INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS
Int. J. Numer. Meth. Fluids 2005; **47**:987–993
Published online 20 January 2005 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/fld.922

On the adjoint solution of the quasi-1D Euler equations: the effect of boundary conditions and the numerical flux function

G. F. Duivesteijn*,†, H. Bijl, B. Koren and E. H. van Brummelen

Faculty of Aerospace Engineering, Delft University of Technology, P.O. Box 5058, 2600 GB Delft, The Netherlands

SUMMARY

This work compares a numerical and analytical adjoint equation method with respect to boundary condition treatments applied to the quasi-1D Euler equations. The effect of strong and weak boundary conditions and the effect of flux evaluators on the numerical adjoint solution near the boundaries are discussed. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: adjoint equation; boundary conditions; numerical flux function; equations

1. INTRODUCTION

For efficient computation of large-scale fluid flow problems, an efficient error estimation and grid adaptation algorithm is desirable. Traditional error estimation or grid adaptation may not suffice, since these may be insufficiently related to relevant engineering quantities. The dual formulation can be used as an efficient *a posteriori* error estimation in the quantity of interest. However, derivation of the dual problem, especially the accompanying boundary conditions, is not a trivial task.

Two ways of formulating the dual problem exist: analytical [1, 2] and numerical [3, 4]. This paper gives an outline of the boundary-condition derivation for both methods. For the analytical method, carefully crafted boundary conditions are needed. For the numerical method, imposing strong or weak boundary conditions to the primal problem has a great influence on the implicitly given boundary conditions for the numerical dual problem. Also, the effect of

*Correspondence to: G. F. Duivesteijn, Faculty of Aerospace Engineering, Delft University of Technology, P.O. Box 5058, 2600 GB Delft, The Netherlands.
†E-mail: g.f.duivesteijn@lr.tudelft.nl

Contract/grant sponsor: Technology Foundation STW
Contract/grant sponsor: Applied Science Division of NWO
Contract/grant sponsor: The Technology Program of the Ministry of Economic Affairs

Received 27 April 2004
Revised 9 December 2004
Accepted 9 December 2004

the numerical flux evaluators of the primal problem on the adjoint solution at the boundaries are discussed.

2. FLOW EQUATIONS AND OUTPUT FUNCTIONAL

A simple test problem was chosen. A subsonic inviscid, compressible gas flow through a convergent–divergent channel is considered. Let $q = (\rho, u, p)^{\mathrm{T}}$ be the solution of the quasi-1D Euler equations:

$$\oint_{\partial\Omega} AF(q)\,\mathrm{d}\partial\Omega - \int_{\Omega} \frac{\mathrm{d}A}{\mathrm{d}x} J(q)\,\mathrm{d}\Omega = 0 \tag{1}$$

with

$$F(q) = \begin{pmatrix} \rho u \\ (\rho u^2 + p) \\ \rho u\left(E + \frac{p}{\rho}\right) \end{pmatrix}, \quad J(q) = \begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix} \tag{2}$$

where ρ, u, p, E, Ω and $\partial\Omega$ are defined as the density, velocity, pressure, total energy, inner domain $x \in \langle -1, 1\rangle$ and the boundary of the domain $x = -1$ and 1, respectively. A denotes the height of the channel and is defined as

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

As boundary conditions, we define typical engineering boundary conditions: $\rho = \rho_{\mathrm{in}}$, $u = u_{\mathrm{in}}$ at inflow and $p = p_{\mathrm{out}}$ at outflow. Extrapolation of Riemann invariants enables us to find the unknown states at the boundaries. The output functional considered is

$$I = \int_{-1}^{1} p(q)\,\mathrm{d}\Omega \tag{3}$$

where $x = -1$ and 1 are the co-ordinates of the inlet and outlet, respectively.

For solving the primal problem, a structured-grid, cell-centred finite-volume solver is applied. We consider Lax and Osher flux evaluators at the cell faces. The steady-state solution of the non-linear system of equations is obtained by a global Newton iteration method.

3. ANALYTICAL ADJOINT APPROACH

Following Reference [2], the analytical adjoint equations are derived as follows: First, the quasi-1D Euler equations are linearized:

$$Lq' = \frac{\partial}{\partial x}\left(\frac{\partial AF(q)}{\partial q} q'\right) - \frac{\mathrm{d}A}{\mathrm{d}x}\frac{\partial J(q)}{\partial q} q' = r' \tag{4}$$

where q' is a small solution perturbation. The change in the output functional due to small perturbations in the flow solution can be written as

$$I' = \int_\Omega \frac{\partial p}{\partial q} q' \, \mathrm{d}x \tag{5}$$

The influence of the change in solution on the functional can be determined by the adjoint equation. Using the continuous Lagrangian multiplier v, where $(Lq' - r') = 0$, the augmented Lagrangian functional becomes:

$$I' = \int_\Omega \frac{\partial p}{\partial q} q' \, \mathrm{d}x - \int_\Omega v(Lq' - r') \, \mathrm{d}x \tag{6}$$

After integration by parts, we obtain

$$I' = \int v \cdot r' \, \mathrm{d}x - \int_\Omega \left(L^* v - \frac{\partial p}{\partial q} \right) q' \, \mathrm{d}x - \left[v \frac{\partial AF(q)}{\partial q} q' \right]_{-1}^{1} \tag{7}$$

where the adjoint operator L^* is defined as

$$L^* v \equiv - \left[\frac{\partial AF(q)}{\partial q} \right]^{\mathrm{T}} v_x - \left[\frac{\mathrm{d}A}{\mathrm{d}x} \frac{\partial J(q)}{\partial q} \right]^{\mathrm{T}} v \tag{8}$$

To remove the dependence of q' in Equation (7), v must satisfy the adjoint equation

$$L^* v = \frac{\partial p}{\partial q} \tag{9}$$

and the boundary term must satisfy

$$q'^{\mathrm{T}} \left[\frac{\partial AF(q)}{\partial q} \right]^{\mathrm{T}} v \bigg|_{-1}^{1} = 0 \tag{10}$$

Equation (9) can be written by using Jacobians based on the non-conservative flow variables $q = (\rho, u, p)^{\mathrm{T}}$, so that the adjoint equation becomes

$$A \begin{pmatrix} q_2 & q_2^2 & \frac{1}{2} q_2^3 \\ q_1 & 2q_1 q_2 & \frac{\gamma}{\gamma-1} q_3 + \frac{3}{2} q_1 q_2^2 \\ 0 & 1 & \frac{\gamma}{\gamma-1} q_2 \end{pmatrix} \frac{\mathrm{d}v}{\mathrm{d}x} = - \begin{pmatrix} 0 \\ 0 \\ 1 + \frac{\mathrm{d}A}{\mathrm{d}x} v_2 \end{pmatrix} \tag{11}$$

For this system of adjoint ordinary-differential equations, complementary boundary conditions have to be defined. In this paper, the primal boundary conditions have been chosen as $\rho = \rho_{\mathrm{in}}$, $u = u_{\mathrm{in}}$ at inflow and $p = p_{\mathrm{out}}$ at outflow. Derivation of associated adjoint boundary conditions is illustrated below.

Considering small perturbations in the whole domain, the perturbed solutions have to obey the boundary conditions. Hence, at the boundaries, perturbations in the prescribed states vanish. This yields the following conditions on the perturbations:

$$W_1 q' = 0, \quad x = -1 \tag{12}$$

$$W_2 q' = 0, \quad x = 1 \tag{13}$$

where

$$W_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad W_2 = (0 \quad 0 \quad 1) \tag{14}$$

This result leaves us with one degree of freedom at inflow and two degrees of freedom at outflow. In other words, we are looking for the null spaces to find the missing vectors in compliance with Equation (10). At $x = -1$, this yields

$$\mathrm{Null}(W_1)^{\mathrm{T}}[AF'(q)]^{\mathrm{T}} v_{\mathrm{in}} = 0 \tag{15}$$

The rank of W_1 is 2, hence, its kernel has dimension 1

$$\mathrm{Null}(W_1) = \mathrm{Span}\{(0 \quad 0 \quad 1)^{\mathrm{T}}\} \tag{16}$$

At $x = 1$, it holds that

$$\mathrm{Null}(W_2)^{\mathrm{T}}[AF'(q)]^{\mathrm{T}} v_{\mathrm{out}} = 0 \tag{17}$$

The rank of W_2 is 1 and the kernel has dimension 2

$$\mathrm{Null}(w_2) = \mathrm{Span}\{(1 \quad 0 \quad 0)^{\mathrm{T}}, \quad (0 \quad 1 \quad 0)^{\mathrm{T}}\} \tag{18}$$

Multiplying the null vectors with the Jacobian gives the following adjoint boundary conditions:

$$v_2 + \frac{\gamma}{\gamma - 1} q_2 v_3 = 0, \quad x = -1 \tag{19}$$

$$\left.\begin{aligned} q_2 v_1 + q_2^2 v_2 + \tfrac{1}{2} q_2^3 v_3 &= 0 \\ q_1 v_1 + 2 q_1 q_2 v_2 + \left(\frac{\gamma}{\gamma - 1} q_3 + \tfrac{3}{2} q_1 q_2^2 \right) v_3 &= 0 \end{aligned}\right\}, \quad x = 1 \tag{20}$$

4. NUMERICAL ADJOINT APPROACH

Whether the residual and output functional are linearized around a given design variable [1] or around a given mesh [3], the Jacobian of the numerical residual $R_h(q_h)$, is needed in order to set up and solve the numerical adjoint equations. Assuming that the boundary conditions for the primal problem are included in the residual vector $R_h(q_h)$, the influence of the primal boundary conditions is included in the Jacobian. When taking the transposed Jacobian for computation of the adjoint solution, the adjoint boundary conditions are automatically included in the system of equations. This constitutes a great advantage of the numerical adjoint approach.

The abstract formulation $R_h(q_h) = 0$ tacitly incorporates the precise formulation of the boundary conditions and of the nonlinear flux evaluators. In the case of strong boundary conditions, the boundary conditions are imposed as constraints on the approximation of the solution, whereas for weak boundary conditions, the boundary conditions are implied by the equations and are accounted for by an appropriate choice of the boundary fluxes. It is to be noted, however, that two different formulations with nearly identical primal conditions can yield very different adjoint solutions. In our numerical experiments, the Jacobian matrix $\partial R_h(q_h)/\partial q$ is evaluated by automatic differentiation [5].

5. NUMERICAL EXPERIMENTS

5.1. Strong versus weak boundary conditions

Strong enforcement of the boundary conditions in the primal residual operator, implies corresponding restrictions for the dual solution space. However, a boundary treatment that yields the correct primal boundary conditions does not automatically yield the correct dual boundary conditions. This difficulty can be avoided by imposing the boundary conditions of the primal residual operator in weak form. Computation of the primal problem with strong boundary conditions leads to significant layers near the boundaries (Figure 1, left), whereas the layers have (almost) disappeared when using weak boundary conditions (Figure 1, right). The advantage is that no additional restrictions to the solution space are necessary and the resulting dual problem is automatically well-posed. This property facilitates implementation of the numerical adjoint method in a general purpose flow solver. The user of the software takes full advantage of adjoint based grid adaptation, without being burdened by setting up a well-posed dual problem.

5.2. Effect of flux evaluators near the boundaries

Another point of interest is the effect of the flux evaluator in the primal problem on the adjoint solution near the boundaries. In general, the numerical adjoint solution should converge to the

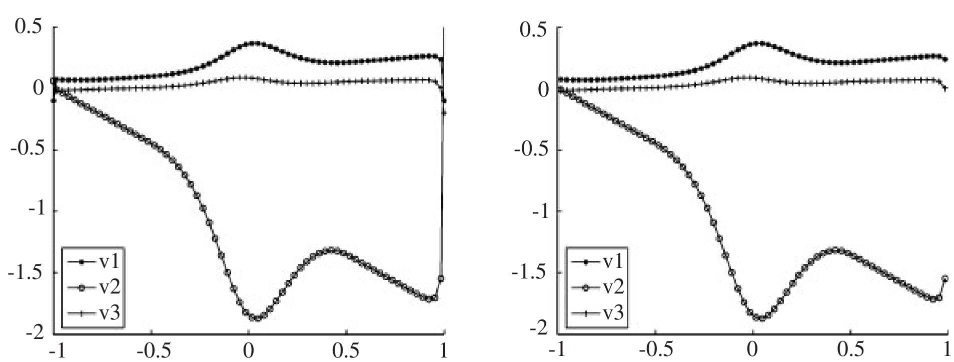

Figure 1. Numerical adjoint solution with strong boundary conditions (left) and weak boundary conditions (right) for the Lax scheme, with $h = \frac{1}{32}$.

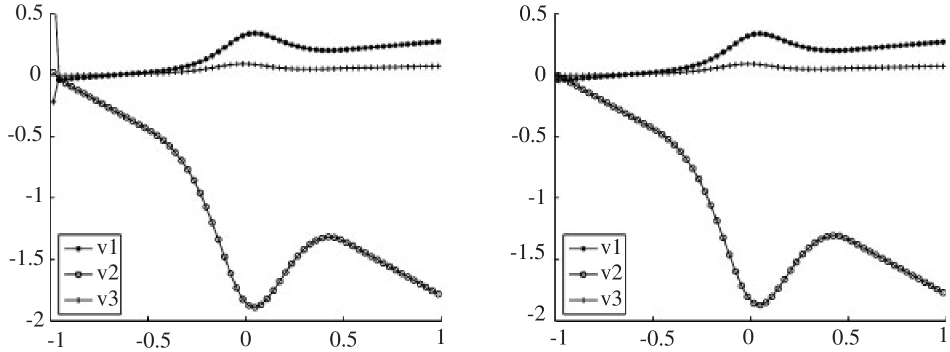

Figure 2. Numerical adjoint solution with weak boundary conditions for the Osher scheme with engineering boundary conditions (left) and Osher scheme with a half Osher path flux evaluation at the boundaries (right), $h=\frac{1}{32}$.

analytical adjoint solution when the mesh is fine enough. When looking at the same mesh and solving the primal problem with different flux evaluators, the corresponding adjoint solutions may have slightly different solutions, especially near the boundaries. Numerical experiments confirm this behaviour. The effects of flux evaluators can be divided into two effects.

The first effect concerns differences in the adjoint solutions when an adjoint variable is not constrained. For instance, as can be seen from the analytical boundary conditions, Equation (19), v_1 is a free variable at $x=-1$. When comparing the adjoint solutions from Lax (Figure 1, right) and Osher (Figure 2, left), v_1 has a different solution near $x=-1$.

The second effect concerns artifacts or layers near the boundaries. The use of non-physical interpolation techniques or flux functions that contain non-physical diffusion terms, like the Lax scheme, can yield entirely incorrect behaviour of the adjoint solution, even if they function properly for the primal solution.

The Lax diffusion term brings state variables from the exterior of the computational area into the interior, without respecting the real physics. A similar behaviour can be found for the Osher scheme when using the engineering boundary conditions $\rho_{\text{in}}, u_{\text{in}}, p_{\text{out}}$. This problem can be overcome when the flux at the boundary is replaced by an appropriate boundary flux, which respects the physics in every aspect. Figure 2 shows the Osher flux at the boundaries from the engineering boundary conditions (Figure 2, left) and the special Osher boundary flux computed by a half Osher path (Figure 2, right) [6, 7].

6. CONCLUSIONS

The main conclusions are listed below:

- In contrast to the numerical adjoint method, the analytical adjoint method requires derivation of adjoint boundary conditions.
- When using the numerical adjoint method, use of weak boundary conditions for the primal problem is advisable in order to prevent erroneous values of the dual solution near the boundaries.

- When a variable of the adjoint problem is not set by boundary conditions, the numerical adjoint solution near that boundary can be dependent on the primal flux evaluator.
- Although the primal solution shows good results, when the primal boundary conditions and/or the boundary flux evaluator does not obey the flow physics, the adjoint solution reacts immediately by showing artifacts near the boundaries.

ACKNOWLEDGEMENTS

This research is supported by the Technology Foundation STW, applied science division of NWO, and the technology program of the Ministry of Economic Affairs.

REFERENCES

1. Giles MB, Pierce NA. Adjoint equations in CFD: duality, boundary conditions and solution behaviour. *AIAA Paper 97-1850*, 1997.
2. Giles MB, Pierce NA. Analytic adjoint solutions for the quasi-one-dimensional Euler equations. *Journal of Fluid Mechanics* 2001; **426**:327–345.
3. Venditti DA, Darmofal DL. Adjoint error estimation and grid adaptation for functional outputs: application to quasi-one dimensional flow. *Journal of Computational Physics* 2000; **164**:204–227.
4. Venditti DA, Darmofal DL. Grid adaptation for functional output: application to two-dimensional inviscid flows. *Journal of Computational Physics* 2002; **176**:40–69.
5. Griewank A. *Evaluating Derivatives*, *Principles and Techniques of Algorithmic Differentiation*. SIAM: Philadelphia, 2000.
6. Duivesteijn GF. Aspects of the numerical adjoint solution of quasi-1D Euler flow, http://www.hsa.lr.tudelft.nl/~gilbert/, Delft University of Technology, 2004.
7. Osher S, Solomon F. Upwind difference schemes for hyperbolic systems of conservation laws. *Mathematics of Computation* 1982; **100**:339–374.

