Least Squares Minimisation and Steepest Descent Methods for the Scalar Advection Equation and a Cauchy-Riemann System on an Adaptive Grid. *

M.E.Hubbard

The University of Reading, Department of Mathematics,

P.O.Box 220, Whiteknights, Reading, Berkshire, RG6 6AX, U.K.

11th September 1997

Abstract

Recently Roe [2] has suggested solving systems of first order conservation laws numerically and simultaneously adapting the computational grid using a least squares minimisation procedure on the fluctuations together with a steepest descent iteration approach to solve the resulting minimisation problem. In this report, the procedure is repeated for the Cauchy-Riemann system written in complex form and suggestions made for other possible functionals to be minimised in the scalar case. In each case, steepest descent updates are written explicitly for simple choices of the functional.

*This work has been carried out as part of the Oxford/Reading Institute for Computational Fluid Dynamics and was funded by EPSRC.

1 Introduction

The problem which will be addressed in this brief report is the minimisation of the functional

$$F \;=\; \frac{1}{2}\sum_{T} \underline{\phi}_T^{\,\mathrm{T}}\, Q_T\, \underline{\phi}_T \;. \tag{1.1}$$

This quantity arises from the numerical solution of systems of first order conservation laws via least squares minimisation of the associated fluctuations $\underline{\phi}_T$. The sum in (1.1) is taken over the grid cells (T) of a triangulated computational domain and the Q_T are positive definite symmetric matrices. The $\underline{\phi}_T$ will be defined precisely later in this report and the Q_T will be chosen appropriately for each case considered.

F can be considered as a function of solution values stored at the grid nodes *and* of the coordinates of the nodes themselves so it can be minimised with respect to any or all of these variables. The minimisation can be achieved iteratively using a steepest descent method which defines the update to a nodal variable, u_j say, in which j is a nodal index, to be

$$\delta u_j \;=\; -\tau\,\frac{\partial F}{\partial u_j}\;, \tag{1.2}$$

where τ is an appropriate relaxation factor. This is equivalent to computing $\underline{\phi}_T$ within each triangle in turn and accumulating adjustments at the nodes of the form

$$\delta(u_j)_T \;=\; -\tau\,\frac{\partial(\underline{\phi}_T^{\,\mathrm{T}}\, Q_T\, \underline{\phi}_T)}{\partial u_j} \tag{1.3}$$

from each triangle T. In this report the contribution (1.3) of an individual cell to a node j will be calculated for two cases where $\underline{\phi}_T$ is a vector quantity:

a) when the fluctuation is divided into more than one component within each triangle.

b) when a complex scalar fluctuation can be derived from a system of equations, based on the 2×2 Cauchy-Riemann system.

In both of the above cases F is minimised with respect to the solution values *and* the coordinates of the grid nodes.

2 Split Scalar Fluctuations

Consider the steady state linear advection equation in two dimensions,

$$\vec{a} \cdot \vec{\nabla} u \;=\; 0 \,, \tag{2.1}$$

where the advection velocity $\vec{a} = (a, b)^{\mathrm{T}}$ is constant over the whole domain. Alternatively, in any case where $\vec{a}$ is divergence-free, equation (2.1) can be written as

$$\vec{\nabla} \cdot \vec{f} = 0 \qquad \text{where} \qquad \vec{f} = u\,\vec{a} \,. \tag{2.2}$$

The fluctuation in a triangle T associated with (2.1) is given by

$$\begin{aligned} \phi_T &= -\int\!\!\int_{\triangle} \vec{a} \cdot \vec{\nabla} u \; \mathrm{d}x \, \mathrm{d}y \\ &= \oint_{\partial\triangle} u\, \vec{a} \cdot \mathrm{d}\vec{n} \,, \end{aligned} \tag{2.3}$$

where $\vec{n}$ represents the inward pointing normal to the boundary of the cell. Under the assumption that u varies linearly over each triangle and its approximation is continuous across the cell edges the discrete fluctuation is evaluated to be

$$\begin{aligned} \phi_T &= \sum_{k=1}^{3} \frac{1}{2} (u_i + u_j)\, \vec{a} \cdot \vec{n}_k \\ &= \sum_{k=1}^{3} -\frac{1}{2} (\vec{a} \cdot \vec{n}_k)\, u_k \,, \end{aligned} \tag{2.4}$$

where k is a vertex of the triangle (i and j are the other two) and $\vec{n}_k$ is the normal to the edge opposite vertex k scaled by the length of that edge.

In [2] ϕ_T is considered as a single scalar quantity but it could be split into components before the steepest descent update is calculated. As an example, the fluctuation could be written as a three component vector,

$$\underline{\phi}_T \;=\; \frac{1}{2} \begin{pmatrix} (u_2 + u_3)\, \vec{a} \cdot \vec{n}_1 \\ (u_3 + u_1)\, \vec{a} \cdot \vec{n}_2 \\ (u_1 + u_2)\, \vec{a} \cdot \vec{n}_3 \end{pmatrix} \,, \tag{2.5}$$

where each of the above components is the contribution from an edge of the triangle to the fluctuation, *cf.* (2.3) and (2.4). In the definition (1.1), Q_T is now a 3×3 positive definite matrix.

The simple choice of $Q_T = \frac{1}{S_T} I$, where S_T is the area of the triangle gives

$$F \;=\; \sum_T \frac{(\phi_T^1)^2 + (\phi_T^2)^2 + (\phi_T^3)^2}{2S_T} \;=\; \sum_T F_T \;, \tag{2.6}$$

and the individual element contributions to this sum can be written

$$\delta F_T \;=\; \sum_{k=1}^{3} \left(\frac{\phi_T^k}{S_T} \, \delta\phi_T^k - \frac{(\phi_T^k)^2}{2{S_T}^2} \, \delta S_T \right) \;. \tag{2.7}$$

Thus, using (2.5) and the fact that

$$S_T \;=\; \frac{1}{2} \sum_{k=1}^{3} x_k \, \Delta_k y \;=\; -\frac{1}{2} \sum_{k=1}^{3} y_k \, \Delta_k x \;, \tag{2.8}$$

where Δ_k is a difference along the edge opposite vertex k taken in an anticlockwise sense, *e.g.* $\Delta_1 x = x_2 - x_3$, leads to the increments to the variables at vertex 1 of a triangle T due to F_T which are given by

$$\begin{aligned}
\delta u_1 &= -\frac{(\phi_T^2)}{2S_T} \vec{a} \cdot \vec{n}_2 - \frac{(\phi_T^3)}{2S_T} \vec{a} \cdot \vec{n}_3 \qquad (2.9)\\
\delta x_1 &= -\frac{b(\phi_T^2)}{2S_T}(u_3 + u_1) + \frac{b(\phi_T^3)}{2S_T}(u_1 + u_2) + \frac{(\phi_T^1)^2 + (\phi_T^2)^2 + (\phi_T^3)^2}{4{S_T}^2}(y_2 - y_3) \\
\delta y_1 &= \frac{a(\phi_T^2)}{2S_T}(u_3 + u_1) - \frac{a(\phi_T^3)}{2S_T}(u_1 + u_2) - \frac{(\phi_T^1)^2 + (\phi_T^2)^2 + (\phi_T^3)^2}{4{S_T}^2}(x_2 - x_3) \;.
\end{aligned}$$

Similar expressions can easily be derived for the contributions to vertices 2 and 3 and the accumulation of these updates over the whole grid leads to the full steepest descent update to the nodal variables.

Note that F only vanishes if the fluctuation components ϕ_T^k all vanish and this will not always be possible since the solution values and grid coordinates do not provide enough degrees of freedom. If the fluctuation remains unsplit then there are N_c quantities set to zero using $3 \times N_n$ unknowns. N_c and N_n are the number of grid cells and nodes respectively.

This splitting in itself is probably of limited use. However, it can be used as the basis for introducing some form of upwinding into the algorithm by weighting the components of $\underline{\phi}_T$ (2.5) in the functional F (2.6) in some manner which depends continuously on all of the dependent variables. For example, one could take

$$\underline{\phi}_T \;=\; \frac{1}{2} \begin{pmatrix} (u_2 + u_3)(\vec{a} \cdot \vec{n}_1)^+ \\ (u_3 + u_1)(\vec{a} \cdot \vec{n}_2)^+ \\ (u_1 + u_2)(\vec{a} \cdot \vec{n}_3)^+ \end{pmatrix} \;, \tag{2.10}$$

where $(\cdot)^+$ indicates the positive part, so that only contributions to the fluctuation from inflow edges are considered in the minimisation of F (2.6).

One further option is to define the fluctuation within each triangle to be dependent only on perturbations of the variables at the upwind vertices, so if the upwind vertices of a chosen cell are 1 and 2 then

$$\delta \underline{\phi}_T = \frac{\partial \underline{\phi}_T}{\partial u_1} \delta u_1 + \frac{\partial \underline{\phi}_T}{\partial u_2} \delta u_2 \tag{2.11}$$

and there is no dependence on δu_3. Effectively, the fluctuation is redefined to be independent of the variables at the dowstream vertices. The disadvantage of the resulting scheme, and of the process of allowing only upwind cells to contribute to the least squares iteration at a node, is that the stencil for the update to a node may change at each iteration, leading to a discontinous change in the definition of F between iterations which may even increase its value. Note that it is more likely that upwinding would be used on the solution variables rather than the grid variables since the former arises from a hyperbolic differential equation.

It may also be possible to combine the ideas behind (2.10) and (2.11) by defining an update of the form

$$\delta \underline{\phi}_T = \frac{\partial \underline{\phi}_T^1}{\partial u_1} \delta u_1 + \frac{\partial \underline{\phi}_T^2}{\partial u_2} \delta u_2 + \frac{\partial \underline{\phi}_T^3}{\partial u_3} \delta u_3 \ , \tag{2.12}$$

where the ϕ_T^k is the k^{th} component of a vector such as (2.10). This does not discount the possibility of discontinuities in the resulting definition of the functional being minimised but does allow more flexibility in the upwinding of the algorithm.

Also, the suggestion for splitting ϕ_T in (2.10) is not unique. Another choice, for example, might be to divide the fluctuation into components proportional to those derived from multidimensional fluctuation distribution schemes [1]. This would lead to different expressions in (2.10) in which ϕ_T^k is now the contribution sent to vertex k by the fluctuation in triangle T. This can be illustrated by considering the PSI scheme [1].

In the case where the whole fluctuation is sent to a single downstream vertex the analysis carries through as in [2], although some weighting similar in nature to that applied in (2.10) would be necessary for the iteration to become genuinely upwind in nature. In the two target case (vertices 2 and 3, say) the distribution before weighting is given by

$$\phi_2 \;=\; -\frac{1}{2}\vec{a}\cdot\vec{n}_2(u_2-u_1)\;,\quad \phi_3 \;=\; -\frac{1}{2}\vec{a}\cdot\vec{n}_3(u_3-u_1)\;, \tag{2.13}$$

and $\phi_1 = 0$. From (2.7) it can easily be deduced that

$$\begin{aligned}
\delta u_1 &= -\frac{(\phi_T^2)}{2S_T}\vec{a}\cdot\vec{n}_2 - \frac{(\phi_T^3)}{2S_T}\vec{a}\cdot\vec{n}_3 \\
\delta x_1 &= \frac{b(\phi_T^2)}{2S_T}(u_2-u_1) - \frac{b(\phi_T^3)}{2S_T}(u_3-u_1) + \frac{(\phi_T^2)^2+(\phi_T^3)^2}{4{S_T}^2}(y_2-y_3) \\
\delta y_1 &= -\frac{a(\phi_T^2)}{2S_T}(u_2-u_1) + \frac{a(\phi_T^3)}{2S_T}(u_3-u_1) - \frac{(\phi_T^2)^2+(\phi_T^3)^2}{4{S_T}^2}(x_2-x_3)\;.
\end{aligned} \tag{2.14}$$

The asymmetry of the chosen splitting of the fluctuation means that the other two sets of updates take a slightly different form so that

$$\begin{aligned}
\delta u_2 &= \frac{(\phi_T^2)}{2S_T}\vec{a}\cdot\vec{n}_2 \\
\delta x_2 &= \frac{b(\phi_T^3)}{2S_T}(u_3-u_1) + \frac{(\phi_T^2)^2+(\phi_T^3)^2}{4{S_T}^2}(y_2-y_3) \\
\delta y_2 &= -\frac{a(\phi_T^3)}{2S_T}(u_3-u_1) - \frac{(\phi_T^2)^2+(\phi_T^3)^2}{4{S_T}^2}(x_2-x_3)\;.
\end{aligned} \tag{2.15}$$

and a very similar expression can be derived for the update to the variables at vertex 3. As before, accumulating these updates over the whole grid leads to the complete steepest descent update.

3 A Cauchy-Riemann System

The second model problem considered here is, as in [2], that of inviscid, irrotational flow arising from a small perturbation of a uniform stream, given by the equations

$$\begin{aligned}
\delta &= (1-M^2)u_x + v_y &= 0 \\
\omega &= v_x - u_y &= 0\;.
\end{aligned} \tag{3.1}$$

In fact, only the elliptic case ($M^2 < 1$) will be considered here, where the transformation

$$\begin{aligned}
X &= x\;, \quad Y = \sqrt{1-M^2}\,y\;, \\
U &= \sqrt{1-M^2}\,u\;, \quad V = v\;,
\end{aligned} \tag{3.2}$$

leads directly to the Cauchy-Riemann equations,

$$\begin{aligned} \delta' &= \frac{\delta}{\sqrt{1-M^2}} &= U_X + V_Y &= 0 \\ \omega' &= \omega &= V_X - U_Y &= 0 \,. \end{aligned} \tag{3.3}$$

In [2] (3.3) was kept as a system of equations with real coefficients and the fluctuation was evaluated as

$$\begin{aligned} \underline{\phi}_T &= -\int\!\!\int_{\triangle} \underline{F}_X + \underline{G}_Y \; \mathrm{d}x\,\mathrm{d}y \\ &= \oint_{\partial\triangle} (\underline{F}, \underline{G}) \cdot \mathrm{d}\vec{n} \,, \end{aligned} \tag{3.4}$$

where $\underline{F} = (U, V)^{\mathrm{T}}$ and $\underline{G} = (V, -U)^{\mathrm{T}}$. When U and V are assumed to vary linearly within each cell (3.4) can be written

$$\underline{\phi}_T = \sum_{k=1}^{3} -\frac{1}{2} (\underline{F}, \underline{G})_k \cdot \vec{n}_k \,, \tag{3.5}$$

and the quantity chosen in [2] to be minimised is

$$F = \frac{1}{2} \sum_T \frac{\underline{\phi}_T{}^{\mathrm{T}} \underline{\phi}_T}{S_T} = \frac{1}{2} \sum_T \frac{(\underline{F}^{\mathrm{T}} \underline{F} + \underline{G}^{\mathrm{T}} \underline{G})_T}{S_T} \,. \tag{3.6}$$

Alternatively, the complex variables

$$W = V + iU \,, \quad Z = X + iY \,, \tag{3.7}$$

can be introduced and (3.3) can be written as a scalar equation with complex coefficients given by

$$\frac{\partial W}{\partial Z} = \frac{\partial W}{\partial X} = \frac{\partial W}{\partial (iY)} \,, \tag{3.8}$$

which, with a small amount of algebraic manipulation becomes

$$(V_X - U_Y) + i(U_X + V_Y) = 0 \tag{3.9}$$

or, equivalently,

$$\vec{\nabla} \cdot \underline{f} = 0 \,, \tag{3.10}$$

where

$$\underline{f} = \underline{F} + i\underline{G} = \begin{pmatrix} V + iU \\ -U + iV \end{pmatrix} \,, \tag{3.11}$$

and finally

$$\vec{a} \cdot \vec{\nabla} W = 0 \,, \tag{3.12}$$

where $\vec{a} = (1, i)^{\mathrm{T}}$ and W is defined in (3.7). Note that (3.12) bears a striking resemblance to the scalar advection equation (2.1) although the coefficients are now complex.

Equations (3.10) and (3.12) are integrated to give the complex fluctuation

$$\begin{aligned} \phi_T &= -\int\!\!\int_{\triangle} \vec{\nabla} \cdot \vec{f} \, \mathrm{d}x \, \mathrm{d}y \\ &= \oint_{\partial\triangle} \vec{f} \cdot \mathrm{d}\vec{n} \\ &= \oint_{\partial\triangle} W \, \vec{a} \cdot \mathrm{d}\vec{n} \ , \end{aligned} \tag{3.13}$$

and the assumption that U and V both vary linearly over each triangle leads to the discrete form of the fluctuation which is given by

$$\phi_T = \sum_{k=1}^{3} -\frac{1}{2} (\vec{a} \cdot \vec{n}_k) \, W_k \ . \tag{3.14}$$

One can now seek to minimise the quantity

$$F = \frac{1}{2} \sum_T \frac{|\phi_T|^2}{S_T} = \frac{1}{2} \sum_T \frac{\overline{\phi_T} \phi_T}{S_T} = \sum_T F_T \ , \tag{3.15}$$

in which the sum is over all of the triangles in the domain and S_T is the area of triangle T. (3.15) is in fact equivalent to (3.6). It follows immediately from (3.15) that an individual element contribution gives

$$\begin{aligned} \delta F_T &= \frac{1}{2S_T} \delta(|\phi_T|^2) + \frac{|\phi_T|^2}{2} \delta \left(\frac{1}{S_T} \right) \\ &= \frac{1}{2S_T} \delta(|\phi_T|^2) - \frac{|\phi_T|^2}{2{S_T}^2} \delta S_T \\ &= \frac{1}{2S_T} (\overline{\phi}_T \delta \phi_T + \phi_T \delta \overline{\phi}_T) - \frac{|\phi_T|^2}{2{S_T}^2} \delta S_T \ . \end{aligned} \tag{3.16}$$

Using a steepest descent method to minimise F leads to iterative updates to the complex variables defined in (3.7) of the form

$$\begin{aligned} \delta W &= \delta V + i \delta U = -\frac{\partial F}{\partial V} - i \frac{\partial F}{\partial U} \\ \delta Z &= \delta X + i \delta Y = -\frac{\partial F}{\partial X} - i \frac{\partial F}{\partial Y} \ . \end{aligned} \tag{3.17}$$

With some algebraic manipulation of (3.16) and using

$$\sqrt{1 - M^2} S_T = \frac{1}{2} \sum_{k=1}^{3} X_k \Delta_k Y = -\frac{1}{2} \sum_{k=1}^{3} Y_k \Delta_k X \ , \tag{3.18}$$

and the fact that

$$\begin{aligned}\phi_T &= -\frac{1}{2}\sum_{k=1}^{3}\left[(V_k\Delta_k Y + U_k\Delta_k X) + i(U_k\Delta_k Y - V_k\Delta_k X)\right] \\ &= \frac{i}{2}\sum_{k=1}^{3} W_k\Delta_k Z \\ &= -\frac{i}{2}\sum_{k=1}^{3} Z_k\Delta_k W \qquad (3.19) \\ &= \frac{1}{2}\sum_{k=1}^{3}\left[(X_k\Delta_k U + Y_k\Delta_k V) + i(Y_k\Delta_k U - X_k\Delta_k V)\right] \;,\end{aligned}$$

where Δ_k as in (2.8) signifies a difference along the edge opposite vertex k taken in an anticlockwise sense, the contribution of a particular cell to its k^{th} vertex can be shown to be

$$\begin{aligned}\delta W_k &= \frac{i}{2S_T}\phi_T\Delta_k\overline{Z} \\ \delta Z_k &= -\frac{i}{2S_T}\phi_T\Delta_k\overline{W} - \frac{i|\phi_T|^2}{4\sqrt{1-M^2}{S_T}^2}\Delta_k Z \;. \qquad (3.20)\end{aligned}$$

The accumulation of these increments leads to the complete steepest descent iteration. This is equivalent to the update derived in [2].

4 Conclusions

In this report, iterative updates have been derived for a steepest descent method designed to minimise a chosen functional, related to a system of partial differential equations, with respect to solution values *and* grid node coordinates. The functional is in each case designed for a least squares minimisation of the fluctuations corresponding to the system of equations.

Two specific cases have been considered, one in which a scalar fluctuation is split into components before the least squares minimisation is applied and another in which a system based on the 2×2 Cauchy-Riemann system is considered. In the latter case it is noted that the system can be written in a complex form which has many similarities to the scalar case.

Acknowledgements

The author would like to thank Prof. M. J. Baines for his contributions to this work and the EPSRC for providing the funding for the author.

References

[1] H.Deconinck, R.Struijs, G.Bourgois and P.L.Roe, 'High resolution shock capturing cell vertex advection schemes for unstructured grids', *Computational Fluid Dynamics*, number 1994–05 in VKI Lecture Series, 1994.

[2] P.L.Roe, 'Compounded of many simples: reflections on the role of model problems in CFD', *Proceedings of Workshop on Barriers and Challenges in CFD*, ICASE, 1996.