could be used in other applications in which it is point quantities, rather than integral quantities, that are of most importance.

Regardless of the area of application, when integral functionals based on approximate PDE solutions are of significant interest, it is worth considering approaches for enhancing the accuracy of these functional approximations. The question to be addressed in the present work is the following: Given an approximate solution to a PDE with boundary conditions, how do errors in the solution affect the accuracy of an integral functional, and how can these functional errors be estimated and used to obtain a more accurate functional approximation?

The key is the solution of the adjoint PDE with inhomogeneous terms appropriate to the functional of interest. We show that it is the adjoint solution that relates the residual error in the primal PDE solution (as measured by the extent to which the numerical solution fails to satisfy the PDE) to the consequent error in the computed value of the functional. Numerical approximations of the adjoint solution and primal residual errors can then be used to correct the error in the functional and obtain a new estimate that is *superconvergent* in that the remaining error is proportional to the product of the errors in the primal and adjoint solutions.

The analysis is closely related to superconvergence results in the finite element literature [3, 4, 5, 6, 15, 26, 28, 29, 34]. The key distinction is that the adjoint error correction term that is evaluated to obtain superconvergence is zero in a large class of finite element methods. Thus, these methods automatically produce superconvergent results for any integral functional without requiring the computation of an approximate adjoint solution. From a finite element perspective, this paper can therefore be viewed as extending superconvergence theory to cover numerical results obtained by any numerical method: finite difference, finite volume, or finite element without natural superconvergence. Moreover, we show that the adjoint recovery technique in this paper can also be used to improve the order of accuracy of the superconvergent functionals obtained from finite element methods.

There are other ways of improving the accuracy of a functional by improving the entire solution. One is defect correction, in which a higher order discretization is used to define a residual error that acts as a source term in calculating a solution correction using a lower order discretization [12, 7, 8]. Another even older approach is to use Richardson extrapolation, assuming that the order of accuracy of the computed solution is reliably known on more than one mesh level [32, 10]. However, the adjoint error correction technique described in this paper can be applied in addition to either of these methods. All that is required is approximate solutions to both the primal problem and its adjoint; if the accuracy of these solutions is improved through the use of defect correction or Richardson extrapolation, then the accuracy of the functional after the adjoint error correction will be correspondingly improved as well.

We begin by describing the approach for linear problems including simple examples of its application to the Poisson equation in one and two dimensions. To illustrate the applicability of the theory to numerical results obtained by any discretization method, the one-dimensional (1D) solutions are obtained using a finite difference method, whereas the two-dimensional (2D) results are based on a finite element discretization. These 2D results demonstrate both the natural superconvergence of the finite element method and the additional orders of accuracy resulting from adjoint error analysis.

Next, we present the approach for nonlinear problems with examples of its use for the quasi-1D Euler equations, a coupled system of three nonlinear ODEs describing inviscid compressible flow in a variable area duct. The examples include cases with a sonic point at which there is a change in direction of one of the hyperbolic characteristics, and a shock at which there is a discontinuity in the flow field. For these cases, numerical results are obtained using a finite volume method typical of those used in aeronautical CFD calculations.

We conclude by discussing the difficulties in and prospects for extending the theory and its implementation to nonlinear PDEs in multiple dimensions on domains of arbitrary shape.

2. Linear Analysis. Let u be the solution of the linear differential equation

$$Lu = f$$

on the domain Ω, subject to homogeneous boundary conditions for which the problem is well-posed when $f \in L_2(\Omega)$. The adjoint differential operator L^* and associated homogeneous boundary conditions are defined by the identity

$$(v, Lu) = (L^*v, u)$$

for all u, v satisfying the respective boundary conditions. Here the notation $(.,.)$ denotes an integral inner product over the domain Ω.

Suppose now that we are concerned with the value of the functional $J = (g, u)$ for a given function $g \in L_2(\Omega)$. An equivalent dual formulation of the problem is to evaluate the functional $J = (v, f)$, where v satisfies the adjoint equation

$$L^*v = g,$$

subject to the homogeneous adjoint boundary conditions. The equivalence of the two forms of the problem follows immediately from the definition of the adjoint operator

$$(v, f) = (v, Lu) = (L^*v, u) = (g, u).$$

Digressing slightly, we note that the dual formulation of the problem is exploited in optimal design [20, 21], in which there is only one function g, corresponding to the objective function in the design optimization, but there are multiple functions f, each corresponding to a different geometric design parameter. Therefore, the dual approach is computationally much more efficient since each design cycle requires just one adjoint calculation, whereas the direct approach would require one calculation for each design variable. The existence of adjoint solution methods for design purposes [2, 11, 22, 31] means that in many cases, the building blocks are already in place for rapid exploitation of the error correction ideas in this paper.

Returning to the subject at hand, suppose that u_h and v_h are approximations to u and v, respectively, and satisfy the homogeneous boundary conditions. The subscript

h denotes that the approximate solutions are derived from numerical computations using a grid with average spacing h. When using finite difference or finite volume methods, u_h and v_h might be created by interpolation through computed values at grid nodes. With finite element solutions, one might more naturally use the finite element solutions themselves, or one could again use an interpolation through nodal values. A last comment is that u_h and v_h do not have to come from a numerical computation; they could, for example, come from an asymptotic analysis yielding a uniformly valid asymptotic approximation to the solution.

Let the functions f_h and g_h be defined by

$$Lu_h = f_h, \quad L^* v_h = g_h.$$

It is assumed that u_h and v_h are sufficiently smooth that f_h and g_h lie in $L_2(\Omega)$. If u_h and v_h were equal to u and v, then f_h and g_h would be equal to f and g. Thus, the *residual errors* $f_h - f$ and $g_h - g$ are a computable indication of the extent to which u_h and v_h are not the true solutions.

Now, using the definitions and identities given above, we obtain the following expression for the functional:

$$\begin{aligned}(g,u) &= (g,u_h) - (g_h, u_h - u) + (g_h - g, u_h - u)\\ &= (g,u_h) - (L^* v_h, u_h - u) + (g_h - g, u_h - u)\\ &= (g,u_h) - (v_h, L(u_h - u)) + (g_h - g, u_h - u)\\ &= (g,u_h) - (v_h, f_h - f) + (g_h - g, u_h - u).\end{aligned}$$

The first term in the final expression is the value of the functional obtained from the approximate solution u_h. The second term is an inner product of the residual error $f_h - f$ and the approximate adjoint solution v_h. The adjoint solution gives the weighting of the contribution of the local residual error to the overall error in the computed functional. Therefore, by evaluating and subtracting this adjoint error term we obtain a more accurate value for the functional.

The third term is the remaining error after making the adjoint correction. If $g_h - g$ is of the same order of magnitude as $v_h - v$ then the remaining error has a bound that is proportional to the product $\|u_h - u\| \, \|v_h - v\|$ (using L_2 norms), and thus the corrected functional value is superconvergent. If the solution errors $u_h - u$ and $v_h - v$ are both $O(h^p)$, so that halving the grid spacing leads to a 2^p reduction in the errors, then the error in the functional is $O(h^{2p})$. Furthermore, the remaining error term can be expressed as $(g - g_h, L^{-1}(f - f_h))$ and so has the computable a posteriori error bound

$$|\text{Error}| \le \|L^{-1}\| \, \|f_h - f\| \, \|g_h - g\|,$$

with $\|L^{-1}\|$ being assumed to be finite due to well-posedness.

If u_h and v_h are taken to be the finite element solutions obtained from a Galerkin finite element method (or more generally any finite element method for which the test and trial spaces for the primal problem are interchanged to become the trial and test spaces for the adjoint problem) the adjoint correction term is always zero because of the orthogonality arising from the weak formulation of the finite element discretization. Thus, the values of all integral functionals are automatically superconvergent. However, if the operator L involves derivatives of up to degree m, then usually $f_h - f = O(h^{p-m})$, and hence the error in any functional is $O(h^{2p-m})$. This loss

of accuracy is due to a lack of smoothness in the finite element solution. If a smoother interpolated solution can be recovered from the finite element solution, then there is a possibility of using the adjoint error correction to recover an improved functional estimate whose error is $O(h^{2p})$. This will be demonstrated in the second of the two examples to follow.

To conclude this section, we return to the topic of boundary conditions. For simplicity in presenting the analysis, we have assumed that the primal problem has homogeneous boundary conditions and that the functional is simply an inner product of the whole domain and does not have a boundary integral term. More generally, inhomogeneous boundary conditions and boundary integrals in the functional are both permissible. Inhomogeneous boundary conditions for the primal problem lead to a boundary integral term for the adjoint formulation, and similarly a boundary integral in the primal form of the functional leads to inhomogeneous adjoint boundary conditions. Although the analysis is slightly more complicated, the final form of the adjoint error correction is exactly the same as before, provided the approximate solutions u_h and v_h still exactly satisfy the inhomogeneous boundary conditions. If they do not, then there is an additional correction term to account for this error [18].

3. Two Linear Examples.

3.1. 1D Finite Difference Calculation. The first example is the 1D Poisson equation,

$$\frac{d^2u}{dx^2} = f,$$

on the unit interval $[0,1]$ subject to homogeneous boundary conditions $u(0)=u(1)=0$. This is approximated numerically on a uniform grid, with spacing h, using a second order finite difference discretization,

$$h^{-2}\delta_x^2 u_j = f(x_j).$$

The approximate solution $u_h(x)$ is then defined by cubic spline interpolation through the nodal values u_j.

The dual problem is the Poisson equation,

$$\frac{d^2v}{dx^2} = g,$$

subject to the same homogeneous boundary conditions, and the approximate adjoint solution v_h is obtained in exactly the same manner.

Numerical results have been obtained for the case

$$f = x^3(1-x)^3, \qquad g = \sin(\pi x).$$

Figure 3.1 shows the residual error $f_h - f$ when $h=\frac{1}{32}$, as well as the three Gaussian quadrature points on each subinterval which are used in the numerical integration of the inner product $(v_h, f_h - f)$. Since u_h is a cubic spline, $f_h \equiv \frac{d^2u_h}{dx^2}$ is continuous and piecewise linear. The best piecewise linear approximation to f has an error whose dominant term is quadratic on each subinterval; this explains the scalloped shape of the residual error. Figure 3.2 shows the approximate adjoint solution v_h, which reveals that the residual error in the center of the domain contributes most to the overall error in the functional.

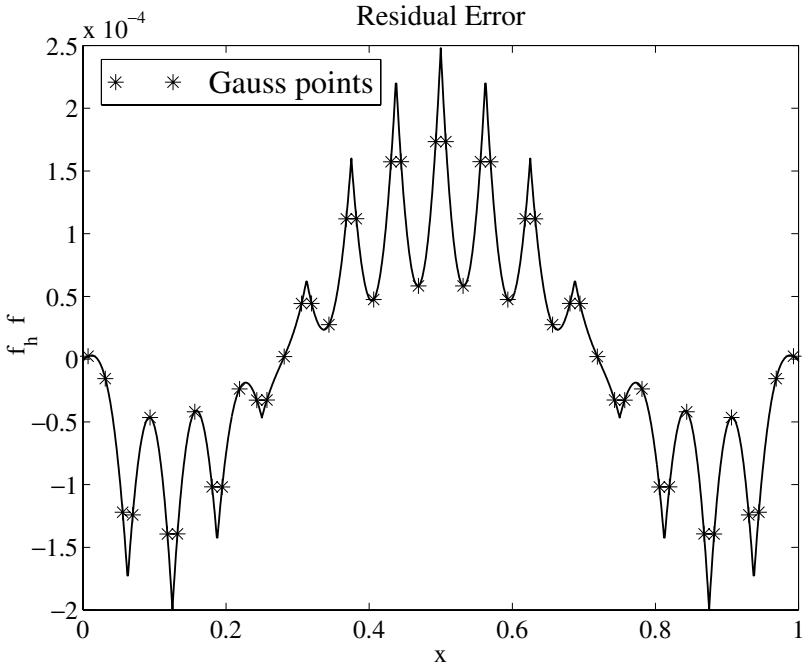

Fig. 3.1 *Residual error for the* 1*D Poisson equation.*

Figure 3.3 depicts a log-log plot of three quantities versus the number of cells: the error in the base value of the functional (g, u_h); the remaining error after subtracting the adjoint correction term $(v_h, f_f - f)$; the a posteriori error bound $\|L^{-1}\| \, \|f_h - f\| \, \|g_h - g\|$. The superimposed lines have slopes of -2 and -4, confirming that the base solution is second order accurate while the error in the corrected functional and the error bound are both fourth order. It is also worth noting that on a grid with 16 cells, which might be a reasonable choice for practical computations, the error in the corrected value of the functional is over 200 times smaller than the uncorrected error.

3.2. 2D Finite Element Calculation. The second example is the two-dimensional Poisson equation,

$$\nabla^2 u = f,$$

on the unit square $[0,1] \times [0,1]$ subject to homogeneous Dirichlet boundary conditions. The dual problem is

$$\nabla^2 v = g$$

with the same boundary conditions.

For this example, the equations are approximated using a Galerkin finite element method with piecewise bilinear elements on a uniform Cartesian grid. Recalling that in the present case, $p = m = 2$, finite element error analysis reveals that the solution error for the primal problem is $O(h^2)$ with a corresponding residual error that is $O(1)$. The inherent superconvergence of the finite element method thus yields a computed functional that is $O(h^2)$. However, by using bicubic spline interpolation through

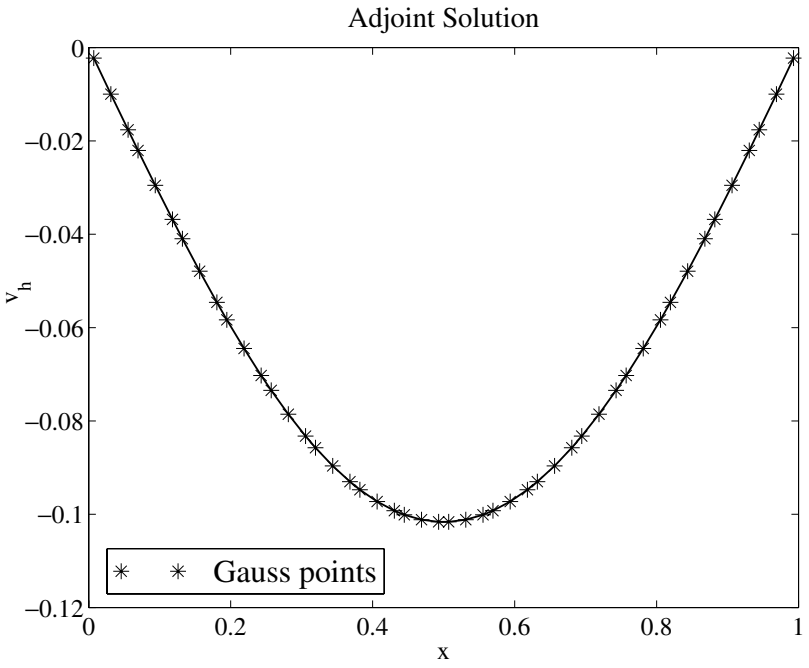

Fig. 3.2 *Adjoint solution for the* $1D$ *Poisson equation.*

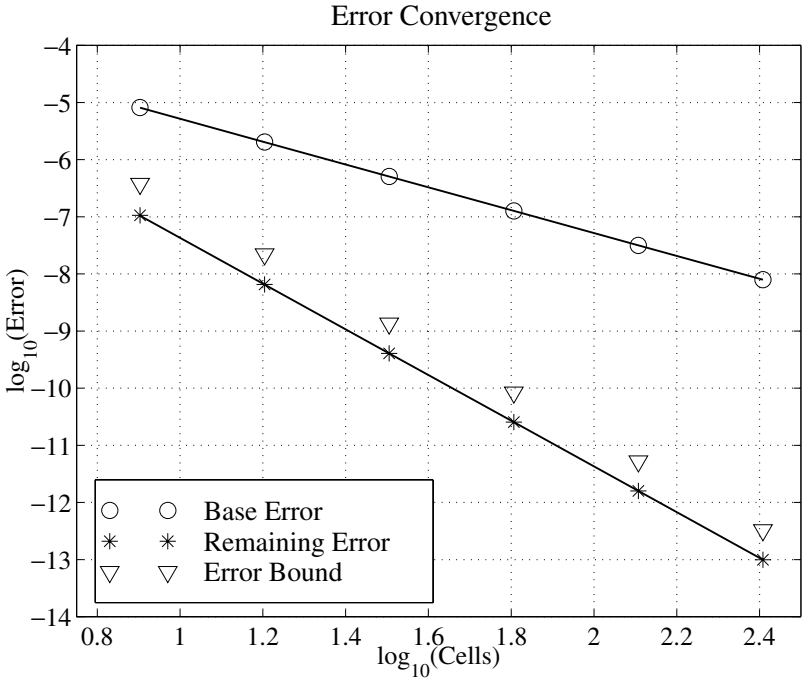

Fig. 3.3 *Functional error convergence for the* $1D$ *Poisson equation.*

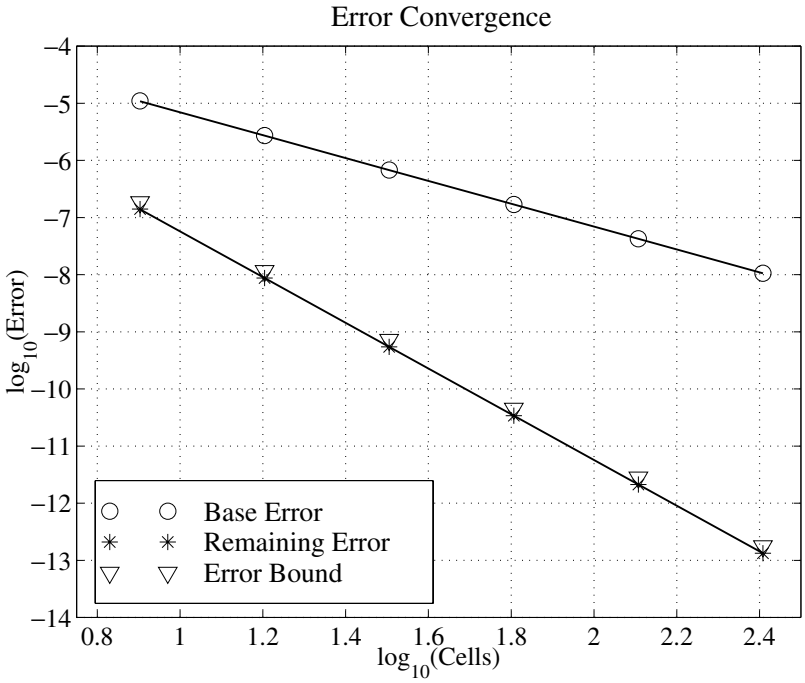

Fig. 3.4 *Functional error convergence for the 2D Poisson equation.*

the computed nodal values, one can reconstruct an improved approximate solution $u_h(x, y)$ with an error that is $O(h^2)$ in the H^2 Sobolev norm, and hence has a residual error that is also $O(h^2)$. Using a similarly reconstructed approximate adjoint solution $v_h(x, y)$, the adjoint error correction term then produces a corrected functional whose accuracy is $O(h^4)$. All inner product integrals are approximated by 3×3 Gaussian quadrature on each square cell to ensure that the numerical quadrature errors are of a higher order.

Figure 3.4 shows the numerical results obtained for the functions

$$f(x, y) = x(1-x)\, y(1-y), \qquad g(x, y) = \sin(\pi x)\, \sin(\pi y).$$

The ordinate is the log of the number of cells in each dimension, and lines of slope -2 and -4 are again superimposed. As predicted by the analysis, the base error in the functional is second order, while the corrected functional error and the error bound are again both fourth order.

4. Nonlinear Analysis. For nonlinear problems, the conceptual approach is very similar, but the mathematical presentation becomes somewhat more involved. Let u be the solution of the nonlinear differential equation

$$N(u) = f,$$

subject to appropriate boundary conditions, and let the functional of interest, $J(u)$, be an integral of a nonlinear algebraic function of u over the domain Ω.

The linear differential operator L_u is defined to be the Fréchet derivative of N,

$$L_u\, \tilde{u} \equiv \lim_{\epsilon \to 0} \frac{N(u + \epsilon \tilde{u}) - N(u)}{\epsilon},$$

and, similarly, the function $g(u)$ is defined by the identity

$$(g(u), \tilde{u}) \equiv \lim_{\epsilon \to 0} \frac{J(u + \epsilon \tilde{u}) - J(u)}{\epsilon}.$$

The corresponding linear adjoint problem is then

$$L_u^* v = g,$$

subject to the appropriate homogeneous adjoint boundary conditions.

We now consider approximate solutions u_h, v_h and define f_h, g_h by

$$N(u_h) = f_h, \quad L_{u_h}^* v_h = g_h.$$

Note the use of $L_{u_h}^*$, the Fréchet derivative based on u_h which is known, instead of L_u^*, based on u which is not known.

In addition, the analysis requires averaged Fréchet derivatives $\overline{L}_{(u,u_h)}$ and $\overline{g}(u, u_h)$ defined by

$$\begin{aligned} \overline{L}_{(u,u_h)} &= \int_0^1 L|_{u+\theta(u_h - u)} \, d\theta, \\ \overline{g}(u, u_h) &= \int_0^1 g(u + \theta(u_h - u)) d\theta, \end{aligned}$$

so that

$$\begin{aligned} N(u_h) - N(u) &= \int_0^1 \frac{\partial}{\partial \theta} N(u + \theta(u_h - u)) \, d\theta \\ &= \overline{L}_{(u,u_h)} \, (u_h - u), \end{aligned}$$

and similarly

$$J(u_h) - J(u) = (\overline{g}(u, u_h), u_h - u).$$

We then obtain the following result:

$$\begin{aligned} J(u) &= J(u_h) - (\overline{g}(u, u_h), u_h - u) \\ &= J(u_h) - (g_h, u_h - u) + (g_h - \overline{g}(u, u_h), u_h - u) \\ &= J(u_h) - (L_{u_h}^* v_h, u_h - u) + (g_h - \overline{g}(u, u_h), u_h - u) \\ &= J(u_h) - (v_h, L_{u_h}(u_h - u)) + (g_h - \overline{g}(u, u_h), u_h - u) \\ &= J(u_h) - (v_h, \overline{L}_{(u,u_h)}(u_h - u)) + (g_h - \overline{g}(u, u_h), u_h - u) \\ &\qquad - (v_h, (L_{u_h} - \overline{L}_{(u,u_h)})(u_h - u)) \\ &= J(u_h) - (v_h, N(u_h) - N(u)) + (g_h - \overline{g}(u, u_h), u_h - u) \\ &\qquad - ((L_{u_h}^* - \overline{L}_{(u,u_h)}^*) v_h, u_h - u) \\ &= J(u_h) - (v_h, f_h - f) + (g_h - \overline{g}(u, u_h), u_h - u) - ((L_{u_h}^* - \overline{L}_{(u,u_h)}^*) v_h, u_h - u). \end{aligned}$$

The first term in the final line is again the functional evaluated using the approximate solution u_h. The second term is again a computable adjoint error correction term which is an inner product of the residual error and the approximate adjoint solution. The last two terms form the remaining error in the corrected functional.

The third term is similar to the remaining error term in the linear case, while the fourth term is associated with the nonlinearity in the operator $N(u)$. If the solution errors for the nonlinear primal problem and the linear adjoint problem are of the same order, and they are both sufficiently smooth that the corresponding residual errors are also of the same order, then the order of accuracy of the functional approximation after making the adjoint correction is twice the order of the primal and adjoint solutions.

An a posteriori error bound is harder to construct than in the linear case. Splitting the remaining error into three pieces,

$$\text{Error} = (g_h - g(u_h), u_h - u) + (g(u_h) - \overline{g}(u, u_h), u_h - u) - ((L^*_{u_h} - \overline{L}^*_{(u,u_h)})v_h, u_h - u),$$

we can obtain asymptotic error bounds by converting each inner product into an alternative representation that is asymptotically equivalent and has a computable bound. With the first inner product we have

$$(g_h - g(u_h), u_h - u) \approx (g_h - g(u_h), L_u^{-1}(f_h - f)).$$

For the second, we define G_u to be the Fréchet derivative of $g(u)$,

$$G_u \tilde{u} = \lim_{\epsilon \to 0} \frac{g(u + \epsilon\tilde{u}) - g(u)}{\epsilon},$$

and then obtain

$$\begin{aligned}(g(u_h) - \overline{g}(u, u_h), u_h - u) &\approx \tfrac{1}{2}(G_u(u_h - u), u_h - u) \\ &\approx \tfrac{1}{2}(L_u^{*\,-1} G_u L_u^{-1}(f_h - f), f_h - f).\end{aligned}$$

For the third inner product, we define the operator $H_{u,v}$ as

$$H_{u,v}\tilde{u} = \lim_{\epsilon \to 0} \frac{L^*_{u+\epsilon\tilde{u}} v - L^*_u v}{\epsilon},$$

so that

$$\begin{aligned}((\overline{L}^*_{(u,u_h)} - L^*_{u_h})v_h, u - u_h) &\approx \tfrac{1}{2}(H_{u,v}(u - u_h), u - u_h) \\ &\approx \tfrac{1}{2}(L_u^{*\,-1} H_{u,v} L_u^{-1}(f - f_h), f - f_h).\end{aligned}$$

Together, these give the approximate asymptotic bound

$$|\ \text{Error}\ | \le c_1 \|f_h - f\|\, \|g_h - g(u_h)\| + c_2 \|f_h - f\|^2,$$

where

$$c_1 = \|L_u^{-1}\|, \qquad c_2 = \tfrac{1}{2}\left\|L_u^{*\,-1}(H_{u,v} - G_u)L_u^{-1}\right\|.$$

The problem in evaluating this a posteriori error bound is that c_1 and c_2 will not be known in general and may be hard to bound analytically. A more practical option may be to estimate them computationally based on the corresponding discrete operators.

5. Nonlinear Finite Volume Examples. The steady quasi-1D Euler equations describe the flow of an inviscid, compressible ideal gas in a variable area duct. The functional of interest is the integral of the pressure along the duct, which serves as a model for the computation of lift and drag on airfoils in two dimensions, and wings and aircraft in three dimensions.

The unsteady quasi-1D Euler equations in conservative form are

$$A\frac{\partial U}{\partial t} + \frac{\partial}{\partial x}(AF) - \frac{dA}{dx}P = 0,$$

where $A(x)$ is the cross-sectional area of the duct and U, F, and P are defined as

$$U = \begin{pmatrix} \rho \\ \rho q \\ \rho E \end{pmatrix}, \qquad F = \begin{pmatrix} \rho q \\ \rho q^2 + p \\ \rho q H \end{pmatrix}, \qquad P = \begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix}.$$

Here, ρ is the density, q is the velocity, p is the pressure, E is the total energy, and H is the stagnation enthalpy. The system is closed by the equation of state for an ideal gas

$$H = E + \frac{p}{\rho} = \frac{\gamma p}{(\gamma - 1)\rho} + \frac{1}{2}q^2,$$

where γ is the ratio of specific heats.

The unsteady quasi-1D Euler equations are a hyperbolic system with three characteristic wave speeds, q, $q + c$, and $q - c$, with $c = \sqrt{\gamma p/\rho}$ being the local speed of sound. Accordingly, the nature of the steady flow solution varies depending on whether the flow is subsonic ($M < 1$) or supersonic ($M > 1$), where $M \equiv q/c$ is the Mach number. In order of increasing difficulty, we will consider the subsonic, isentropic transonic, and shocked transonic flows depicted in terms of Mach number in Figure 5.1.

Steady flow solutions are obtained by marching the nonlinear unsteady system to a steady state using a standard second order finite volume method with characteristic smoothing on a uniform computational grid. The linear adjoint problem is approximated by linearizing the nonlinear flow equations, constructing the analytic adjoint equations and boundary conditions, and then forming a discrete approximation to these on the same uniform grid as the flow solution [21, 2]. Previous research has confirmed that this produces a consistent approximation to the analytic adjoint solution, which has been determined in closed form for the quasi-1D Euler equations [17], [19].

The approximate solution $u_h(x)$ is constructed from the discrete flow solution by cubic spline interpolation of the cell-centered values of the three components of the state vector U (except in the shocked case to be described later). The flow residual f_h is then formed using analytic derivatives of this reconstruction. The approximate adjoint solution $v_h(x)$ is also obtained by cubic spline interpolation of the cell-centered values of the three components of the discrete adjoint solution. The integrals that form the base value for the functional and the adjoint correction are then approximated using three-point Gaussian quadrature.

5.1. Subsonic Flow. As a first case, consider smooth subsonic flow in a converging-diverging duct. The error convergence of the computed functional is shown in Figure 5.2, where the superimposed lines of slopes -2 and -4 demonstrate that the base error is second order and the error in the corrected functional is fourth order. This

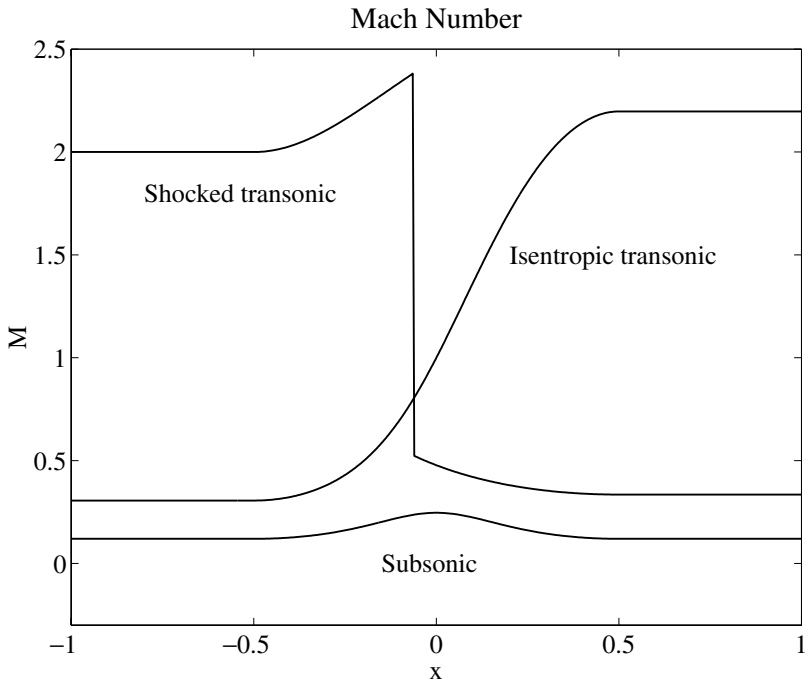

Fig. 5.1 *Mach number distributions for quasi-1D Euler equation test cases.*

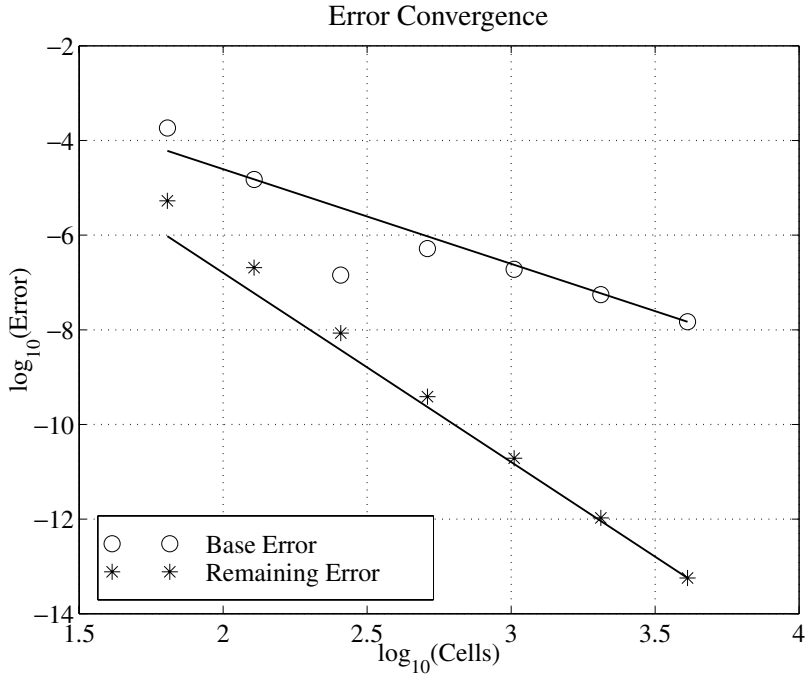

Fig. 5.2 *Error convergence for quasi-1D subsonic flow.*

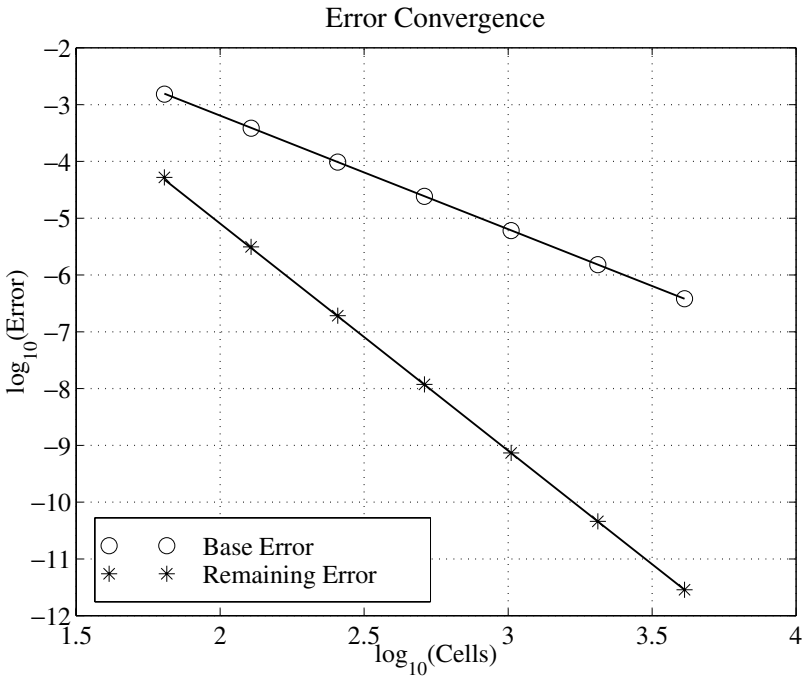

Fig. 5.3 *Error convergence for quasi-1D shock-free transonic flow.*

is in agreement with an a priori error analysis [30], based on the nonlinear convergence theory of Keller [23] and Sanz-Serna [25, 33] and stability bounds of Kreiss [24], which proves that $u_h - u$, $v_h - v$, and their first derivatives are all $O(h^2)$ for the present finite volume scheme, and hence the error in the corrected functional is $O(h^4)$.

5.2. Isentropic Transonic Flow. The error convergence for a transonic flow in a converging-diverging duct is shown in Figure 5.3. The flow is subsonic upstream of the throat and supersonic downstream of the throat. Again the results show that the base error is second order while the remaining error after the adjoint correction is fourth order.

The accuracy of the corrected functional in this case is a little puzzling because the adjoint solution has a logarithmic singularity at the throat [17], [19], as shown in Figure 5.4. Therefore, $v_h - v$ is $O(1)$ in a small region of size $O(h)$ on either side of the throat. Based on this, one might expect that the remaining error would be $O(h^3)$ since the numerical results confirm that the solution error $u_h - u$ and the consequent residual error for the nonlinear equations are both $O(h^2)$. The explanation for the fourth order convergence must lie in a cancellation of the leading order terms within the remaining error, but the reason for this is not yet understood.

5.3. Shocked Transonic Flow. The final case is a shocked flow in a diverging duct where the flow is wholly supersonic upstream of the shock and subsonic downstream of it. At the shock, the analytic adjoint solution is continuous and has zero gradient [17], [19] and so the adjoint variables pose no special difficulty in this case.

The challenge is the reconstruction of the approximate solution $u_h(x)$ from the cell-centered quantities produced by the finite volume calculation. The analytic so-

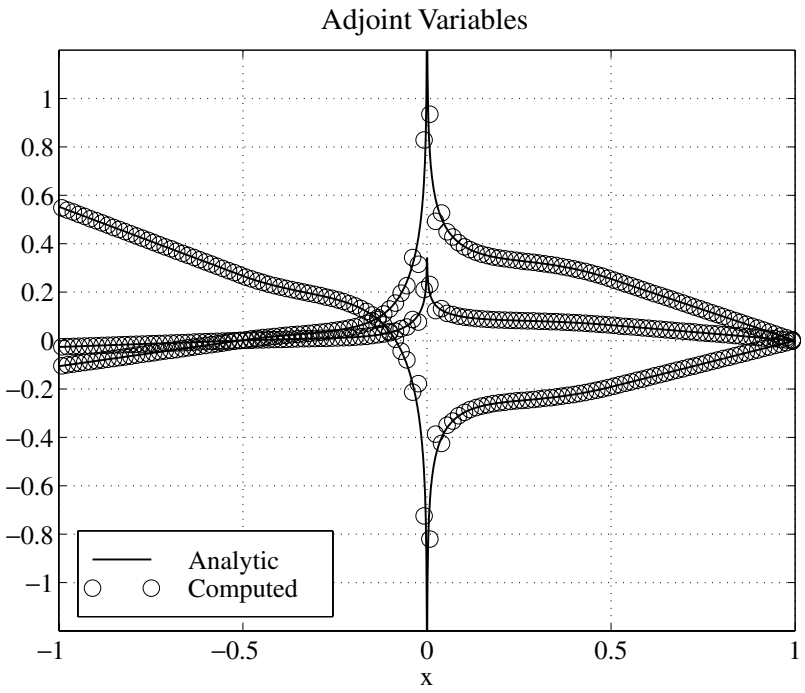

Fig. 5.4 *Adjoint solution for quasi-1D shock-free transonic flow.*

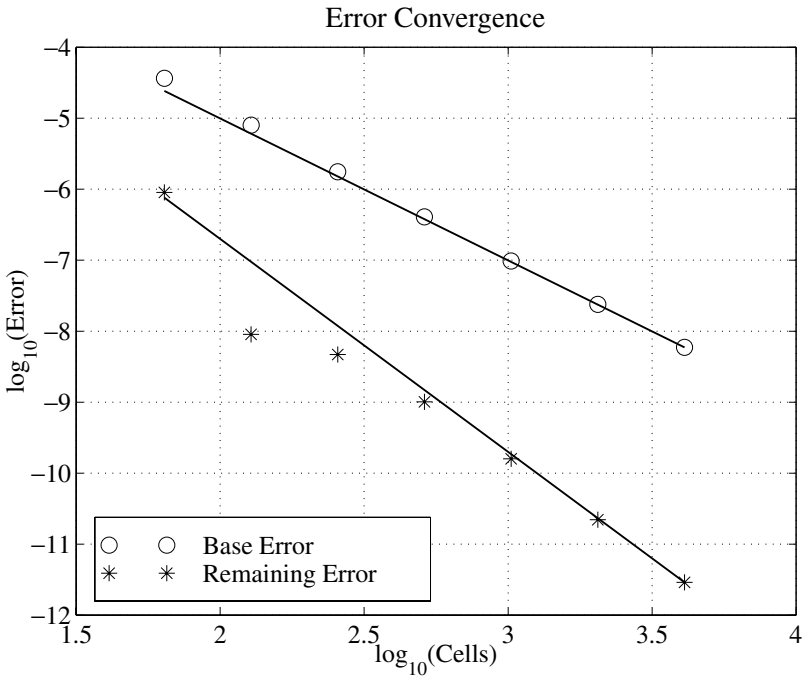

Fig. 5.5 *Error convergence for quasi-1D shocked flow.*

lution is discontinuous at the shock and satisfies the Rankine–Hugoniot shock jump relations which require that there is no discontinuity in the nonlinear flux F. To recover a discontinuous approximate solution $u_h(x)$, we first interpolate the computed values of F, which is known to be continuous across a shock. From these one can deduce the conservation variables U by solving a quadratic equation, one branch of which gives a subsonic flow solution, the other being supersonic. Therefore, given a shock position, one can reconstruct a supersonic solution on the upstream side, a subsonic solution on the downstream side, and automatically satisfy the Rankine–Hugoniot shock jump conditions at the shock itself.

To determine the shock position, we rely upon the fact that the integrated pressure along the duct is correct to second order when using a finite volume method that is conservative and second order accurate in smooth flow regions [13]. Therefore, we iteratively adjust the position of the shock until the reconstructed solution has the same base functional value (i.e., without the adjoint correction) as the original numerical approximation, thereby obtaining the correct shock position to second order.

The form of the adjoint error correction term is exactly the same as before. This conclusion follows from a slight extension of the nonlinear formulation to take the shock into account as an internal boundary. The corresponding adjoint linearization includes perturbations to the shock position, which lead to an internal boundary condition for the adjoint equations [17], [19].

The baseline error is expected to remain second order for shocked flow, but in the neighborhood of the shock, there is an $O(h)$ error in $u_h(x)$, so the corrected error is expected to be third order rather than fourth. This behavior is confirmed by the error convergence results shown in Figure 5.5, where the superimposed lines have slopes of -2 and -3.

6. Conclusions and Future Challenges. This paper presents a method for estimating the value of an integral functional with twice the order of accuracy of the numerical PDE solution on which the functional is based. The additional cost is the computation of an approximate solution to the associated adjoint problem. The formulation of the method for linear and nonlinear problems is relatively simple although some further complications arise when considering inhomogeneous boundary conditions and boundary integral terms in the functional. Given that many researchers are developing adjoint solvers because of their importance in optimal design, there is the potential for rapid exploitation of this error correction technique in a variety of engineering applications in which integral functionals are of interest.

In cases where the functional is a point quantity, the above theory could be applied using a distribution function for g. However, the loss of smoothness in g will often result in a poorer order of accuracy for the approximate adjoint solution v_h, leading to a consequent reduction in the order of accuracy of the corrected functional. To circumvent this difficulty, it may be possible to follow the approach of inner and outer matched asymptotic expansions, to combine an approximate analytic near-field solution with a computed far-field solution. Alternatively, one could use the technique of Babuška and Miller [3] to convert the point quantity into an equivalent integral representation.

A number of challenges will arise in applying the theory to more complex nonlinear problems in multiple dimensions. For curved boundaries, the computational domain covered by a grid is only an approximation to the true domain, and so there may be complications in extending the numerical solution to cover the full domain.

Likewise, there is the problem of ensuring that the approximate solution u_h exactly satisfies the boundary conditions imposed on the analytic solution u. Otherwise, an additional adjoint correction term associated with the residual error in the boundary conditions must be computed. In multiple dimensions, the functionals of interest are often boundary integrals rather than integrals over the whole domain. The formulation must then be modified by the introduction of inhomogeneous boundary conditions in the adjoint problem [16, 18].

Possibly the biggest challenge in multiple dimensions will be the treatment of discontinuities and singularities. In one dimension, reconstructive shock-fitting is relatively straightforward, but in multiple dimensions it will likely prove infeasible, especially when there are shock junctions. A more practical approach may be to use local grid refinement at the shock to reduce its width to $O(h^2)$, where h is the average cell width in the rest of the grid. In this way, it may be possible to ensure that the error from the shock region is of the same order as the error from the rest of the domain. Similarly, there are singularities in the adjoint Euler equations in multiple dimensions [16] that will need to be well resolved to achieve the desired superconvergence in the corrected functional.

This leads to the whole topic of optimal grid adaptation [6, 28, 34, 14]. The magnitude of the adjoint error correction term $(v_h, f_h - f)$ is minimized by adapting the grid in the regions in which the product $v_h^T(f_h - f)$ is largest. Alternatively, if grid adaptation is to be used in conjunction with adjoint error correction, then the remaining error is perhaps best minimized by adapting the grid where the residual errors $f_h - f$ and $g_h - g$ are largest.

Another interesting topic to be pursued in the future is the combination of adjoint error correction with defect correction. As discussed in the introduction, defect correction methods can be used to construct approximate solutions u_h and v_h which are of a higher order of accuracy. Applying adjoint error correction to these improved solutions will then lead to a corrected functional of an even higher order of accuracy. Given that adjoint error correction already requires the development of algorithms and software for the smooth reconstruction of an approximate solution from nodal values, the idea that immediately arises is to use the residuals from this smooth reconstruction to define the defect correction source term. This is slightly different from the usual defect correction approach in which one uses a higher order numerical discretization to define the residual. The proposed method thus avoids the difficulty of constructing a higher order discretization on an unstructured grid.

We conclude this paper with an open question. As discussed earlier in presenting the linear approach, Galerkin finite element methods automatically provide superconvergent estimates of order h^{2p-m} for integral functionals with sufficiently smooth weighting functions. From this result it can be deduced that the solution error is $O(h^{2p-m})$ when measured in an appropriate negative Sobolev norm. The question is under what conditions it is possible to reconstruct from the finite element solution a smoother approximate solution u_h for which the residual error is also $O(h^{2p-m})$, leading to an adjoint error correction that produces functionals with accuracy $O(h^{4p-2m})$! The numerical results for the 2D Poisson equation confirm that it is possible in the case when $p = m = 2$, but it is not clear to what extent this result can be generalized.

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