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ON THE DESIGN OF CONSERVATIVE BOUNDARY CONDITIONS FOR A HIGH-ORDER NUMERICAL MODEL

BY

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C A NASH

1. INTRODUCTION

In a physical problem described by fluid transport equations, eg the Navier-Stokes equations, it is common for the prognostic equations to contain flux divergence terms, such as those representing advection or diffusion. These terms have the property that they conserve the transported quantity in a volume integrated sense and there are no net sources or sinks, except perhaps on the boundaries of the fluid region.

For a numerical model to accurately represent such behaviour it is usual to constrain the differencing to satisfy similar requirements and **indeed, conservation of** quadratic functions of the model variables can be a convenient way of ensuring stability during an extended time-integration (Arakawa 1966). In practice designing a conservative form of differencing for the interior points of a discrete grid is relatively easy and the simplest numerical schemes often conserve linear quantities. Equally for **schemes second-order accurate in space,** ensuring the interior conservation under advection of quadratic properties, such as kinetic energy, is also fairly straightforward (Bryan (1966), Lilly (1965)) in the case of an incompressible fluid. Piacsek and Williams (1970) have proposed a quadratically conservative scheme which does not require zero divergence of the velocity field but is weakly non-conservative of linear quantities. Methods have also been devised to give energy conservation in compressible atmospheric models (Haltiner and Williams (1980)). However it should be noted that most methods only conserve the relevant properties to the accuracy of the time integration scheme.

To complete the specification of a numerical scheme boundary conditions must be specified and these must also be consistent with the required conservation properties. For a second-order accurate scheme the boundary conditions need only be first order accurate and this gives sufficient freedom to design such conditions relatively simply (eg Clark (1977)). However for higher order schemes, when the boundary conditions must be no more than one order less than the interior scheme in accuracy (Gustafsson et al 1972), the design of suitable conditions becomes very complex.

This note describes a simple constructive method for such conditions and is illustrated by an example at a rigid boundary in a 4th order accurate model. In particular this provides a method for the design of the boundary conditions in the proposed Met 0 15 mesoscale model (Nash 1983).

2. THE METHOD

Consider a transport equation for a variable ϕ that contains a flux divergence term, viz

$$\frac{\partial \phi}{\partial t} = \frac{\partial F}{\partial x} + S \qquad (1)$$

where S represents any remaining terms and the domain is $0 < x < 1$. The equation is semi-discretised using a spatial grid X_i, where $X_i = (i - 1)/(N - 1)$, $(i = 0, 1, 2, \ldots, N)$ are the grid points, and the finite difference equivalent of (1) is

$$\frac{\partial \phi_i}{\partial t} = \delta_x F_i + S_i \qquad (2)$$

where $\phi_i = \phi(x_i)$, $\quad \delta_{px} F_i = \left(F(x_{i+\frac{p}{2}}) - F(x_{i-\frac{p}{2}})\right)/p\Delta x$ †
is a finite difference representation for the flux divergence term, and F is a known function on all the half-grid points $i = 1/2, \ldots, N + 1/2$. The scheme is assumed to be accurate to order m, that is

$$\frac{\partial F}{\partial x} = \delta_x F + O(\Delta x^m) \qquad (3)$$

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† $\Delta x = 1/(N-1)$

Integrating equation (1) gives

$$\frac{\partial}{\partial t} \int_0^1 \phi \, dx = F(1) - F(0) + \int_0^1 S \, dx \qquad (4)$$

and we would like the numerical differencing to satisfy an analogous constraint. Clearly $\delta_x F$ and ϕ are only known at the grid points X_i so that the integral in equation (4) must be replaced by a numerical quadrature to give an equation linking these parameters.

Let Q be an nth order quadrature such that

$$Q(\phi_i, i = 0, 1, \ldots, N) = \int_0^1 \phi \, dx + O(\Delta x^n) \qquad (5)$$

Since $\delta_x F$ is known at i = 1, 2, 3, ..., N, the numerical constraint consistent with equation (4) is

$$Q\left((\delta_x F)_i \, , i = 0, 1, \ldots, N \right) = F(1) - F(0) \qquad (6)$$

This is sufficient to determine $(\delta_x F)_0$ and becomes the conservative lower boundary condition for the scheme. It is necessary to check the accuracy of this expression as an approximation to $\partial F / \partial x$ at X = 0. By definition,

$$\int_0^1 \frac{\partial F}{\partial x}\, dx = F(1) - F(0)$$

and using the quadrature (5), it follows that

$$Q\left((\partial F/\partial x)(x = x_i),\, i = 0,1,..,N \right) = F(1) - F(0) + O(\Delta x^n) \quad (7)$$

Substituting from equation (3) gives

$$Q\left((\partial F/\partial x)(x = x_0),\, (\delta_x F)_i,\, i = 1,..,N \right) = F(1) - F(0) \quad (8)$$

$$+ O(\Delta x^n) + O(\Delta x^m)$$

since integrating the $O(\Delta x^m)$ term over an interval with length of order unity gives a term that is also $O(\Delta x^m)$. (Note that if $\delta_x F$ is $O(\Delta x^{m-1})$ on a small number (r) of the grid points where r<<N, then the integrated error term is still $O(\Delta x^m)$.

Comparing equations (6) and (8) shows that $(\delta_x F)_0$, defined by equation (6), must satisfy

$$(\delta_x F)_0 = (\partial F/\partial x)(x = x_0) + O(\Delta x^{\min(m,n)-1}) \quad (9)$$

where the error order decreases by unity since $(\delta_x F)_0$ appears in Q in a linear combination weighted by a multiplier which is $O(\Delta x)$.

Thus the numerical boundary condition (9) is accurate to an order one less than the accuracy of the quadrature (5) and the interior differencing (3). Since it is possible to choose Q of arbitrary order accuracy the method will specify boundary conditions of sufficient accuracy for any order of differencing in principle. Clearly as $\delta_x F$ must be known at all but one of the grid points, $\delta_x F$ must be calculated by one-sided differences at any other point that lies too close to the boundaries to use the interior (centred) form. This restriction appears to limit the utility of the method to deducing only one of the boundary conditions at X = 0 and X = 1 but not both. However this is not the case as will be demonstrated in the example described in the next section.

3. AN EXAMPLE

Consider an equation of the form (1) given by

$$\frac{\partial \phi}{\partial t} = \frac{\partial \phi}{\partial x} + S \qquad 0 < x < 1 \qquad (10)$$

where $\partial \phi / \partial x$ is differenced in the interior by the fourth-order accurate expression

$$\delta_x F = \frac{4}{3} \delta_x \overline{\phi}^{x} - \frac{1}{3} \delta_{2x} \overline{\phi}^{2x} \qquad (11)$$

where $\overline{\phi_i}^{px} = \frac{1}{2}(\phi_{i+\frac{p}{2}} + \phi_{i-\frac{p}{2}})$. The operator (11) is a function of five points and so is defined for X_i, i = 2, 3, ..., N - 2 if ϕ_i is known on the entire grid at a given timestep. Assume two computational points at X_{-1} and X_{N+1} with ϕ values given by $o(\Delta x^4)$ extrapolation, (Nash 1983), eg

$$\phi_{-1} = 4\phi_0 - 6\phi_1 + 4\phi_2 - \phi_3 \qquad (12)$$

Then equation (11) can be calculated at X_1 and X_{N-1} and is an $o(\Delta x^3)$ approximation to $\partial \phi / \partial x$ there. The method of section 2 will now be used to deduce a finite difference approximation for $\partial \phi / \partial x$ at X_o and X_N that is conservative and $O(\Delta x^3)$ accurate.

The integration formula given by

$$\int_0^1 f\,dx \simeq \Delta x \sum_{i=3}^{N-3} f_i + \frac{\Delta x}{24}\Big\{9f_0 + 28f_1 + 23f_2$$

$$+ 23f_{N-2} + 28f_{N-1} + 9f_N\Big\} \qquad (13)$$

$$= Q(f_i)$$

has an error of $O(\Delta x^4)$ and is therefore of sufficient accuracy to derive an $O(\Delta x^3)$ boundary condition. (The quadrature was designed to be symmetric in the interior so that substantial cancellation should occur for the summation of flux-like terms and thus results in a strictly local boundary condition : Simpson's rule, for example, would not have this property).

Substituting $\delta_x F$ for f in equation (13) gives

$$Q(f_i) = \frac{1}{24}\Big\{9\Delta x(\delta_x F)_0 - 28F_{\frac{1}{2}} + 5F_{1\frac{1}{2}} - F_{2\frac{1}{2}}$$

$$+ 28F_{N-\frac{1}{2}} - 5F_{N-1\frac{1}{2}} + F_{N-2\frac{1}{2}} \qquad (14)$$

$$+ 9\Delta x(\delta_x F)_N\Big\}$$

Then putting $Q(f_i)$ into the conservation constraint (6), gives one equation but two unknowns. Equation (14) is clearly satisfied if $(\delta_x F)_0$ and $(\delta_x F)_N$ are given by the pair of equations

$$\frac{1}{24}\left\{9\Delta x(\delta_x F)_0 - 28F_{\frac{1}{2}} + 5F_{1\frac{1}{2}} - F_{2\frac{1}{2}}\right\} = -\phi(0)$$

(15)

$$\frac{1}{24}\left\{9\Delta x(\delta_x F)_N + 28F_{N-\frac{1}{2}} - 5F_{N-1\frac{1}{2}} + F_{N-2\frac{1}{2}}\right\} = \phi(1)$$

which can be considered to be the applicable forms of equation (6) for solving two related half-infinite problems: that is, $0 < x < \infty$ such that $F \to 0$ as $x \to \infty$ and $-\infty < x < 1$ with $F \to 0$ as $x \to -\infty$. The splitting of equation (7) into two equalities is also physically reasonable since the nature of the flux term suggests that $(\delta_x F)$ should always be a function of ϕ values local to itself.

Without loss of generality only the lower boundary condition will be evaluated. Substituting for F in the first of equations (15) and using the extrapolation (12)

$$(\delta_x F)_0 = \frac{1}{108\Delta x}\left\{-\phi_4 + 40\phi_3 - 168\phi_2 + 328\phi_1 + 89\phi_0\right\} - \frac{24}{9\Delta x}\phi(0) \quad (16)$$

Defining $\phi(0)$ equal to ϕ_0, it may be confirmed that this expression has an error $O(\Delta x^3)$ as intended. The final form of the lower boundary condition is

$$(\delta_x F)_0 = \frac{1}{108\Delta x}\left\{-\phi_4 + 40\phi_3 - 168\phi_2 + 328\phi_1 - 199\phi_0\right\} \quad (17)$$

4. EXTENSIONS AND STABILITY

The method presented in section 2 can be used to construct conservative boundary conditions of arbitrary order. Whilst the accuracy is assured the method does not guarantee stability of the resulting scheme. For an inflow or rigid boundary stability is probably less sensitive to the boundary formulation (Oliger (1972)) but on outflow more care is required in designing a stable scheme. In practice the method described is unlikely to be used at other than rigid boundaries, for which a definite zero-flux constraint exists.

However in principle the method could be used to ensure quadratic conservation and stability would then necessarily follow. For example, consider the advection of a passive quantity ϕ in a two-dimensional incompressible fluid with velocity components u and w. Then equation (1) is generalised to

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x}(u\phi) + \frac{\partial}{\partial z}(w\phi) = 0 \tag{18}$$

and the velocity components satisfy a continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0 \tag{19}$$

Then the quadratic ϕ^2 is conserved by the advection since from equation (18)

$$\frac{\partial}{\partial t}\left(\frac{\phi^2}{2}\right) + \frac{\partial}{\partial x}\left(u\frac{\phi^2}{2}\right) + \frac{\partial}{\partial z}\left(w\frac{\phi^2}{2}\right) + \frac{\phi^2}{2}\left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z}\right) = 0 \qquad (20)$$

and the last term is zero due to equation (19). Equation (20) shows that the total ϕ^2 integrated over a closed domain can only be changed by boundary fluxes.

A finite difference scheme for equations (18) and (19) can often be similarly manipulated. Consider the second order semi-discrete system

$$\frac{\partial \phi}{\partial t} = -\delta_x\left(\overline{u}^x\,\overline{\phi}^x\right) - \delta_z\left(\overline{w}^z\,\overline{\phi}^z\right) \qquad (21)$$

It may be shown that

$$\frac{\partial}{\partial t}\left(\frac{\phi^2}{2}\right) = -\delta_x\left(\overline{u}^x\,\frac{\widetilde{\phi\phi}^x}{2}\right) - \delta_z\left(\overline{w}^z\,\frac{\widetilde{\phi\phi}^z}{2}\right)$$

$$- \frac{\phi^2}{2}\left(\delta_x\overline{u}^x + \delta_z\overline{w}^z\right) \qquad (22)$$

where $\widetilde{\phi\phi}^x = \phi\,(x+\Delta x/2).\phi\,(x-\Delta x/2)$.

If the continuity equation is approximated as

$$\delta_x \overline{u}^x + \delta_z \overline{w}^z = 0 \tag{23}$$

then the advection of ϕ is described by a flux process in the numerical system. Then the method of section 2 may be applied to the flux terms alone in equation (22) to deduce quadratically conserving boundary conditions for the finite difference scheme (21). In general only one constraint per boundary can be applied by these methods and linear conservation may then be sacrificed. However quadratic conservation is an attractive property due to its guarantee of stability.

5. SUMMARY

A method has been presented that allows boundary conditions for a numerical model to be constructed satisfying certain **spacial conservation** constraints.

In some cases either linear or quadratic conservation may be incorporated but not both. The method has its main application in designing conditions for higher order finite difference schemes when a heuristic approach becomes very difficult.

Boundary conditions were designed for a fourth-order centred difference scheme as an illustration of the approach. This example is directly relevant for the proposed Met 0 15 mesoscale Model.

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