Understanding the Shu–Osher Conservative Finite Difference Form

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Shu and Osher introduced a conservative finite difference discretization for hyperbolic conservation laws using nodal values rather than the traditional cell averages. Their form was obtained by introducing mathematical relations that simplify the resulting numerical methods. Here we instead "derive" their form from the standard cell average approach. In the process, we clarify the origin of their relations and the properties of this formulation. We also investigate the extension of their form to non-uniform grids. We show the strict conservation form only extends to grids with quadratic or exponential stretching. However, a slight generalization can be applied to all smoothly stretched grids with no loss of essential properties.

1. INTRODUCTION

To discretize a hyperbolic conservation law,

$$\frac{du}{dt} + \frac{df(u)}{dx} = 0, \tag{1}$$

on a grid $\{x_i\}$, it is common practice to simply integrate the equation over each grid cell $[x_i, x_{i+1}]$ to obtain the "cell averaged conservation form"

$$\frac{d\bar{u}_{i+\frac{1}{2}}}{dt} + \frac{(f(u_{i+1}) - f(u_i))}{\varDelta x} = 0, \tag{2}$$

where $\bar{u}_{i+\frac{1}{2}}$ denotes the average value of u over the cell, and $u_i = u(x_i)$ denotes the nodal value at node x_i.

It is well known (as the Lax–Wendroff Theorem [4, p. 129]) that such a "conservative difference form" is essential because it insures that discontinuities (shocks or contacts) in the flow move at the correct speed dictated by physical conservation.

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This could not be guaranteed by the traditional notion of numerical accuracy, which is based on approximating *smooth* solutions.

The standard conservative difference form (2) automatically combines both cell averages $\bar{u}_{i+\frac{1}{2}}$ and nodal values u_i, and thus requires the use of both reconstruction and averaging procedures to pass between these representations of *u*. This complicates the numerical algorithms, especially in multiple dimensions.

In order to simplify the numerical schemes, Shu and Osher [6, 7] introduced a discretization based solely on nodal values. They first postulate the functional relation

$$\frac{df}{dx} = \frac{(h(x + \frac{\Delta x}{2}) - h(x - \frac{\Delta x}{2}))}{\Delta x}, \tag{3}$$

so that the original differential equation takes on a conservative difference form

$$\frac{du}{dt} + \frac{(h(x + \frac{\Delta x}{2}) - h(x - \frac{\Delta x}{2}))}{\Delta x} = 0, \tag{4}$$

which we will refer to as the "Shu–Osher form". This can then be discretized conservatively in terms of nodal values simply by imposing the equation at the nodes

$$\frac{du_i}{dt} + \frac{(h_{i+\frac{1}{2}} - h_{i-\frac{1}{2}})}{\Delta x} = 0, \tag{5}$$

assuming we can construct $h_{i+\frac{1}{2}} = h(x_i + \frac{\Delta x}{2})$ in terms of the local nodal values of *f* in some convenient fashion. Towards this end, Shu and Osher [7] provide two functional relations between *f* and *h*: a power series asymptotic expansion for *h*

$$h(x) = a_0 f(x) + a_2 f''(x) \Delta x^2 + a_4 f''''(x) \Delta x^4 + \cdots + a_{2n} f^{(2n)}(x) \Delta x^{2n} + \cdots, \tag{6}$$

where the coefficients are deduced from the defining relation (4), to be $a_0 = 1$, $a_2 = -1/24$, $a_4 = 7/5760,\ldots$, and also a integral "primitive" for *h*,

$$f(x) = \frac{\int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} h(x) \, dx}{\Delta x}. \tag{7}$$

Either of these relations can be used to compute $h_{i+\frac{1}{2}}$ from local nodal values $f_j = f(u_j)$ to any desired order of accuracy in Δx. In particular, Shu and Osher provide an elegant divided difference construction using the primitive relation [7], and this is a major algorithmic component of the resulting family of Essentially Non-Oscillatory (ENO) schemes.

We have three goals in this paper. First, we want to relate the Shu–Osher conservation form (4) back to the traditional cell average form (2) in a way that illuminates the origins of the *h* function and its relations given by Eqs. (3), (6), and (7). We provide a derivation of the Shu–Osher form from cell averages, and show why *h* and its relations are indeed natural and essential. Second, we want to clarify why the nodal value form provides a simplification over cell averages, given that both forms require reconstruction processes. We show that the relative simplicity of

the nodal form becomes clear in multiple dimensions. Finally, we want to investigate the extent to which the Shu–Osher form extends to non-uniform grids, since the original presentation [7] assumes a uniform spatial grid. We will show the strict conservation form applies only to quadratically or exponentially stretched grids, but a slightly generalized form can be applied to any smoothly stretched grid.

2. DERIVING THE SHU-OSHER FORM

We first give a formal derivation of the Shu–Osher form (4), starting from the standard cell average form (2). Let $\mathscr{A}$ denote the cell average operator, which we define generally as a functional that acts on $u(x)$ to give

$$\mathscr{A}[u](x) = \frac{\int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} u(x)\, dx}{\Delta x}. \tag{8}$$

Here Δx is the "grid spacing", which for now is simply a constant. Applying $\mathscr{A}$ to the general hyperbolic conservation law (1) gives the cell average conservative difference form

$$\frac{d\mathscr{A}u}{dt} + \frac{\Delta f}{\Delta x} = 0 \tag{9}$$

where

$$\Delta f(x) = f\left(x + \frac{\Delta x}{2}\right) - f\left(x - \frac{\Delta x}{2}\right) \tag{10}$$

is the generalized central difference operator, and $f(x) = f(u(x))$. Simply inverting $\mathscr{A}$ off the cell averaged Eq. (9) gives

$$\frac{du}{dt} + \frac{\mathscr{A}^{-1}\Delta f}{\Delta x} = 0, \tag{11}$$

and, since $\mathscr{A}^{-1}$ and Δ commute, we have

$$\frac{du}{dt} + \frac{\Delta(\mathscr{A}^{-1}f)}{\Delta x} = 0. \tag{12}$$

This is precisely the same form as the Shu–Osher form in (4), but here we naturally encounter the conservative difference of the function

$$h = \mathscr{A}^{-1}f. \tag{13}$$

Thus we have derived the Shu–Osher form in a way that shows it to be a natural consequence of the cell average form, rather than being a wholly independent formulation. This has an important consequence for properly interpreting the nodal value form. In general, pointwise values are ambiguously defined at discontinuities (shocks, contacts) in the solution u, hence there is a mathematically justified bias towards describing solutions in terms of well-defined local (or cell) averages.

However, this anti-pointwise bias should not be applied to the Shu–Osher "nodal value" form, since it is merely a mathematically transformed version of the cell average form. At the discretized level, this means the nodal values $\{u(x_j)\}$ computed from this form should *not* be thought of as true pointwise values, but rather as being the best-estimate values as inferred by applying $\mathscr{A}^{-1}$ to the computed cell average values $\{\bar{u}_{j+\frac{1}{2}}\}$. Thus the $\{u(x_j)\}$ and $\{\bar{u}_{j+\frac{1}{2}}\}$ are equivalent, with the cell averages being the primary, well-defined quantities, and the "nodal values" being a derived set of data. The Shu–Osher formulation simply allows us to compute this derived set directly, avoiding the need to ever compute the underlying cell averages.

We now consider the origin of the various Shu–Osher relations involving h, in light of our derivation. Comparing the nodal form (12) to the original conservation law (1), we see that we must have the functional relation $\Delta h/\Delta x = f'$, which was used as the defining relation for h, (3), by Shu and Osher. Also, to express h, which is natural defined by (13), in terms of standard operations, we must invert that relation and write

$$f = \mathscr{A}h, \tag{14}$$

which is precisely the primitive relation (7) of Shu and Osher. This relation was particularly puzzling in their original presentation [7], since they dealt only with nodal values yet this cell average operation appeared spontaneously. Here we see this is a necessary consequence of using the operator $\mathscr{A}$ to convert between between the cell average (f) and nodal value (h) based forms of the conservation law.

As for the power series expansion relation (6), we simply point out that this expansion can be obtained in a closed form via the Fourier transform. Fourier transforming the functional difference relation (3) that defines h gives

$$-ik\hat{f} = -i\frac{2}{\Delta x}\sin\left(k\frac{\Delta x}{2}\right)\hat{h}, \tag{15}$$

or, isolating $\hat{h}$ and transforming back,

$$h = \theta\csc(\theta)\,f, \tag{16}$$

where $\theta = i\frac{\Delta x}{2}\frac{d}{dx}$, which is a closed form for h as a (pseudo-)differential operator on f. This relation can be made explicit by substituting for θ in the Taylor series expansion [1, p. 85, formula 4.5.65]

$$\theta\csc(\theta) = 1 + \frac{1}{6}\theta^2 + \frac{7}{360}\theta^4 + \frac{31}{15120}\theta^6 + \cdots + (-1)^{n+1}\frac{(2^{2n}-2)\,B_{2n}}{(2n)!}\theta^{2n} + \cdots, \tag{17}$$

where the B_n are the Bernoulli numbers [1, p. 804]. In particular, this shows that the coefficients for h in the power series (6) given by Shu and Osher are $a_0 = 1$, $a_2 = -1/24$, $a_4 = 7/5760$, $a_6 = -31/967680$, $a_8 = 127/154828800$, $a_{10} = -73/3503554560,\ldots$, with the general formula being

$$a_{2n} = (-1)^{n+1}\frac{(2^{2n}-2)\,B_{2n}}{2^{2n}(2n)!} \tag{18}$$

for $n \geqslant 0$.

3. THE MULTI-DIMENSIONAL ADVANTAGE

Since both the standard cell average form and the Shu–Osher nodal form have reconstruction processes (u from $\bar{u}$ or h from f), it is not clear that there is any real difference in simplicity between them. However, repeating our derivation in the multi-dimensional setting makes this distinction clear. Consider a general scalar conservation law in three spatial dimensions,

$$\frac{du}{dt}+\frac{dF_x}{dx}+\frac{dF_y}{dy}+\frac{dF_z}{dz}=0, \tag{19}$$

where $F=(F_x, F_y, F_z)$ is the vector flux of the conserved quantity $u(x, y, z, t)$. Let $\mathscr{A}_x$ denote the 1-D cell averaging operator in x,

$$\mathscr{A}_x[u](x, y, z)=\frac{\int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} u(x, y, z)\, dx}{\Delta x}, \tag{20}$$

where Δx is a constant, and let Δ_x denote the 1-D central difference in x,

$$\Delta_x f(x, y, z)=f\left(x+\frac{\Delta x}{2}, y, z\right)-f\left(x-\frac{\Delta x}{2}, y, z\right). \tag{21}$$

Similarly, let $\mathscr{A}_y$, Δ_y and $\mathscr{A}_z$, Δ_z be the 1-D averaging and difference operators in y and z.

The full 3-D cell average over a $\Delta x \times \Delta y \times \Delta z$ cell centered at (x, y, z) is given by the composition of 1-D averages, $\mathscr{A}=\mathscr{A}_x\mathscr{A}_y\mathscr{A}_z$, and these 1-D averages freely commute with each other. Applying this cell average to the conservation law (19) and using $\mathscr{A}_x \frac{d}{dx}=\Delta_x/\Delta x$, and similarly for y and z, gives the standard cell average conservation form

$$\frac{d(\mathscr{A}_x\mathscr{A}_y\mathscr{A}_z u)}{dt}+\frac{\Delta_x(\mathscr{A}_y\mathscr{A}_z F_x)}{\Delta x}+\frac{\Delta_y(\mathscr{A}_x\mathscr{A}_z F_y)}{\Delta y}+\frac{\Delta_z(\mathscr{A}_x\mathscr{A}_y F_z)}{\Delta z}=0. \tag{22}$$

To obtain the Shu–Osher form, we again simply apply $\mathscr{A}^{-1}=\mathscr{A}_x^{-1}\mathscr{A}_y^{-1}\mathscr{A}_z^{-1}$ and use the fact that all the 1-D operators commute with each other to get the Shu–Osher form

$$\frac{du}{dt}+\frac{\Delta_x(\mathscr{A}_x^{-1}F_x)}{\Delta x}+\frac{\Delta_y(\mathscr{A}_y^{-1}F_y)}{\Delta y}+\frac{\Delta_z(\mathscr{A}_z^{-1}F_z)}{\Delta z}=0. \tag{23}$$

This is easily conservatively discretized via nodal values on a $\{x_i\} \times \{y_j\} \times \{z_k\}$ grid by evaluating it at the nodes (x_i, y_j, z_k). Thus in 3-D we naturally encounter three 1-D Shu–Osher flux functions

$$\begin{aligned}
h_x &= \mathscr{A}_x^{-1}F_x, \\
h_y &= \mathscr{A}_y^{-1}F_y, \\
h_z &= \mathscr{A}_z^{-1}F_z,
\end{aligned} \tag{24}$$

each of which are obtained through the standard, purely 1-D reconstruction relations from Eqs. (6) or (7) applied along the grid in the respective directions. This is the so-called "dimension-by-dimension" discretization process. If we contrast the cell average and Shu–Osher forms, we see that each term in the cell average form (22) involves operations in all three of the x, y and z directions, where as in the Shu–Osher form (23) the x-term involves only operations in the x-direction, the y-term only operations in the y direction, and the z-term only operations in the z-direction, and further all three contributions can be computed using the same 1-D procedure. Moreover, there is never a need to do a "fully 3-D" reconstruction such as reconstructing u from the triple averaged $\mathscr{A}_x\mathscr{A}_y\mathscr{A}_y u$, nor is there ever a need to do any 2-D integrations of fluxes such as $\mathscr{A}_y\mathscr{A}_z F_x$.

Thus we see that in multiple dimensions, the inversion leading to Shu–Osher form yields a conservative difference form equivalent to cell averages, but which separates out the operations dimension-by-dimension. This in turn corresponds to a real algorithmic simplification in multiple dimensions, since multidimensional calculations simply recycle the same basic 1-D procedure. In practice this greatly facilitates producing computer programs that solve equations in any number of spatial dimensions, since they can be implemented as a simple dimension-by-dimension loop over the basic 1-D code. This easy extensibility favors the 1-D Shu–Osher ENO method over the otherwise comparable 1-D cell average form, which does not enjoy such a simple multidimensional extension. Thus, in the context of ultimately wanting to do multidimensional flow calculations, the Shu–Osher form is generally favored by its simplicity.

4. EXTENDING SHU–OSHER FORM TO NON-UNIFORM GRIDS

In problems where the solution has localized fine scale structure that must be fully resolved, it is computationally efficient to do local grid refinement. Such situations can arise in purely hyperbolic problems, for example due to shock wave focusing or merging of material contact discontinuities. Thus it is desirable that discretization methods for conservation equations have extensions to non-uniform grids.

The standard cell average discretization procedure leading to (2) extends naturally to arbitrary non-uniform grids, although the reconstruction of values from the cell averages can become quite complicated, depending on the complexity of the grid structure.

In contrast, if we try and repeat our derivation of the Shu–Osher finite difference form from the cell average discretization, the argument breaks down because the cell-average operator $\mathscr{A}$ no longer commutes with the finite difference operator $\varDelta$. This suggests that the Shu–Osher form may not extend to non-uniform grids. Indeed, we will show that in general it does not, even for smoothly stretched non-uniform grids, although it is possible for the special cases of exponentially or quadratically stretched grids. However, we will also show how the Shu–Osher form can easily be employed in a way that does extend to all smoothly stretched 1-D grids (and the product of such grids, in higher dimensions), retaining all the desirable properties of accuracy, simplicity and shock-capturing form.

We will not address the practically important and difficult problem of extending these methods to grids that have abrupt changes in cell size, but the analytical techniques presented here may be of use in these situations as well. Also, in section (4.4) we briefly describe one general framework for adaptive gridding that is in principle compatible with the Shu–Osher form.

4.1. Failure of the Derivation for Non-Uniform Grids

First we will consider in detail what goes wrong when we attempt to derive the Shu–Osher form from the cell average form, since this is the underlying reason for the difficulties on non-uniform grids. To facilitate the discussion we need to generalize our conception of a grid and the associated operators. We will assume a grid on x in 1-D is produced by a smooth, monotone mapping function $x(\alpha)$ applied to a uniform grid on α of spacing $\Delta\alpha$. The cell average operator is given by essentially the same form as before,

$$\mathscr{A}[f](x(\alpha)) = \int_{x(\alpha - \frac{\Delta\alpha}{2})}^{x(\alpha + \frac{\Delta\alpha}{2})} f(x)\, dx, \tag{25}$$

but we no longer divide by Δx in order to simplify the subsequent analysis. Similarly, the associated central finite difference operator becomes

$$\Delta f(x(\alpha)) = f\left(x\left(\alpha + \frac{\Delta\alpha}{2}\right)\right) - f\left(x\left(\alpha - \frac{\Delta\alpha}{2}\right)\right). \tag{26}$$

Using this generalized notation, we can follow the derivation leading to the standard Shu–Osher form (4) starting from cell averages. We can proceed as before up to the point of interchanging the order of cell averaging and finite differencing

$$\mathscr{A}^{-1}\Delta f = \Delta\mathscr{A}^{-1}f, \tag{27}$$

but the derivation fails at this point. One can easily show that if this relation is generally valid, the grid must be uniform. Specifically, if we evaluate the equivalent measure of commutivity $\mathscr{A}\Delta - \Delta\mathscr{A}$, we find that for any function g,

$$(\mathscr{A}\Delta - \Delta\mathscr{A})[g](x(\alpha)) = \int_{\alpha - \frac{\Delta\alpha}{2}}^{\alpha + \frac{\Delta\alpha}{2}} \mathscr{C}(\alpha; g, x, \Delta\alpha)\, d\alpha \tag{28}$$

where the integrand is

$$\mathscr{C}(\alpha; g, x, \Delta\alpha) = g\left(x\left(\alpha + \frac{\Delta\alpha}{2}\right)\right)\left(x'\left(\alpha + \frac{\Delta\alpha}{2}\right) - x'(\alpha)\right)$$
$$- g\left(x\left(\alpha - \frac{\Delta\alpha}{2}\right)\right)\left(x'\left(\alpha - \frac{\Delta\alpha}{2}\right) - x'(\alpha)\right). \tag{29}$$

If the commutator integral (28) is to be zero for all choices of $g(x)$ and $\Delta\alpha$, then we must have $\mathscr{C}$ vanish for all g and $\Delta\alpha$ as well, and hence we must have $x'(\alpha + \frac{\Delta\alpha}{2}) = x'(\alpha)$ for all $\Delta\alpha$. Thus x' is constant, which means the grid $x(\alpha)$ is uniform.

Simply summarized, when the grid is not uniform, the cell averaging operation $\mathscr{A}$ is not translation invariant and thus does not commute with the translation operator Δ. This is the fundamental reason why the Shu–Osher form cannot be derived in this case.

However, this breakdown of the derivation does not strictly imply the Shu–Osher form does not exist for such grids. In fact, to derive a Shu–Osher conservation form in greatest generality, we do not actually need the exact commutation relation

$$\mathscr{A}^{-1}\Delta - \Delta\mathscr{A}^{-1} = 0. \tag{30}$$

It would suffice for this commutator itself to be a conservation-form difference of some operator $\mathscr{G}$ (that must be conveniently constructable from f), i.e.,

$$\mathscr{A}^{-1}\Delta - \Delta\mathscr{A}^{-1} = \Delta\mathscr{G}, \tag{31}$$

since then we would obtain the generalized Shu–Osher form

$$\frac{du}{dt} + \frac{\Delta H}{\Delta x} = 0, \tag{32}$$

where $H = \mathscr{A}^{-1}f + \mathscr{G}[f] = h + \mathscr{G}[f]$. The main drawback of this more general form is that only h can be constructed using the elegant divided difference techniques given in $[7]$—$\mathscr{G}[f]$ would presumably have to be constructed by a series expansion, comparable to that for h in (6).

If we rewrite this most general commutation relation (31) in terms of the more tractable operator $\mathscr{A}$ instead of $\mathscr{A}^{-1}$, it becomes

$$\Delta\mathscr{A} - \mathscr{A}\Delta = \mathscr{A}\,\Delta\mathscr{G}\mathscr{A}. \tag{33}$$

Because of the complexity of the right hand side and the unspecified nature of $\mathscr{G}$, this relation (33) is not of practical value for deciding when a given non-uniform grid allows the general Shu–Osher form. Its main value is to show the possibility that some exceptional non-uniform grids may still allow this form, although in those cases it will not be possible to rely (solely) on the elegant Shu–Osher divided difference reconstruction technique. We will give a complete characterization of these "exceptional" non-uniform grids in the subsequent sections.

4.2. Non-Uniform Grids that Allow the Shu–Osher Form

Now we will show directly that the Shu–Osher finite difference form exists only for special classes of smoothly stretched grids.

4.2.1. The General Condition

The precise question is this: given a non-uniform grid $x(\alpha)$, is it is possible to obtain the exact functional relation

$$\frac{df}{dx} = \frac{\Delta H}{\Delta x} \tag{34}$$

where Δ is the difference operator associated with $x(\alpha)$, and $H[f](x)$ is an "essentially locally constructable" functional of f, i.e., to any given order of accuracy in $\Delta\alpha$, $H(x(\alpha))$ can be expressed in terms of local f values, $f(x(\alpha + j\,\Delta\alpha))$, $j = -k,..., k$, where k depends only the desired order. The local constructability of H is essential for a practical numerical algorithm, and is carried out by the upwind biased divided difference table reconstruction in the standard uniform grid Shu–Osher finite difference method [7], where $H = h$. The alternative series expansion for h in Eq. (6) gives a more concrete example of what it means to be essentially locally constructable. There we see that formally h could *not* be computed using a local stencil, since it depends on derivatives of all orders of f. But, up to any desired order of accuracy in $\Delta\alpha$, $h(x)$ depends on only a finite number of derivatives of f at x and thus can be approximated using a local stencil on the grid near x—hence the "essentially" locally constructable.

Note that the defining relation (34) trivially implies a unique solution for H on any given grid $\{x(\alpha_j)\}$, obtained by summing the relation from an arbitrary starting point $x_0 = x(\alpha_0)$ to get

$$H(x_{n+\frac{1}{2}}) = H(x_{0-\frac{1}{2}}) + \sum_{j=0}^{j=n} f'(x_j)\,\Delta x_j \tag{35}$$

where $x_j = x(\alpha_j)$, $\alpha_j = \alpha_0 + j\,\Delta\alpha$, and $\Delta x_j = x(\alpha_j + \frac{\Delta\alpha}{2}) - x(\alpha_j - \frac{\Delta\alpha}{2})$. Thus, on any given grid there is no ambiguity as to what H must be, and we immediately have an exact—but *nonlocal*—expression for H. The only remaining question is under what conditions there exists (to any desired order of accuracy) a local expression for H as well. We already know that in the case of a uniform grid such an expression exist, as exhibited by the series expansion for h in Eq. (6).

4.2.2. A Negative Example

We will give a simple example that shows such local expressions do not always exist, so it is not possible to obtain the Shu–Osher form in general. Let $x_j = j\,\Delta x$ be a uniform grid with spacing Δx, and let $X(\alpha)$ be a grid identical to the uniform one, $X(j\,\Delta x) = x_j$, except that a single grid node J is displaced, $X(J\,\Delta\alpha) = x_J + \beta\,\Delta x$, where $0 < \beta < 1$. Let h be the standard Shu–Osher function corresponding to the uniform grid x, and let H be the function defined by the nonlocal summation for grid X via the summation formula (35). Then, comparing their respective explicit summation forms, we see they differ only in the J term, so that at any point x_n we have

$$H(x_{n+\frac{1}{2}}) = \underbrace{h(x_{n+\frac{1}{2}})}_{\text{local}} + \underbrace{(f'(X_J)\,\Delta X_J - f'(x_J)\,\Delta x)}_{\text{non-local}}. \tag{36}$$

This shows H equals an essentially locally constructable part (since h is), expressible via f values near x_n, plus a "truly nonlocal" error term that fundamentally depends on values of f near the remote point x_J, thus no essentially local expression for H can be possible. Specifically, if there were some local expression

$$H(x_{n+\frac{1}{2}}) = L(x_{n-k(p)},..., x_{n+k(p)}) + O(\Delta\alpha^p) \tag{37}$$

it would imply a relation between f values near x_J and near x_n

$$(f'(X_J)\,\Delta X_J - f'(x_J)\,\Delta x) = G(x_{n-k(p)},..., x_{n+k(p)}) + O(\Delta\alpha^p) \tag{38}$$

for arbitrarily large p, and x_n arbitrarily far from x_J, yet no such relation (with a truly small $O(\Delta\alpha^p)$ error term) is possible for general smooth f.

The example given uses an "unresolved" non-uniform grid x, i.e., with abrupt change in cell size at the particular $\Delta\alpha$ considered. This was for simplicity and is not essential to the argument. The same argument can be applied to a grid that is smoothly distorted from uniform near x_J, such as

$$x(\alpha) = \alpha + b(\alpha - x_J) \tag{39}$$

where b is a smooth bump of compact support and with $|b'| < 1$, and $\Delta x \ll 1$, yielding the same result that $H(x_{n+\frac{1}{2}})$ has a truly nonlocal dependence on the values of f near the distant point x_J.

4.2.3. Solving the General Condition

Now that we have demonstrated that local expressions are not always possible, we return to the general question of whether a local expression exists for H. We will need the Euler–Maclaurin summation formula [1, p. 806, formula 23.1.30], which for our purposes says: for a uniform grid α_i of spacing $\Delta\alpha$, and any smooth $F(\alpha)$, the midpoint rule summation and corresponding integral differ only by terms depending on F at the endpoints as follows

$$\sum_{i=0}^{n} F(\alpha_i)\,\Delta\alpha = \int_{\alpha_{0-\frac{1}{2}}}^{\alpha_{n+\frac{1}{2}}} F(\alpha)\,d\alpha + \mathscr{E}[F](\alpha_{n+\frac{1}{2}}) - \mathscr{E}[F](\alpha_{0-\frac{1}{2}}) \tag{40}$$

where the $\mathscr{E}[F]$ is a functional given formally by an asymptotic series expansion

$$\mathscr{E}[F](\alpha) = c_0 F(\alpha) + c_1 F'(\alpha)\,\Delta\alpha + c_2 F''(\alpha)\,\Delta\alpha^2 + \cdots + c_n F^{(n)}(\alpha)\,\Delta\alpha^n + \cdots \tag{41}$$

for certain coefficients c_n. (Note: the Euler–Maclaurin summation formula is usually written with integration limits α_0 and α_n; the altered form we use here must including corresponding terms in $\mathscr{E}[F]$ that compensate for shifting the endpoints by $\frac{\Delta\alpha}{2}$.)

Applying this to the sum that occurs in the summation form for H in (35), we obtain

$$\sum_{j=0}^{j=n} f'(x_j)\,\Delta x_j = \sum_{j=0}^{j=n} f'(x(\alpha_j)) \frac{(x(\alpha_j + \frac{\Delta\alpha}{2}) - x(\alpha_j - \frac{\Delta\alpha}{2}))}{\Delta\alpha}\,\Delta\alpha$$

$$= \int_{\alpha_{0-\frac{1}{2}}}^{\alpha_{n+\frac{1}{2}}} f'(x(\alpha)) \left(\frac{(x(\alpha + \frac{\Delta\alpha}{2}) - x(\alpha - \frac{\Delta\alpha}{2}))}{\Delta\alpha} \right) d\alpha$$

$$+ \mathscr{E}[Gf'](\alpha_{n+\frac{1}{2}}) - \mathscr{E}[Gf'](\alpha_{0-\frac{1}{2}}) \tag{42}$$

where $G(\alpha) = \Delta x / \Delta \alpha$ as indicated. We change variable in the integral from α to x via $dx = x'\, d\alpha$, and adopt a more succinct notation to obtain

$$\sum_{j=0}^{j=n} f'(x_j)\, \Delta x_j = \int_{x_{0-\frac{1}{2}}}^{x_{n+\frac{1}{2}}} f'(x)\, g(x)\, dx + \mathscr{E}[gx'f']_{n+\frac{1}{2}} - \mathscr{E}[gx'f']_{0-\frac{1}{2}} \qquad (43)$$

where $g(x) = g(x(\alpha)) = \frac{x(\alpha + \frac{\Delta\alpha}{2}) - x(\alpha - \frac{\Delta\alpha}{2})}{x'(\alpha)\, \Delta\alpha} = G/x'$.

Using result (43) in the summation formula for H, (35), we get

$$H(x_{n+\frac{1}{2}}) = \mathscr{E}[gx'f'](\alpha_{n+\frac{1}{2}}) + \int_{x_{0-\frac{1}{2}}}^{x_{n+\frac{1}{2}}} f'(x)\, g(x)\, dx + H_0, \qquad (44)$$

where we will from now on absorb all x_0 terms into the constant term H_0. Integrating by parts to take the derivative off f gives

$$H(x_{n+\frac{1}{2}}) = \mathscr{E}[gx'f'](\alpha_{n+\frac{1}{2}}) + f(x_{n+\frac{1}{2}})\, g(x_{n+\frac{1}{2}}) - \int_{x_{0-\frac{1}{2}}}^{x_{n+\frac{1}{2}}} f(x)\, g'(x)\, dx + H_0. \quad (45)$$

The only nonlocal term (i.e., away from x_n) in this expression is the integral, and thus H has a local expression only if this integral vanishes for all smooth f. This is possible only if $g'(x) = 0$, i.e., if $g(x)$ is constant. In this case we can write $g(x) = \gamma(\Delta\alpha)$, depending only on $\Delta\alpha$, and we get

$$H(x) = \gamma(\Delta\alpha)(\mathscr{E}[x'f'](\alpha(x)) + f(x)) + H_0 \qquad (46)$$

as the essentially local construction of H from f. Given the general form of $\mathscr{E}$ coming from the Euler–Maclaurin error term (41), this is an asymptotic series expansion for H in terms of derivatives of f and $\Delta\alpha$.

As noted, this local form exists only for grids for which $g(x) = \gamma(\Delta\alpha)$ is constant, which implies

$$x\left(\alpha + \frac{\Delta\alpha}{2}\right) - x\left(\alpha - \frac{\Delta\alpha}{2}\right) = \gamma(\Delta\alpha)\, x'(\alpha)\, \Delta\alpha. \qquad (47)$$

If we Taylor expand the left side in $\Delta\alpha$ we obtain a relation between all odd order derivatives of x,

$$x'(\alpha)\, \Delta\alpha + 2\, \frac{x'''(\alpha)\, \Delta\alpha^3}{3!} + \cdots = \gamma(\Delta\alpha)\, x'(\alpha)\, \Delta\alpha. \qquad (48)$$

There are only two ways such a (pseudo-)differential equation can be satisfied—either all odd order derivatives of x must be nontrivially proportional to x', in which case x must have the exponential form

$$x(\alpha) = ae^{c\alpha} + be^{-c\alpha} \qquad (49)$$

for arbitrary constants a, b, and c (which could be complex, allowing sinusoidal solutions as well), and $\gamma = (e^{c\Delta\alpha/2} - e^{-c\Delta\alpha/2})/c$, or x''' and all higher odd order derivatives must simply vanish, in which case x must be a quadratic function

$$x(\alpha) = a + b\alpha + c\alpha^2. \tag{50}$$

for arbitrary constants a, b and c, and $\gamma = 1$.

As an aside, note the analysis in this section solves the "paradox" of how the apparently nonlocal explicit summation form for H (or h) in Eq. (35) can collapse into a local form—under the right circumstances, the summation can be expressed entirely as integrals of derivatives (this is the basis of the Euler–Maclaurin error formula as well), which all integrate to just endpoint values.

4.2.4. Exceptional Grids in Practical Application

We have shown that only two special types of non-uniform grid—exponentially stretched and quadratically stretched—allow the Shu–Osher form, and in these cases local construction of H from f is provided only by the asymptotic series in Eq. (46). Since both forms of stretching may be useful for resolving a fine scale feature near one end of the grid, the Shu–Osher form for these grids may be of practical value in special cases. However, the standard Shu–Osher divided difference construction from [7] cannot be used to construct H. This added bit of complexity may make it more desirable to use the more flexible, less exact, approach of the next section, even though these special non-uniform grids in principle allow the exact Shu–Osher finite difference conservation form.

However, we will further develop the H construction for these special cases, which may enhance their practical value. Foremost, we can derive the unspecified coefficients c_n in the required series expansion (41). Note that our general derivation of H applies to the special case of a uniform grid, $x(\alpha) = \alpha$, in which case $H = h$ and we already have the Shu–Osher series expansion for h given succinctly in Eq. (16). Thus the series derived here in (46) must be identical, i.e. we must have (using $x' = 1$ and $\gamma = 1$ in this case)

$$\mathscr{E}[f'] + f = \theta \csc \theta f. \tag{51}$$

Since this holds for all smooth f, it determines the general coefficients c_n for $\mathscr{E}$ in (41). Indeed, we get that $c_k = 0$ for all even $k \geqslant 0$, and

$$c_{2n-1} = a_{2n} \, \Delta\alpha \tag{52}$$

for all $n > 0$, where a_{2n} are the same coefficients for the Shu–Osher series (18). Given this close relation between the series expansions for h and H, its seems possible that the standard Shu–Osher reconstruction from primitives procedure in [7] may also have a closely related reconstruction for H, even though we have no obvious apriori primitive relation for H comparable to that for h (7).

As an amusing aside, note that the c_n-defining relation (51) is valid for any smooth f, and thus provides a novel closed form expression for the error term in (our slightly modified form of) the Euler–Maclaurin summation formula (40).

4.3. A Shu–Osher Form Suitable for General Non-Uniform Grids

Fortunately, the Shu–Osher finite difference form can easily be employed in a way suitable for all smoothly stretched grids. In this case, using

$$\frac{df}{dx} = \frac{df}{d\alpha}\frac{d\alpha}{dx}$$
$$= g(x)\frac{df}{d\alpha} \tag{53}$$

where $g(x) = 1/x'$, we can rewrite the conservation law in equivalent form as

$$\frac{dU}{dt} + \frac{df}{d\alpha} = 0, \tag{54}$$

where $U(x,t) = u(x,t)/g(x)$. This form can be semi-discretized using the standard Shu–Osher form on the uniform α grid,

$$\frac{dU}{dt} + \frac{\Delta h}{\Delta \alpha} = 0, \tag{55}$$

where h is the Shu–Osher function $h(\alpha)$ from $f(\alpha) = f(x(\alpha))$. Of foremost importance, this conservation form will ensure that discontinuities in U—and hence in u, since they are related by a smooth multiplier—move at the right speed. The h function is obtained from the standard construction on the uniform α grid. In practice this simply means using the standard divided difference table reconstruction on the nodal f values on the x_i grid, but using $\Delta\alpha$ instead of Δx as the grid spacing parameter. Thus it is a trivial modification of the standard construction procedure.

Multiplying this form by g to transform back to the standard unknown u shows that

$$\frac{du}{dt} + g(x)\frac{\Delta h}{\Delta \alpha} = 0 \tag{56}$$

is a suitable generalization of the Shu–Osher form, even though it is not itself in strict conservation form. In practice $g = 1/x'$ may need to be computed using numerical derivatives. Because it is smooth, it suffices to use central difference of the desired order of accuracy to evaluate this factor.

Thus we see that the standard Shu–Osher form and h construction both carry over directly to the case of a smoothly stretched grid, although instead of

$$\sum u_i\,\Delta x_i \tag{57}$$

being the discretely conserved quantity, it will now be

$$\sum u_i\,dx_i \tag{58}$$

where $dx_i = x_i'\,\Delta\alpha$.

In [5], Osher and Chakravarthy developed this smoothly stretched grid approach in detail for an earlier class of conservative difference schemes. They include the treatment of multiple dimensions, boundary conditions and the Euler Equations, as well as a detailed proof that this special non-conservative form is sufficient to ensure that converged solutions are indeed weak solutions of the governing conservation laws. Their developments can be directly applied to the Shu–Osher discretization outlined here.

4.4. An Alternative Extension for Adaptive Grid Refinement

We conclude our discussion of non-uniform grids by mentioning that Harten [2] has introduced an alternative approach that allows use of the standard Shu–Osher form with locally refined grids. In his framework, only uniform grids are used for discretization, but a multiresolution hierarchy of such grids is maintained, allowing local refinement via passage to a finer grid only where needed. The development of this approach was disrupted by Harten's untimely death, but further research can be found in Harten's series of unpublished technical reports [3]. These early results are promising and suggest that it may be possible to develop a full (multidimensional space and time) adaptive gridding version of the Shu–Osher finite difference ENO. Making the Shu–Osher form compatible with robust adaptive gridding remains one of the outstanding problems in the development of the highly successful class of ENO methods, and it is both a challenging and important problem for future research efforts.

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