Non-Oscillatory Third Order Fluctuation Splitting Schemes

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ABSTRACT. This paper addresses the issue of constructing non-oscillatory, higher than second order, multidimensional, fluctuation splitting methods on unstructured triangular meshes. It highlights the reasons why current approaches fail and proposes a potential solution to these problems. The results presented for a simple steady state scalar advection problem show significant improvements on previous methods.

RÉSUMÉ. Ce papier aborde la question de l'élaboration de schémas non-oscillants, d'ordre supérieur à deux, multidimensionnels et de type "fluctuation splitting" sur des maillages triangulaires non-structurés. Il expose les raisons de l'échec des approches actuelles et propose une solution potentielle à ces problèmes. Les résultats obtenus pour un problème simple d'advection scalaire stationnaire montrent des améliorations significatives par rapport aux méthodes existantes.

KEYWORDS: Fluctuation splitting, monotonicity, high order. MOTS-CLÉS : "Fluctuation splitting", monotonicité, ordre élevé.

1. Introduction

The fluctuation splitting approach to approximating multidimensional systems of conservation laws has developed to a stage where it can be used reliably to produce accurate simulations of complex steady state fluid flow phenomena using unstructured meshes [DSA 00]. For steady state computations, second order methods are deemed accurate enough in the majority of practical situations and, within the fluctuation splitting framework, the PSI scheme [DSBR 94] has shown itself to provide an ideal basis for a range of highly successful methods. It is an upwind scheme which is second order accurate at the steady state, guarantees monotonicity (even in the presence of discontinuities), and gives rapid convergence to the steady state, all without the necessity for additional artificial viscosity.

More recently, research has focused on the development of higher order methods. This has largely been with a view to approximating time-dependent problems, which require the discrete forms of both temporal and spatial derivative terms to be much higher order (typically orders of accuracy of between three and five are preferred), if any degree of accuracy is to be maintained over long times. They should also prove useful in the approximation of higher order derivatives (*cf.* the Boussinesq equations for shallow water flow), even for steady state computations.

The first method to achieve third order accuracy did so by integrating the temporal derivative terms in a manner consistent with the spatial derivative terms (in the context of a Petrov-Galerkin finite element method) [Fer 97, Mär 96] but it relied heavily on the structure of the computational mesh for success. A number of approaches have subsequently been proposed, all of which are based on alternative methods of constructing a higher order representation of the underlying flow variables, *e.g.* piecewise quadratics lead to a third order method. This is used to construct a high order fluctuation which, if distributed completely using bounded distribution coefficients, gives the high order method [Abg 01, AM 03]. Caraeni et al. [CCF 01] created the quadratic representation within each mesh cell via the reconstruction of local gradients of the dependent variables at the mesh nodes using the surrounding data. It was distributed using the non-monotone LDA scheme so, although the results shown for smooth Navier-Stokes flows were excellent, unphysical oscillations can still occur at high Reynolds number. Abgrall, along with Roe [AR 03] and Mezine and Andrianov [AAM 05, AM 04] have used a similar idea, but constructed the higher order fluctuation using extra information about the dependent variable stored at the additional nodes created by a uniform global subdivision of the mesh, and updated the solution using a distribution on the subtriangles. The proposed schemes are third (and higher) order and *almost* non-oscillatory. The approach of Hubbard and Laird [HL 05] obtained higher order by extending the stencil of the distribution for a lower order fluctuation. This can be linked with the methods of Abgrall *et al.* by noting that the high order fluctuation on each mesh cell can, in simple cases, be written in terms of low order fluctuations on the subcells.

Each approach has achieved higher than second order accuracy for the scalar advection equation, and that of Caraeni *et al.* has already shown a great deal of promise in more practical situations. However, none of them has yet achieved the higher accuracy without losing monotonicity, except with the aid of a post-processing step, such as the Flux-Corrected Transport algorithm [LMVBB 88, Zal 79] used by Ferrante [Fer 97] and Hubbard and Roe [HR 00]. This paper is concerned with the search for this ideal combination. It will consider the scalar advection equation, summarising the previous methods and discussing the reasons why they have not yet succeeded completely. It will offer some suggestions for how the problem might be overcome and show some preliminary results which improve significantly on those of the previous methods.

2. Fluctuation Splitting

Consider the two-dimensional scalar conservation law given by

$$u_t + f_x + g_y = 0$$
 or $u_t + \vec{\lambda} \cdot \vec{\nabla} u = 0$ (1)

on a domain Ω , with u(x, y, t) = g(x, y, t) imposed on the inflow part of the boundary $\partial \Omega$. $\vec{\lambda} = \left(\frac{\partial f}{\partial u}, \frac{\partial g}{\partial u}\right)^T$ defines the advection velocity associated with the conservation law (1). This equation has an associated fluctuation, assumed here to be calculated over a triangular mesh cell \triangle and given by

$$\phi = -\int \int_{\Delta} \vec{\lambda} \cdot \vec{\nabla} u \, d\Omega = \oint_{\partial \Delta} u \, \vec{\lambda} \cdot d\vec{n}$$
⁽²⁾

in which \vec{n} represents the inward pointing normal to the cell boundary. When u is assumed to have a piecewise linear continuous representation with values stored at the mesh nodes, the discrete counterpart of ϕ is evaluated using an appropriate (conservative) linearisation [DSBR 94]. Ideally, this allows the integration in Equation (2) to be carried out exactly, giving

$$\phi = -S_{\triangle} \hat{\vec{\lambda}} \cdot \vec{\nabla} u = -\frac{1}{2} \sum_{i \in \triangle} u_i \hat{\vec{\lambda}} \cdot \vec{n}_i \tag{3}$$

where S_{\triangle} is the cell area and the symbol $\hat{}$ indicates an appropriately linearised quantity. The index *i* loops over the vertices of \triangle , and \vec{n}_i is the inward unit normal to the i^{th} edge (opposite the i^{th} vertex) multiplied by the length of that edge. This linearisation is straightforward in the special case of linear advection [DSBR 94].

A simple forward Euler discretisation of the time derivative leads to an iterative update of the nodal solution values which is generally written [DSBR 94] as

$$u_i^{n+1} = u_i^n + \frac{\Delta t}{S_i} \sum_{j \in \bigcup \triangle_i} \alpha_i^j \phi_j \tag{4}$$

where Δt is the time-step, S_i is the area of the median dual cell corresponding to node i (one third of the total area of the triangles with a vertex at i), α_i^j is the distribution coefficient which indicates the appropriate proportion of the fluctuation ϕ_j to be sent from cell j to node i, and $\bigcup \Delta_i$ represents the set of cells with vertices at node i. Conservation is assured as long as

$$\sum_{i \in \Delta_j} \alpha_i^j = 1 \qquad \forall j \tag{5}$$

where \triangle_j represents the set of nodes at the vertices of cell *j*, *i.e.* the whole of each fluctuation is sent to the nodes. Note that the distribution has been restricted here so that a cell can only make contributions to nodes at its own vertices. This allows the

scheme to be implemented very efficiently. The time derivative term in this construction is included here purely as a device for iterating to the steady state, but its presence would be necessary for time-dependent problems when it must be integrated in a manner consistent with the underlying representation of u if the order of accuracy of the steady state approach is to be maintained [AAM 05, CCF 01].

2.1. The N Scheme

The attempts to impose monotonicity on the higher order schemes presented here rely heavily on the low order, non-oscillatory fluctuation distribution scheme known as the N-scheme [DSBR 94], which is defined as follows:

(1) For each triangle, locate the downstream vertices, *i.e.* those for which $\vec{\lambda} \cdot \vec{n_i} > 0$, where $\vec{n_i}$ is the inward pointing normal to the edge opposite vertex *i*.

(2a) If a triangle has a single downstream vertex, node i_1 say, then that node receives the whole fluctuation ϕ , so

$$u_{i_1} \to u_{i_1} + \frac{\Delta t}{S_{i_1}} \phi \tag{6}$$

while the values of u at the other two vertices remain unchanged.

(2b) Otherwise, the triangle has two downstream vertices, i_1 and i_2 say, and the fluctuation ϕ is divided between these two nodes so that

$$u_{i_1} \to u_{i_1} + \frac{\Delta t}{S_{i_1}} \phi_{i_1} \qquad u_{i_2} \to u_{i_2} + \frac{\Delta t}{S_{i_2}} \phi_{i_2}$$
(7)

where

$$\phi_{i_1} = -\frac{1}{2}\hat{\vec{\lambda}} \cdot \vec{n}_{i_1}(u_{i_1} - u_{i_3}) \qquad \phi_{i_2} = -\frac{1}{2}\hat{\vec{\lambda}} \cdot \vec{n}_{i_2}(u_{i_2} - u_{i_3}) \qquad (8)$$

in which i_3 denotes the remaining (upstream) vertex of the triangle. It is easily shown that $\phi_{i_1} + \phi_{i_2} = \phi$ (for conservation).

The distribution coefficients, α_i^j in Equation (4), can be derived easily from Equations (6)–(8) [DSBR 94]. The resulting scheme is globally positive and therefore the iteration given by (4) is conditionally stable, the appropriate restriction on the time-step being

$$\Delta t \leq \frac{S_i}{\sum_{j \in \cup \Delta_i} \max\left(0, \frac{1}{2}\hat{\vec{\lambda}} \cdot \vec{n}_i^j\right)}.$$
(9)

Results: The test case used here to illustrate the properties of each scheme consists of advection in a circle, with velocity $\vec{\lambda} = (y, -x)^T$ and over the domain $[-1, 1] \times [0, 1]$, of the initial profile given by

$$u(x, y, 0) = \begin{cases} G(x) & \text{for } -0.65 \le x \le -0.35, \ y = 0 \\ 0 & \text{otherwise} \end{cases}$$
(10)

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This is also imposed as the boundary function g(x, y, t) on the inflow boundaries of the domain while the experiment is run to steady state. The exact solution is u(x,y) = G(r) for $0.35 \le r = \sqrt{x^2 + y^2} \le 0.65$ and zero elsewhere. Results are shown in Figure 1 for a subdivided (see Section 3) uniform but genuinely unstructured triangular mesh consisting of 984 nodes and 1846 cells. The two cases shown use G(r) = 1 (Test Case A), which illustrates the monotonicity of the scheme and $G(r) = \cos^2(10\pi(r+0.5)/3)$ (Test Case B), which is more appropriate for determining the order of accuracy. Both show the significant level of numerical diffusion incurred.

Figure 1. The N scheme applied to Test Case A (left) and Test Case B (right).

2.2. The PSI Scheme

The PSI scheme, devised by Struijs [Str 94] and formulated algebraically by Sidilkover and Roe [SR 95], is the most commonly used of the second order non-oscillatory fluctuation splitting schemes, and is easily defined once the N-scheme has been described.

Given that the contribution made by cell j to node i by the N scheme can be written as $(\phi_i^j)^N = (\alpha_i^j)^N \phi_j$, where ϕ_j is the fluctuation in cell j (see (3)), the contributions due to the PSI scheme can be defined as follows:

$$(\phi_i^j)^{PSI} = \frac{[(\alpha_i^j)^N]^+}{\sum_{k \in \Delta_j} [(\alpha_k^j)^N]^+} \phi_j = (\alpha_i^j)^{PSI} \phi_j$$
(11)

in which $[]^+$ denotes the positive part of the quantity within the square brackets. This scheme has a number of notable properties (for all nodes *i* and cells *j*):

$$\begin{split} &-\sum_{k\in \bigtriangleup_j} (\alpha_k^j)^{PSI} = \sum_{k\in \bigtriangleup_j} (\alpha_k^j)^N = 1, \text{ so the scheme is conservative.} \\ &- (\alpha_i^j)^{PSI} (\alpha_i^j)^N \geq 0, \text{ so the scheme is non-oscillatory.} \end{split}$$

 $-|(\alpha_i^j)^{PSI}| \le |(\alpha_i^j)^N|$, so the limit on the time-step given by (9) is sufficient to maintain this monotonicity.

 $-(\alpha_i^j)^{PSI}$ is bounded, so the order of accuracy of the steady state scheme is equivalent to the order of accuracy with which ϕ is represented (in this case second order) [Abg 01, AM 03]. This is often referred to as linearity preservation.

Results: The results for the PSI scheme are shown in Figure 2 using the same mesh as before. The improvement in accuracy over the N scheme is clear, as is the lack of oscillations.

Figure 2. The PSI scheme applied to Test Case A (left) and Test Case B (right).

3. A Third Order Method

The scheme proposed by Abgrall and Roe [AR 03] is based on a simple generalisation of the above procedure. The main difference is that the fluctuation ϕ is approximated to higher order. The procedure generalises to arbitrary order and three space dimensions, but only the two-dimensional, third order case will be considered here. In this situation the dependent variable u is taken to be a continuous piecewise quadratic function with the unknowns stored at the nodes of a globally refined mesh, created by subdividing each triangular cell into four congruent subcells. This allows the construction of a unique local quadratic interpolating polynomial on each cell of the original mesh. The fluctuation (2) can be evaluated exactly on any subcell using an appropriate quadrature rule, and these can then be distributed to the nodes of the refined mesh. The method proposed is based on

$$(\phi_i^j)^{HO} = \frac{[(\alpha_i^j)^N]^+}{\sum_{k \in \Delta_j} [(\alpha_k^j)^N]^+} (\phi_j)^{HO} = (\alpha_i^j)^{HO} (\phi_j)^{HO}$$
(12)

in which $(\phi_j)^{HO}$ is calculated by evaluating (2) exactly, according to the high order (HO) representation of u. Note that the distribution remains local to each subcell.

Remark: There is no obvious reason why the approach of Caraeni *et al.* [CCF 01] could not be used to obtain an alternative construction for the high order fluctuations $(\phi_j)^{HO}$, without the necessity for mesh subdivision. However, it would suffer from similar problems to those discussed below so adjustments would also be required (probably to the local reconstruction of the solution gradients) if monotonicity were to be sought.

Results: The results for the Abgrall-Roe scheme are shown in Figure 3 using the same mesh as before. An improvement in accuracy is apparent in the profile at outflow of both test cases (illustrated more clearly by the error measures given in Table 1). However, this is at the expense of small oscillations just visible at the discontinuities close to the inflow boundary in Test Case A (see also Table 1.

Figure 3. The Abgrall-Roe scheme applied to Test Case A (left) and Test Case B (right).

	N	PSI	Abgrall-Roe	Modified Abgrall-Roe
Test Case A: $\min(u)$	0.0000	0.0000	-0.0593	0.0000
Test Case A: $\max(u)$	1.0000	1.0000	1.0131	1.0000
Test Case B:				
$\max(u)$ at outflow	0.5877	0.8346	0.9702	0.9109

 Table 1. Accuracy measures (none of the "non-oscillatory" results goes negative).

3.1. The Problem

There are two significant issues here, neither of which arises in the discussion of the PSI scheme because in that case, in the terminology used below, $(\phi_j)^{HO} \equiv (\phi_j)^{LO}$.

(1) $(\phi_j)^{HO} (\phi_j)^{LO} < 0$ for some subcells j: the high and low order (LO) fluctuations have different signs. This is most damaging in subcells where the N scheme gives only non-negative distribution coefficients $(\alpha_i^j)^N$. In such situations the scheme (12) gives only zero distribution coefficients, clearly violating conservation. Abgrall and Roe proposed a modification to avoid this [AR 03], but this defaulted to a central discretisation, $\alpha_i^j = \frac{1}{3}$, $\forall i \in \Delta_j$, in such situations, which is not monotone.

(2) $|(\phi_j)^{HO}| \gg |(\phi_j)^{LO}|$ for some subcells j, even when $(\phi_j)^{HO} (\phi_j)^{LO} \ge 0$. The magnitude of the high order fluctuation can be much higher than that of the low order fluctuation, even when they have the same sign. (A similar comment holds for the nodal contributions.) This not only places a more restrictive condition than (9) on the time-step if the scheme is to be monotone, but also affects the monotonicity of the steady state.

In some circumstances, which occur repeatedly in Test Case A, $(\phi_j)^{HO}$ can be nonzero in a subcell for which $u_{i_1} = u_{i_2} = u_{i_3}$. In such situations it becomes impossible to distribute $(\phi_j)^{HO}$ to the vertices of subcell j in a conservative manner while maintaining local or, in some cases, global positivity. Hence, for a monotone scheme of this type, the stencil of the distribution of the subcell fluctuations must be extended. The most obvious (and efficient) extension is to allow distribution to the subvertices of the associated mesh cell J. It is always possible to distribute $(\phi_J)^{HO} = \sum_{\Delta_k \in \Delta_J} (\phi_k)^{HO}$ to the six subvertices of cell J in a manner which is both conservative and locally positive (although it is not yet clear what an appropriate monotone time-step restriction would be, cf. (9)).

Remark: At this stage of the development of a high order non-oscillatory finite volume scheme a limiter would be introduced to combine the low order monotone and the high order non-monotone schemes. Here, unfortunately, this would lead to a mismatch in the calculations of fluctuations in neighbouring cells and the edge contributions in the boundary integrals in (2) would no longer cancel at internal edges, leading to a non-conservative scheme. It is worth noting though that Abgrall and Barth [AB 02] have demonstrated that this may not always be a problem in practice.

3.2. A Modified Scheme

It is clear that there are many possible alternatives for distributing $(\phi_J)^{HO}$ to the six subvertices of cell J in a manner which improves the monotonicity properties of the scheme. Two questions which should be considered when making an appropriate choice are as follows.

- Should the distribution be upwind? This clearly relates to the nature of the physical problem and tends to aid convergence to the steady state, but it has yet to be proved that it is possible (or not) in every situation while maintaining conservation and linearity preservation.

– Should the adjustments to the scheme be made to the subcell fluctuations before distribution or directly to the contributions they make to the vertices? In order to remain local the latter procedure would have to be applied before the updates were accumulated at the nodes, otherwise the Flux-Corrected Transport algorithm [Fer 97, HR 00, LMVBB 88, Zal 79] might as well be applied.

The approach proposed here is upwind (in the sense that no contribution is made to the upstream vertices of the upstream subtriangles) and the adjustments are applied directly to the subcell fluctuations, for simplicity. It takes the form of a simple postprocessing step (similar in character to the redistribution step of Hubbard and Roe [HR 00]). The following steps are applied to each mesh cell *J* in turn.

(1) Accumulate from each subcell j the fluctuations due to the Abgrall-Roe scheme which would be of the "wrong" sign, *i.e.* for which $(\phi_j)^{HO} (\phi_i^j)^{LO} \leq 0 \quad \forall i \in \Delta_j$ and $(\phi_j)^{HO} \neq 0$. Reset the fluctuations in the offending subcells to zero.

(2) Add to these a proportion of the high order fluctuations from any subcell j for which they are of an allowable sign but of significantly larger magnitude than the low order fluctuation on that subcell. In this work $(\phi_i^j)^{HO} - K(\phi_i^j)^{LO}$ was redistributed, leaving $K(\phi_i^j)^{LO}$ with the subcell (with K chosen, rather arbitrarily, to be 5).

(3) Add the fluctuations accumulated in steps (1) and (2) to the unaffected fluctuation of largest magnitude.

This process is guaranteed to be conservative, but not yet proved to be monotone, and the distribution coefficients for each of the subcell fluctuations are still bounded $(\alpha_i^j \in [0, 1])$.

Results: The results for the modified Abgrall-Roe scheme are shown in Figure 4, using the same mesh again. The accuracy seems similar (see also Table 1) and the oscillations close to the inflow boundary have completely disappeared from Test Case A, though at the expense of a slight distortion of the outflow profile.

4. Conclusion

It is an extremely challenging problem to construct a conservative fluctuation splitting scheme which is both higher than second order accurate and monotone. Many of the issues associated with this have been discussed, along with a suggested modification to an existing high order scheme which may ultimately lead to an approach which can be proved to have all of the desired properties. However, the work is still in progress.

Figure 4. The modified Abgrall-Roe scheme applied to Test Case A (left) and Test Case B (right).

As things stand, the oscillations have been completely removed in the chosen test case, although preliminary results that the new scheme does not retain the full third order accuracy of the Abgrall-Roe approach. It is left to future work to (i) confirm that the method (or a slight modification of it) genuinely is monotone, conservative and high order, (ii) prove that it is, (iii) apply it to nonlinear systems of equations, for which it may be necessary to construct an appropriate linearisation for system decomposition or matrix distribution (*cf.* [PDW 97]), and (iv) extend it to time-dependent problems, ideally in combination with a high order, non-oscillatory time-stepping scheme, such as the Runge-Kutta schemes presented in [SO 88].

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