Comput Visual Sci 6: 113–121 (2004)
Digital Object Identifier (DOI) 10.1007/s00791-003-0115-y

Computing and
Visualization in Science

Regular article

Progress in adjoint error correction for integral functionals

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Received: 20 July 2002 / Accepted: 23 March 2003
Published online: 23 January 2004 –

Communicated by: M.S. Espedal, A. Quarteroni, A. Sequeira

Abstract. When approximating the solutions of partial differential equations, it is a few key output integrals which are often of most concern. This paper shows how the accuracy of these values can be improved through a correction term which is an inner product of the residual error in the original p.d.e. and the solution of an appropriately defined adjoint p.d.e. A number of applications are presented and the challenges of smooth reconstruction on unstructured grids and error correction for shocks are discussed.

1 Introduction

In performing aeronautical CFD calculations, engineers are interested in the entire flow over an aircraft, but they are most interested in the values of the lift, drag and moment on the aircraft, each of which can be expressed as an integral over the surface of the aircraft [17]. 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 modelling, or the net seepage of a pollutant into an aquifer when modelling soil contamination.

Integral outputs are also important in other disciplines as well. For example, in electrochemical simulations of the behavior of sensors, the quantity of interest is the total current flowing into an electrode [1], and in radar cross-section calculations the scattered field propagating from an aircraft in a particular direction can be evaluated by a convolution integral over a closed surface surrounding the aircraft [8, 18].

In structural mechanics, the output of interest is sometimes the total force or moment exerted on a surface [22], but more often it is a point quantity such as the maximum stress or temperature. Even then, it is possible to use auxiliary functions to convert point values into integral quantities which can be approximated with much greater accuracy [4].

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The above examples are to motivate the subject of this paper, improving the accuracy of integral output functionals. There are a number of possible approaches one might take, including adaptive grid refinement, increasing the order of accuracy of the discretization, iterative refinement of the numerical solution via defect correction, or Richardson extrapolation. All of these approaches can be used to improve global solution accuracy, yielding corresponding increases in functional accuracy. However, for problems in which the value of a functional is the most important quantitative output of a simulation, another approach introduced by Giles and Pierce [12, 20] is to use the approximate solution of an appropriately defined adjoint problem to accurately estimate the error in the functional due to the residual error in approximating the original partial different equation. By using this estimate as a correction, one can often obtain twice the order of accuracy for the output functional compared to the underlying global numerical solution.

The significance of the adjoint PDE for error analysis and adaptivity has long been realized within the finite element community [2–7, 15, 16, 18, 22, 23, 25, 26, 29, 30], where it is well known that many finite element methods enjoy natural superconvergence for functional estimates. The adjoint error correction technique extends these results to approximate solutions obtained by finite volume methods (or other means of approximation) as well as offering the potential for further improvement in the inherent finite element superconvergence.

In this paper we present the progress in applying the adjoint error correction ideas to a range of two-dimensional problems, and discuss two areas of current research, performing smooth reconstructions on unstructured grids, and adjoint error correction when there is a shock in the underlying flow solution. The paper begins with a presentation of the linear theory, and its application to the 2D Poisson equation, on both structured and unstructured grids. It continues with the nonlinear theory, including the complications introduced by boundary conditions and boundary integrals. The nonlinear applications include Burgers equations and a modified form of the 2D Euler equations. In each case the order of accuracy of output functionals is doubled through the use of adjoint error correction. The difficulty of adjoint error correction with a shock is then discussed before making some final conclusions.

2 Linear analysis

2.1 Adjoint error correction

The explanation of the linear theory with homogeneous boundary conditions follows that given in [14], which provides additional background on the use of adjoint error correction in algebraic applications.

Let u be the solution of the linear differential equation

$$Lu = f\,,$$

on some domain Ω, subject to homogeneous boundary conditions for which the problem is well-posed when $f \in L_2(\Omega)$ (meaning that f is a square-integrable function).

The adjoint differential operator L^* and associated homogeneous boundary conditions are defined by the identity

$$(v, Lu) = (L^* v, u)\,, \tag{1}$$

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

$$(v, Lu) \equiv \int_\Omega v^T Lu \;\mathrm{d}V\,,$$

allowing for the possibility that u, and hence v, may be a vector function rather than just a scalar.

The appropriate definition for L^* can be constructed by integration by parts, starting from (v, Lu), until all of the derivatives are acting on v rather than u. In the process, the adjoint boundary conditions come from the requirement that the boundary terms that arise from the integration by parts must be zero. Examples of this will be given later.

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.

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

Suppose that u_h and v_h are approximations to u and v, respectively, and satisfy the homogeneous boundary conditions. The subscript h indicates that the approximate solutions are derived from a numerical computation 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 simply use the finite element solutions themselves, or one could again use interpolation through nodal values and thereby obtain approximate solutions that are smoother than the finite element solutions.

It is assumed that u_h and v_h are sufficiently smooth that Lu_h and $L^* v_h$ lie in $L_2(\Omega)$. If u_h and v_h were equal to u and v, then the *residual errors* $Lu_h - f$ and $L^* v_h - g$ would be zero. Thus, the magnitude of the residual errors is 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:

$$\begin{aligned}(g, u) &= (g, u_h) - \left(L^* v_h, u_h - u\right) + \left(L^* v_h - g, u_h - u\right)\\ &= (g, u_h) - (v_h, L(u_h - u)) + \left(L^*(v_h - v), u_h - u\right)\\ &= (g, u_h) - (v_h, Lu_h - f) + (v_h - v, L(u_h - u))\,. \end{aligned} \tag{2}$$

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 $Lu_h - f$ 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 $Lu_h - f = L(u_h - u)$ is of the same order of magnitude as $u_h - u$ 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. For example, if the solution errors $u_h - u$ and $v_h - v$ are both $O(h^p)$ then the error in the functional is $O(h^{2p})$.

Furthermore, the remaining error term can be expressed as

$$\begin{aligned}(v_h - v, L(u_h - u)) &= \left(v_h - v, L\,L^{-1}\,(Lu_h - f)\right)\\ &= \left(L^*\,(v_h - v)\,, L^{-1}\,(Lu_h - f)\right)\\ &= \left(L^* v_h - g, L^{-1}\,(Lu_h - f)\right)\,.\end{aligned}$$

This has the computable *a posteriori* bound

$$\left\|L^{-1}\right\|\,\left\|Lu_h - f\right\|\,\left\|L^* v_h - g\right\|\,.$$

The problem with this bound is obtaining a value for the operator norm $\|L^{-1}\|$. This can be calculated analytically in the simplest cases, but for harder problems it may be necessary to estimate it numerically.

If the approximate solutions u_h and v_h are the finite element solutions from a Galerkin finite element discretisation, then the correction term

$$(v_h, Lu_h - f)$$

is automatically zero, due to the requirement that the finite element residual is orthogonal to all members of the finite element space [24]. Thus, the Galerkin finite element method gives naturally superconvergent estimates for integral outputs, in the sense that a single order of accuracy improvement in the solution, through increasing the degree of the polynomials in the finite element space, leads to two orders of accuracy improvement in the value of the functional.

However, there is usually a loss of accuracy because of a lack of smoothness in the finite element solution. Typically, if the solution errors are $O(h^p)$, then the residual error $Lu_h - f$ is $O(h^{p-m})$ where m is the degree of the differential operator, the degree of the highest derivative in the operator. Hence, the remaining error in the functional is $O(h^{2p-m})$.

If one takes the finite element solution and reconstructs smoother solutions u_h and v_h, then there is the possibility of recovering $O(h^{2p})$ accuracy for the functional, at the cost of carrying out an adjoint calculation to evaluate the adjoint error correction. This will be demonstrated in the following example.

2.2 2D Poisson equation on structured grids

Consider 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, and the adjoint identity is easily verified,

$$\int_\Omega v\,\nabla^2 u\ \mathrm{d}A = -\int_\Omega \nabla v \cdot \nabla u\ \mathrm{d}A = \int_\Omega \nabla^2 v\ u\ \mathrm{d}A\,.$$

For this example, the equations are approximated using a Galerkin finite element method with piecewise bilinear elements on a uniform Cartesian grid. Finite element error analysis reveals that the solution error for the primal problem, and the error in the computed functional using the finite element solution are both $O(h^2)$.

However, we can obtain an improved value for the functional by first using bi-cubic spline interpolation through the computed nodal values to construct an improved approximate solution $u_h(x,y)$ with an error whose value and gradient are both $O(h^2)$ [19]. Using a similarly reconstructed approximate adjoint solution $v_h(x,y)$, one can then compute the adjoint error correction term resulting in a corrected functional whose accuracy is $O(h^4)$.

In the numerical implementation, 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 1 shows the results obtained for the functions

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

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

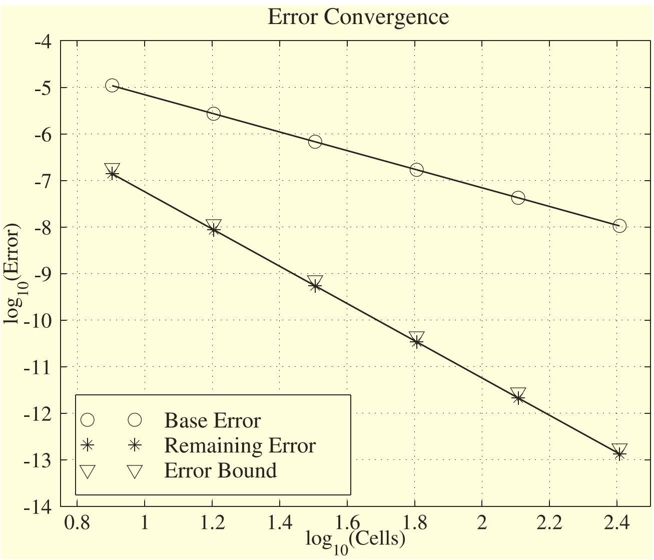

Fig. 1. Error in output integral from 2D Poisson equation on structured grids, with and without adjoint error correction. Superimposed lines have slope -2 and -4

2.3 2D Poisson equation on unstructured grids

With unstructured grids, the problem is how to construct a smooth approximation u_h given a finite element solution U_h. The aim is that the smooth reconstruction should have the same L_2 accuracy as the underlying finite element solution, but the H_1 error, being a weighted combination of the error in the solution and its gradient, should have an improved order of accuracy so that the adjoint correction will produce an output functional with an improved order of accuracy.

It can be shown that a one-dimensional cubic spline $u_h(x)$ minimises the "spline energy" $\int (u_h'')^2\,\mathrm{d}x$ subject to satisfying the specified knot conditions $u_h(x_j) = u(x_j)$, and appropriate end conditions.

Building on this idea, it seems a natural extension to define a 2D unstructured grid reconstruction by minimising

$$\iint (\Delta u_h)^2 + h^{-s}\,(u_h - U_h)^2\ \ \mathrm{d}A\,.$$

The first term in the integral ensures that u_h is smooth, the second term that it does not deviate too significantly from the finite element solution. The minimisation gives the Euler–Lagrange equation

$$h^s\,\Delta^2 u_h + u_h = U_h\,. \tag{3}$$

The issue now is the choice of the exponent s. Suppose that U_h is the piecewise linear solution to the same 2D Poisson equation on an unstructured triangular grid such as that shown in Fig. 2. The L_2 error in U_h is $O(h^2)$ but the piecewise constant gradient gives a first order H_1 error. Choosing $s \ge 2$ ensures that the L_2 error in u_h is still $O(h^2)$. Within this range, a lower value for s will provide more smoothing, so $s=2$ as the choice most likely to make the H_1 error $O(h^2)$. Despite this, however, the best that we are currently able to prove for the Poisson equation on a periodic domain [15], is that the choice $s = 8/5$ leads to a reconstructed solution u_h whose H_1 error is $O(h^{8/5})$.

The numerical results in Figs. 3 and 4 use the smoothing coefficient $0.01h^2$. The reconstruction p.d.e. is approximated with quintic Argyris finite elements, and solved using the FEMLAB package [9]. Figure 3 shows the improvement in

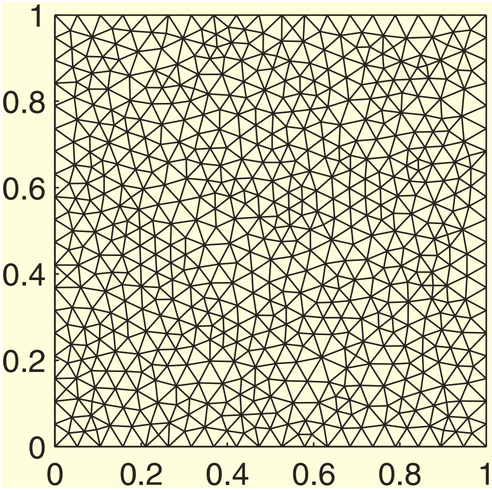

Fig. 2. One of the unstructured grids used for the Poisson equation approximation and reconstruction

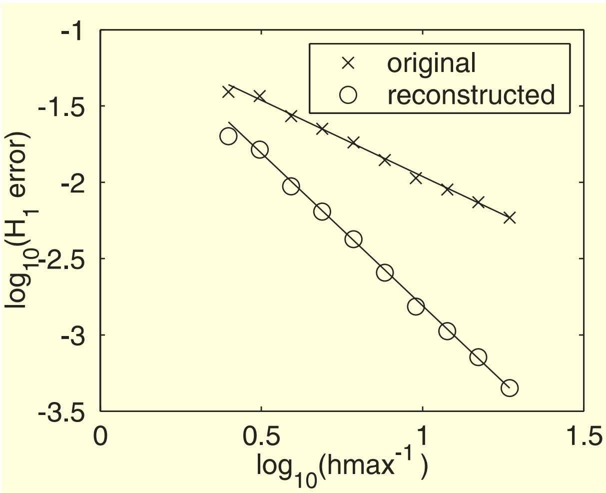

Fig. 3. H_1 error in approximate 2D Poisson solution on unstructured grids, with and without smooth reconstruction. Superimposed lines have slope -1 and -2

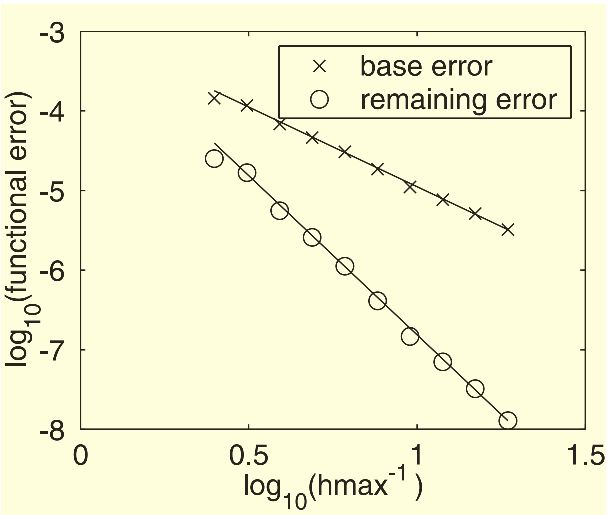

Fig. 4. Error in output integral from 2D Poisson equation on unstructured grids with smooth reconstruction. Superimposed lines have slope -2 and -4

the H_1 error. The original piecewise linear finite element solution has an H_1 error which is $O(h)$, whereas the Argyris reconstruction is $O(h^2)$. Figure 4 shows the corresponding improvement in the output functional through using adjoint error correction. As expected, it is $O(h^2)$ before correction, and $O(h^4)$ afterwards.

It should be noted that solving the reconstruction equation with its bi-quadratic smoothing is quite an expensive procedure. For the application here it is not cost-effective; it would be much more efficient to use quadratic elements for the original finite element discretisation. However, it could well be a very efficient approach for applications involving the nonlinear systems of p.d.e.'s. For such applications, the cost of the iterative solution of the nonlinear discrete equations may far exceed the cost of the symmetric positive-definite scalar reconstruction equations for each component of the solution.

3 Nonlinear analysis

3.1 Adjoint error correction

Let u be the solution of the nonlinear differential equation

$$N(u) = 0\,,$$

in the domain Ω, 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 to be the Fréchet derivatives of N and D, respectively,

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

$$B_u\,\tilde{u} \equiv \lim_{\varepsilon\to 0} \frac{D(u+\varepsilon\tilde{u}) - D(u)}{\varepsilon}\,.$$

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

$$\lim_{\varepsilon\to 0} \frac{J\,(u+\varepsilon\tilde{u}) - J(u)}{\varepsilon} = (g(u), \tilde{u}) + (h, C_u\tilde{u})_{\partial\Omega}\ .$$

Here the dimension of the operator C_u (which may be differential) is required to equal the dimension of the adjoint boundary operator B_u^*, to be defined shortly.

The corresponding linear adjoint problem is

$$L_u^* v = g(u)$$

in Ω, 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

$$(v, L_u\tilde{u}) + \left(C_u^* v, B_u\tilde{u}\right)_{\partial\Omega} = \left(L_u^* v, \tilde{u}\right) + \left(B_u^* v, C_u\tilde{u}\right)_{\partial\Omega}\ , \quad (4)$$

for all $\tilde{u}$, v.

We now consider approximate solutions u_h, v_h of the primal and dual problems, respectively. The analysis will use the quantities

$$L^*_{u_h} v_h\,, \quad B^*_{u_h} v_h\,, \quad C^*_{u_h} v_h\,.$$

Note that these can be evaluated since u_h and v_h are both known, whereas we would not be able to evaluate the Fréchet derivatives based on the unknown analytic solution u.

The analysis also requires averaged Fréchet derivatives defined by

$$\overline{L}_{(u,u_h)} = \int_0^1 L|_{u+\theta(u_h-u)}\, \mathrm{d}\theta\,,$$

$$\overline{B}_{(u,u_h)} = \int_0^1 B|_{u+\theta(u_h-u)}\, \mathrm{d}\theta\,,$$

$$\overline{C}_{(u,u_h)} = \int_0^1 C|_{u+\theta(u_h-u)}\, \mathrm{d}\theta\,,$$

$$\overline{g}(u,u_h) = \int_0^1 g(u+\theta(u_h-u))\, \mathrm{d}\theta\,,$$

so that,

$$N(u_h) - N(u) = \overline{L}_{(u,u_h)}\,(u_h-u)\,,$$
$$D(u_h) - D(u) = \overline{B}_{(u,u_h)}\,(u_h-u)\,,$$
$$J(u_h) - J(u) = \left(\overline{g}(u,u_h), u_h-u\right) + \left(h, \overline{C}_{(u,u_h)}(u_h-u)\right)_{\partial\Omega}.$$

We now obtain the following:

$$\begin{aligned}
&J(u_h) - J(u)\\
&= \left(\overline{g}(u,u_h), u_h-u\right) + \left(h, \overline{C}_{(u,u_h)}(u_h-u)\right)_{\partial\Omega}\\
&= \left(L^*_{u_h}v_h, u_h-u\right) + \left(B^*_{u_h}v_h, C_{u_h}(u_h-u)\right)_{\partial\Omega}\\
&\quad - \left(L^*_{u_h}v_h - \overline{g}(u,u_h), u_h-u\right)\\
&\quad - \left(h, \left(C_{u_h} - \overline{C}_{(u,u_h)}\right)(u_h-u)\right)_{\partial\Omega}\\
&\quad - \left(B^*_{u_h}v_h - h, C_{u_h}(u_h-u)\right)_{\partial\Omega}\\
&= \left(v_h, L_{u_h}(u_h-u)\right) + \left(C^*_{u_h}v_h, B_{u_h}(u_h-u)\right)_{\partial\Omega}\\
&\quad - \left(L^*_{u_h}v_h - \overline{g}(u,u_h), u_h-u\right)\\
&\quad - \left(h, \left(C_{u_h} - \overline{C}_{(u,u_h)}\right)(u_h-u)\right)_{\partial\Omega}\\
&\quad - \left(B^*_{u_h}v_h - h, C_{u_h}(u_h-u)\right)_{\partial\Omega}\\
&= \left(v_h, \overline{L}_{(u,u_h)}(u_h-u)\right) + \left(C^*_{u_h}v_h, \overline{B}_{(u,u_h)}(u_h-u)\right)_{\partial\Omega}\\
&\quad - \left(L^*_{u_h}v_h - \overline{g}(u,u_h), u_h-u\right)\\
&\quad - \left(h, \left(C_{u_h} - \overline{C}_{(u,u_h)}\right)(u_h-u)\right)_{\partial\Omega}\\
&\quad - \left(B^*_{u_h}v_h - h, C_{u_h}(u_h-u)\right)_{\partial\Omega}\\
&\quad + \left(v_h, \left(L_{u_h} - \overline{L}_{(u,u_h)}\right)(u_h-u)\right)\\
&\quad + \left(C^*_{u_h}v_h, \left(B_{u_h} - \overline{B}_{(u,u_h)}\right)(u_h-u)\right)_{\partial\Omega}\\
&= \left(v_h, N(u_h)\right) + \left(C^*_{u_h}v_h, D(u_h)\right)_{\partial\Omega}\\
&\quad - \left(L^*_{u_h}v_h - \overline{g}(u,u_h), u_h-u\right)\\
&\quad - \left(h, \left(C_{u_h} - \overline{C}_{(u,u_h)}\right)(u_h-u)\right)_{\partial\Omega}\\
&\quad - \left(B^*_{u_h}v_h - h, C_{u_h}(u_h-u)\right)_{\partial\Omega}\\
&\quad + \left(v_h, \left(L_{u_h} - \overline{L}_{(u,u_h)}\right)(u_h-u)\right)\\
&\quad + \left(C^*_{u_h}v_h, \left(B_{u_h} - \overline{B}_{(u,u_h)}\right)(u_h-u)\right)_{\partial\Omega}\,.
\end{aligned}$$

In the final result, the first line is the adjoint correction term taking into account the residual errors in satisfying both the p.d.e. and the boundary conditions. The other lines are the remaining errors, which include the consequences of nonlinearity in L, B, C and g as well as residual errors in approximating the adjoint problem.

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. However, rigorous *a priori* and *a posteriori* analysis of the remaining errors is much harder than in the linear case [19] and practical *a posteriori* error bounds have yet to be obtained for the quasi-1D and 2D Euler equations.

3.2 Burgers equation

The first nonlinear test case involves Burgers equation.

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{1}{2}u^2\right) = 0\,.$$

This is to be solved on the interval $0 < x < 1$, for $0 < t < 0.3$, subject to the initial conditions

$$u(x,0) = u_0(x) \equiv -\tanh(2x-1)\,.$$

Since the value $u(x,t)$ is constant along characteristics defined by

$$\frac{\mathrm{d}x}{\mathrm{d}t} = u\,,$$

the solution along characteristics leading from the initial conditions is given implicitly by $u(x,t) = u_0(x_0)$ where x_0 is the root of the equation

$$x = x_0 + u_0(x_0)\, t\,.$$

The Dirichlet boundary conditions at $x = 0$ and $x = 1$ are chosen to be consistent with this, for the same function $u_0(x)$, so that this solution is extended to include the characteristics entering through the side boundaries, as illustrated in Fig. 5.

The functional of interest is chosen to be the integral

$$\int_0^1 u^4(x,T)\, \mathrm{d}x$$

evaluated at the final time $T = 0.3$.

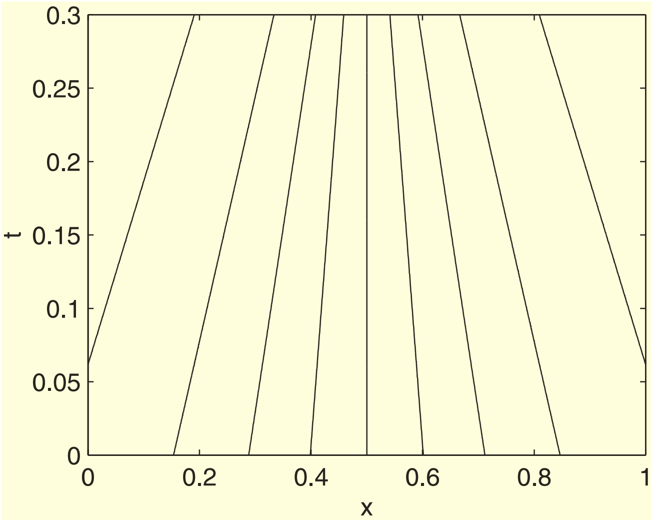

Fig. 5. Characteristics of Burgers equation testcase

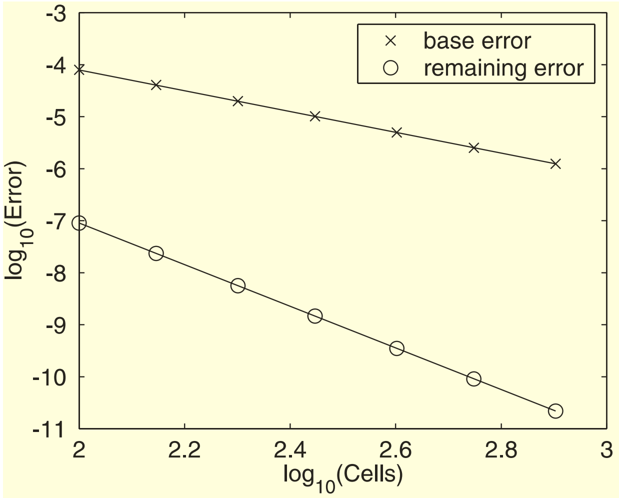

Fig. 6. Error in Burgers equation output integral, with and without adjoint error correction. Superimposed lines have slope −2 and −4

Given a smooth solution $u(x,t)$, the linearised equation is

$$\frac{\partial \tilde{u}}{\partial t} + \frac{\partial}{\partial x}(u\tilde{u}) = 0\,,$$

and the linearised output functional is

$$\int_0^1 4u^3(x,T)\tilde{u}(x,T)\ \mathrm{d}x$$

The corresponding adjoint equation is

$$\frac{\partial v}{\partial t} + u\,\frac{\partial v}{\partial x} = 0\,,$$

subject to the final conditions $v(x,T) = 4u^3(x,T)$.

After further analysis, it is found that the appropriate adjoint boundary operator is $C_u v \equiv u\,v$ on $x=0$ and $x=0$, and $C_u v \equiv v$ on $t=0$.

The original nonlinear Burgers equation and the linear adjoint equation are both approximated using the Lax–Wendroff method. This gives approximate solutions u_j^n and v_j^n at a discrete set of uniformly spaced grid points, and uniformly spaced time levels.

The reconstructed solutions u_h and v_h are defined by piecewise bilinear interpolation on each (x,t) computational cell. Because of the second order accuracy of the Lax–Wendroff discretisation, this gives approximate solutions which are second order accurate. However, the space and time derivatives are only first order accurate, so the residual error from the nonlinear equation will be only first order, and it would appear therefore that the remaining error after adjoint error correction will be third order accurate.

Despite this, the results in Fig. 6 show the adjoint error correction yields fourth order accuracy. A similar result has been obtained previously for the steady quasi-1D Euler equations, with piecewise linear interpolation of a second order solution [19]. In that case, it was proved that the remaining error was indeed fourth order because the leading order component of the first order residual error was orthogonal to the leading order component of the adjoint solution error. A similar explanation must hold for the current test case as well.

One key feature of this testcase was the importance of the adjoint correction term associated with the boundary conditions. The piecewise linear interpolation on the boundaries gives a second order error in satisfying the Dirichlet boundary conditions. In the absence of the adjoint boundary correction term, this leads to a second order error in the functional, so it is vital to include this term in the correction.

3.3 Modified 2D Euler equations

The second nonlinear testcase is based on the 2D Euler equations governing the inviscid flow of a compressible, ideal gas. These can be written as

$$\frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0$$

where

$$F = \begin{pmatrix} \rho q_x \\ \rho q_x^2 + p \\ \rho q_x q_y \\ \rho q_x H \end{pmatrix}, \quad G = \begin{pmatrix} \rho q_y \\ \rho q_x q_y \\ \rho q_y^2 + p \\ \rho q_y H \end{pmatrix},$$

with ρ being the density, q_x, q_y the velocity components, p the pressure, and H the stagnation enthalpy define by

$$H = \frac{\gamma}{\gamma-1}\frac{p}{\rho} + \frac{1}{2}\left(q_x^2 + q_y^2\right)\,.$$

One difficulty with using the 2D Euler equations is the lack of suitable testcases for which an analytic solution is known. This difficulty is avoided here by modifying the Euler equations so that a known $u \equiv (\rho, q_x, q_y, p)^T$ is a solution of the modified equations [21]. The testcase uses a 2D duct with a very mild variation in duct height, as shown in Fig. 7. The 2D solution is constructed from the analytic solution to

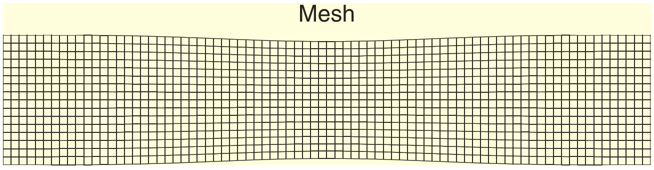

Fig. 7. Grid for modified 2D Euler equation testcase

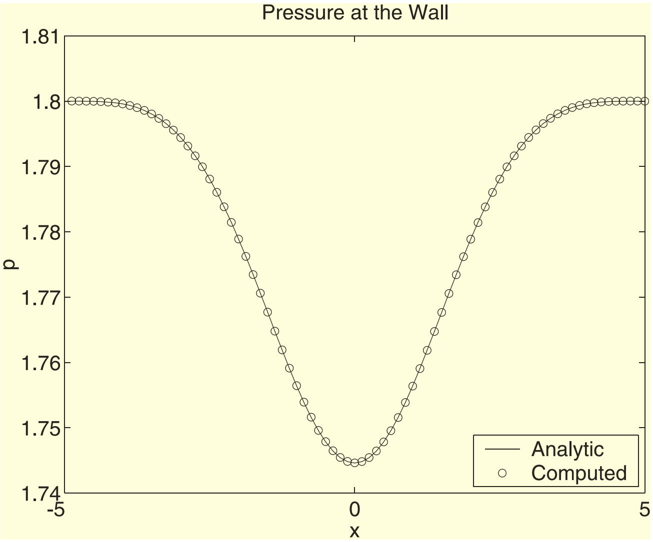

Fig. 8. Analytic and computed surface pressure distribution

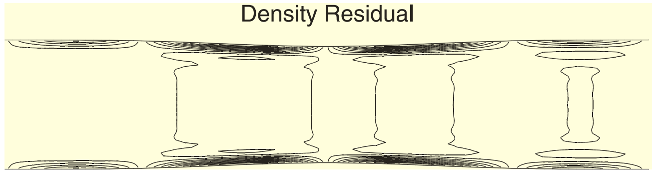

Fig. 9. Density equation residual error for reconstructed solution

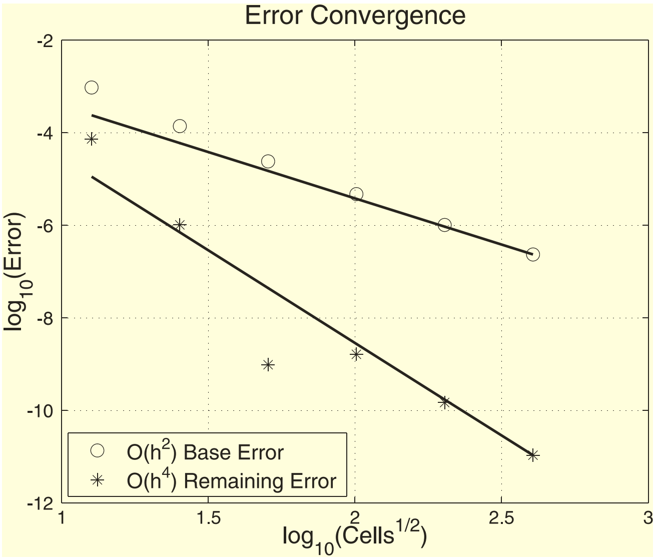

Fig. 10. Error in 2D Euler surface pressure integral, with and without adjoint error correction. Superimposed lines have slope −2 and −4

the quasi-1D Euler equations

$$\frac{\partial}{\partial x}\begin{pmatrix} A\rho q_x \\ A\rho q_x^2 \\ A\rho q_x H \end{pmatrix} + A\frac{\partial}{\partial x}\begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix} = 0\,,$$

where $A(x)$ is the duct height, and the stagnation enthalpy H depends solely on ρ, q_x, p, each of which are functions only of x. q_y is then defined to vary linearly across the duct, satisfying the flow tangency boundary condition on either side.

This constructed solution is not an exact solution of the 2D Euler equations, but instead is the exact solution of an equation

$$\frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S\,,$$

for an appropriately defined source term $S(x, y)$. This then is the modified form of the 2D Euler equations which is used in this testcase. In practice, the magnitude of $S(x, y)$ is extremely small, so it is thought this is a fair test of the applicability of the adjoint error correction methodology to the 2D Euler equations.

The nonlinear equations and the corresponding linear adjoint equations are approximated using a variant of Jameson's SYN82 CFD code. This uses second order central differencing with a scalar numerical dissipation on a cell-centred grid [21]. The values at dummy points outside the computational domain are computed by second order extrapolation, and then the approximate solutions u_h and v_h defined by bi-cubic spline interpolation. As usual, all integrals are approximated by Gauss quadrature, use 3×3 points in each cell for the 2D integrals.

It is observed that the residual error, obtained by substituting the approximate solutions into the modified Euler equations, has second order magnitude over most of the domain, but it is first order in an area of size $O(h)$ adjacent to the upper and lower walls. This residual boundary layer is clearly seen in Fig. 9. Since it is expected that the nonlinear and adjoint solutions will be second order accurate throughout the domain, this leads one to expect that the remaining error will be $O(h^4)$. The results presented in Fig. 10 confirm that the adjoint error correction yields fourth order accuracy, whereas the uncorrected results are only second order accurate. The remaining error data point which looks anomalous is due to a change in the sign of the error. Since we are plotting the logarithm of the magnitude of the error, it produces this unusually low value before then settling into its asymptotic behaviour demonstrating fourth order convergence.

3.4 Quasi-1D flow with a shock

Flows with shocks pose a major challenge to both adjoint calculations and adjoint error correction. The correct formulation of the inviscid adjoint equations has to consider linearised perturbations to the shock location. Using this approach, Giles & Pierce showed that the adjoint equations corresponding to the steady quasi-1D Euler equations require the specification of an interior boundary condition at the shock location, and derived closed form analytic solutions [13]. Numerical results using either the "continuous" approach (approximating the analytic 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 [11].

Ulbrich has recently developed the analytic formulation of the adjoint equations for unsteady 1D equations with scalar fluxes, such as Burgers equations [27, 28]. However, numerical results by Giles [10] indicate that the "discrete" adjoint approach does not necessarily yield convergent results, unless one uses numerical smoothing which leads to an increasing smoothing of the shock. It seems likely that there will be similar problems with the convergence of solutions to the steady adjoint 2D Euler equations, although such convergence errors may be very small for weak shocks.

In addition to these problems in calculating adjoint solutions, there is the further problem for adjoint error correction that any reconstructed solution which is continuous must necessarily have a residual error at the shock location which does not tend to zero as the grid is refined. Even worse, it is likely to be inversely proportional to the grid spacing and therefore increase without bound. Also, the local error in the solution will be $O(1)$. This undermines the whole basis for the adjoint error correction which assumes small errors, allowing a linearised treatment which leads naturally to the linear adjoint flow equations.

It appears the only solution to this problem is to approach it from the perspective of well-resolved viscous shocks. Let u_ε be the solution of the "viscous" quasi-1D Euler equations

$$\frac{\partial}{\partial x}\begin{pmatrix} A\rho q_x \\ A\rho q_x^2 \\ A\rho q_x H \end{pmatrix} + A\frac{\partial}{\partial x}\begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix} = A\varepsilon\frac{\partial^2}{\partial x^2}\begin{pmatrix} \rho \\ q_x \\ p \end{pmatrix}$$

In the limit $\varepsilon \to 0$, u_ε will converge to the discontinuous inviscid solution u at every point other than at the shock point. Furthermore, if $J(u)$ represents an output functional such as the integral of the pressure, then a matched inner and outer asymptotic analysis reveals that

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

for some constant a, and accordingly,

$$J(u) = J(u_\varepsilon) - \varepsilon\frac{\mathrm{d}}{\mathrm{d}\varepsilon}J(u_\varepsilon) + O\big(\varepsilon^2\big)\,.$$

This gives a method for correcting for the functional error introduced by the viscosity ε. Furthermore, the quantity $\frac{\mathrm{d}}{\mathrm{d}\varepsilon}J(u_\varepsilon)$ can be evaluated by the adjoint approach since by definition the gradient with respect to ε is based on infinitesimal perturbations to the viscous solution.

This gives half of the approach to handling shocks. The other half involves a discrete approximation $u_{\varepsilon,h}$ to the viscous solution. If the discrete approximation resolves the viscous shock sufficiently well, the difference $J(u_\varepsilon) - J(u_{\varepsilon,h})$ can be estimated by the adjoint error correction method, and combined with the viscous correction to produce a superconvergent approximation to the true inviscid functional.

In the numerical results presented in Fig. 11, $\varepsilon = N^{-2}$ where N is the number of grid points. Adaptive grid refinement is used so that the shock region has a fixed fraction of the grid points, giving a very well-resolved shock as N increases.

The error in the viscous error correction will be $O(\varepsilon^2) = O(N^{-4})$. The numerical discretisation is second order accurate, and cubic spline interpolation is used as usual, so it was hoped that the error remaining after the adjoint error correction, correcting for both the viscous and discretisation errors, would be $O(N^{-4})$. However, the results in Fig. 12 show the remaining error after adjoint error correction is $O(N^{-3.5})$.

This is a substantial improvement on the second order accuracy of the uncorrected functional, but not the fourth order accuracy which was hoped for. It is thought the explanation for this is that the $O(N^{-2})$ residual error upstream and downstream of the shock leads to an $O(N^{-2})$ displacement in the shock position. The shock width is also $O(N^{-2})$, so this shock displacement leads to a solution error which is $O(1)$ within the shock. Even though this error is over an extremely small region of size $O(N^{-2})$, it invalidates the linearisation basis for the adjoint error correction, preventing the $O(N^{-4})$ convergence.

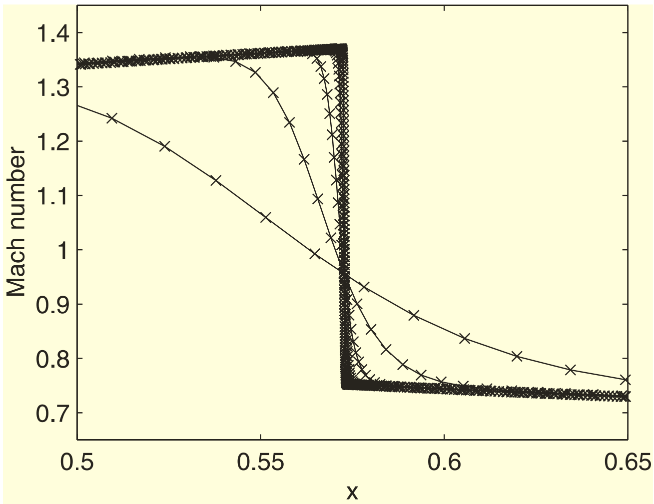

Fig. 11. Quasi-1D Mach number distributions on a sequence of grids with adaptive resolution of the shock

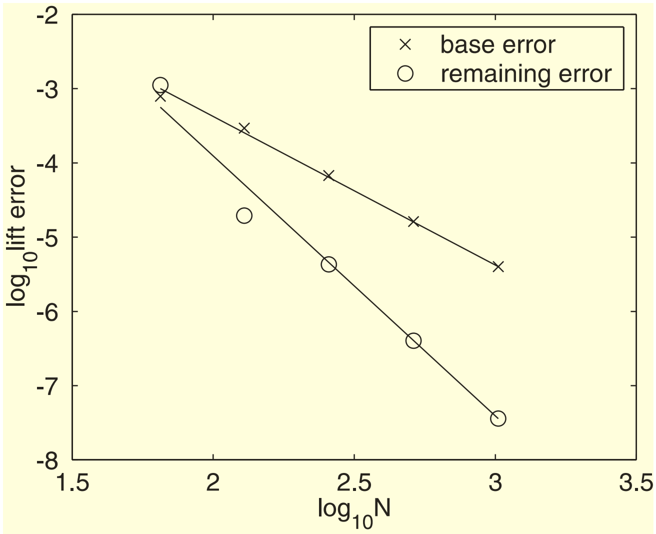

Fig. 12. Error in the quasi-1D pressure integral, with and without adjoint error correction. Superimposed lines have slope −2 and −3.5

Currently, the reason for the $O(N^{-3.5})$ convergence is not understood. Research into this is continuing, and it is still hoped to obtain fourth order convergence. This may require the inclusion of deforming grids into the adjoint error analysis, because in practice the $O(N^{-2})$ shock displacement would lead to a corresponding displacement of the grid points, because of the grid adaptation, and so there would not be an $O(1)$ perturbation to the flow values at the grid points. Indeed, it is more likely that the perturbation would be $O(N^{-2})$, fully allowing accurate adjoint error correction.

4 Conclusions

This paper has reviewed the theory behind adjoint error correction, and presented results showing the progress in applying it to a range of two-dimensional linear and nonlinear applications.

The two main challenges being addressed currently are the reconstruction of smooth approximate solutions on unstructured grids, and error correction when there are shocks. Initial results for the unstructured grid reconstruction have been obtained through the solution of a p.d.e. with biharmonic smoothing. The results provide the anticipated improvement in the output functional, doubling its order of convergence, but the computational cost is very significant. If alternative, cheaper reconstruction methods cannot be developed, this approach will only be worthwhile in cases in which the solution of the primal and adjoint equations is itself extremely expensive.

For the error correction with shocks, the key is the use of discrete solutions with a well-resolved viscous shock. The adjoint error correction is then split into two parts, one dealing with the consequences of the viscosity and the other the effect of the numerical discretisation. The initial results are very promising, with a convergence order of 3.5, but further research is needed to understand the origin of this convergence rate, and to modify the procedure to achieve the fourth order convergence being sought.

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