

Combining high-order accuracy with non-oscillatory methods through monotonicity preservation[‡]

W. J. Rider^{1,*}, J. A. Greenough² and J. R. Kamm¹

¹*Los Alamos National Laboratory, NM 87545 Los Alamos, U.S.A.*

²*Lawrence Livermore National Laboratory, Livermore, CA 94550, U.S.A.*

SUMMARY

We have extended the usual notions used in high-resolution methods. Rather than applying a single principle such as monotonicity or essentially non-oscillatory stencil selection, we hybridize multiple principles applying them where they are most effective. We define methods that blend high-order accuracy with essentially non-oscillatory methods when monotonicity conditions are violated. The methods can be defined with a number of variants leading to results with differing properties. We also focus on the impact of the selection of the high-order accurate stencil on the overall method. Published in 2005 by John Wiley & Sons, Ltd.

KEY WORDS: high-order; non-oscillatory; monotonicity preserving

1. INTRODUCTION

There are a wide variety of high-resolution numerical methods for hyperbolic conservation laws. These methods are based on several different operating principles leading to properties that are advantageous under different conditions. These methods include a wide variety of methods operating on monotonicity principles such as van Leer's MUSCL algorithm [1] or PPM [2]. Other methods are based on choosing the smoothest stencils in some sense. These are the uniformly and essentially non-oscillatory (ENO) [3,4]. More recently, the weighted ENO methods have largely superseded the ENO methods in common use [5]. During the mid-to late-1990s Huynh and Suresh made progress in combining these two design principles into a single algorithm [6,7]. In this paper, we extend their algorithms in terms of accuracy and overall computational efficiency.

*Correspondence to: W. J. Rider, Los Alamos National Laboratory, Applied Physics Division, MS F699, NM 87545 Los Alamos, U.S.A.

†E-mail: rider@lanl.gov

‡This article is a U.S. Government work and is in the public domain in the U.S.A.

Contract/grant sponsor: Accelerated Strategic Computing Program; contract/grant number: W-7405-ENG-36

Received 27 April 2004

Revised 5 August 2004

Accepted 6 October 2004

Published in 2005 by John Wiley & Sons, Ltd.

Here, we discuss principles by which these different methods can be merged so that they operate locally in a more optimal fashion. The basic design principle is to use high-order linear differencing locally whenever the effective polynomial reconstruction is monotone. If monotonicity is threatened, then the local data are interrogated to determine whether the field is locally monotone and under-resolved or at an extremum. If the flow is locally monotone, but under-resolved, the reconstruction is replaced with either an (weighted) essentially non-oscillatory stencil or the monotone bounding stencil. Should the local data contain valid extrema, the smoother local stencil is chosen (either the ENO/WENO or the original high-order).

We implement the method in two algorithms. One is a piecewise linear method plus uniformly non-oscillatory (UNO) limiting and the second is piecewise parabolic with ENO/WENO limiting. When the accuracy per unit CPU time is considered, the methods are shown to be extremely efficient as compared to the two classes of methods that the design draws upon. In this paper, we will focus more of our attention on the PPM variant of our method.

2. ELEMENTS OF METHOD DESIGN AND OPTIMAL METHODS

In this section of the paper, we discuss the degrees of freedom we will exercise in defining our methods. This includes the base high-order stencil, the low-order (dissipative) stencil and a non-oscillatory method. These methods are woven together via a hybridization that builds upon concepts originally introduced in high-resolution methods by Boris [8] and van Leer [9]. Our operating principle is to use the high-order stencil as much as possible, but employ (weighted) essentially non-oscillatory differencing if the high-order stencil violates conditions for monotonicity. Our ultimate selection is based upon which stencil is bounded by the other two available choices.

2.1. Base PPM algorithm

The PPM algorithm that we use differs from those in the literature in several important ways. Our method uses characteristic variables for differencing in both time and space in a manner that is otherwise equivalent to the direct Eulerian (PPMDE) version of the method. The key steps are given here for clarity. To begin the spatial differencing we transform the variables into characteristic variables using $\mathbf{w}_k = L_j(\mathbf{U}_j)\mathbf{U}_k$, which is the projection of conserved variables on to characteristic variables using the left eigenvector evaluated in the j th zone. This transformation is made locally with a stencil wide enough to evaluate the polynomial reconstruction in the j th zone.

Once the variables \mathbf{w}_k are available, the edge values $\mathbf{w}_{j\pm 1/2}$, for a zone are reconstructed using some high-order approximation. Part of this work will replace the standard approximation with some higher order ones. From these values and the cell average quantity, w_j , a unique parabola can be determined, $p(\theta) = p_0 + p_1\theta + p_2\theta^2$, where $\theta = (x - x_j)/\Delta x$ and $p_0 = \frac{3}{2}w_j - (\mathbf{w}_{j-1/2} + \mathbf{w}_{j+1/2})/4$, $p_1 = \mathbf{w}_{j+1/2} - \mathbf{w}_{j-1/2}$, and $p_2 = 3(\mathbf{w}_{j-1/2} + \mathbf{w}_{j+1/2}) - 6w_j$. This polynomial is examined for monotonicity using the following conditions. $\mathbf{w}_{j\pm 1/2} := \text{median}(\mathbf{w}_j, \mathbf{w}_{j\pm 1/2}, \mathbf{w}_{j\pm 1})$, $\mathbf{w}_{j\pm 1/2} := \text{median}(\mathbf{w}_j, \mathbf{w}_{j\pm 1/2}, 3\mathbf{w}_j - 2\mathbf{w}_{j\mp 1/2})$, where $:=$ means *replace*, and the median function returns the argument bounded by the other two. It is this step of the method that is replaced with our more elaborate step.

This is followed by a time-centring which can be expressed by $-1/v \int_{1/2}^{1/2-v} p(\theta) d\theta$ and $-1/v \int_{-1/2}^{-1/2-v} p(\theta) d\theta$. This evaluates to $\mathbf{w}_{j+1/2}^{n+1/2} = p(\frac{1}{2}) - v/2 p_1 + (-v/2 + v^2/3) p_2$ and $\mathbf{w}_{j-1/2}^{n+1/2} = p(-\frac{1}{2}) - v/2 p_1 + (v/2 + v^2/3) p_2$ with $v = \lambda \Delta t / \Delta x$, where λ is the eigenvalue associated with the characteristic field w . Then the variables are transformed back to the original variables, $\mathbf{U}_{j\pm 1/2}^{n+1/2} = R(\mathbf{U}_j) \mathbf{w}_{j\pm 1/2}^{n+1/2}$, where R is the right eigenvector. The algorithm proceeds with advancing the equations through a conservative update. This will involve a Riemann solution as the edge variables are double-valued.

2.2. High-order method

Typically, the high-order method used in high-resolution methods is second-order accurate. While the usual monotonicity-preserving (i.e., TVD) method is limited to second-order accuracy, the use of higher than second-order accurate stencils can be shown to improve method efficiency. The high-order stencils can take numerous forms, which are usually based on centred or upwind biased stencils. This approach is effective; however, we will explore stencils that are anti-dissipative, and optimal stencils that seek to minimize numerical error over some band of Fourier modes [10].

The anti-dissipative stencils can be derived through the use of the derivative of the primitive function polynomial [2, 3]. This approach can be used with a piecewise parabolic method (PPM) using the slope and curvature obtained from the second and third derivatives of the polynomial giving edge values used in the parabolic interpolation using sixth-order slopes and curvatures

$$\mathbf{w}_{j-1/2} = \frac{-111\mathbf{w}_{j+1} + 887\mathbf{w}_{j+2} - 3010\mathbf{w}_{j+1} + 8510\mathbf{w}_j + 6445\mathbf{w}_{j-1} - 1349\mathbf{w}_{j-2} + 148\mathbf{w}_{j-3}}{11\,520}$$

and

$$\mathbf{w}_{j+1/2} = \frac{-111\mathbf{w}_{j-1} + 887\mathbf{w}_{j-2} - 3010\mathbf{w}_{j-1} + 8510\mathbf{w}_j + 6445\mathbf{w}_{j+1} - 1349\mathbf{w}_{j+2} + 148\mathbf{w}_{j+3}}{11\,520}$$

The parabolic interpolation is defined by these two points and the parabola that preserves the cell average value, \mathbf{w}_j .

Optimal edge values can be derived to minimize errors over a waveband in Fourier space. We seek methods with high fidelity at large wavenumbers, therefore, we will optimize over the range, $[0, 3\pi/4]$. The method is also constrained to some specified order-of-accuracy. This procedure can be easily implemented using symbolic algebra software such as Mathematica. Following this path for the edge values for PPM gives

$$\begin{aligned} \mathbf{w}_{j+1/2} = & 0.6810564693289125(\mathbf{w}_j + \mathbf{w}_{j+1}) - 0.22991803732670166(\mathbf{w}_{j+2} - \mathbf{w}_{j-1}) \\ & + 0.0488615679977887(\mathbf{w}_{j+3} - \mathbf{w}_{j-2}) \end{aligned}$$

The edge $\mathbf{w}_{j-1/2}$ is identical with an index shift of -1 .

For the primitive variable derived slopes, the method becomes mildly anti-dissipative for CFL numbers away from zero and one and for low wavenumbers. The use of the monotonicity preserving limiters overcomes this weak instability in all calculations. The optimal slope minimizes the error at the higher wavenumbers at the cost of somewhat larger errors at small wavenumbers.

For PPM the higher order edge values improve the phase error while leaving the leading order dissipation unchanged. The parabolic primitive function edge values reduce both the amplitude and the phase error.

2.3. Low-order method and dissipation

While there is a large degree of latitude with low-order methods, we will use a single method here. This will be a first-order Godunov method with an iterative Riemann solver that reconstructs the rarefaction as a linear function in similarity space. This method is a slightly simplified version of that used by Rider [11]. This Riemann solver provides an effective and robust method for strong shocks and is free from many common pathologies afflicting many linearized Riemann solvers.

2.4. Non-oscillatory methods

Other important elements of our methods are ENO methods. Used alone, these methods are effective shock capturing techniques although they tend to be rather dissipative compared with methods such as MUSCL [12]. The method works effectively by choosing the smoothest local stencil for the differencing. For our purposes, this character may well be an advantage because of the relative safety in dissipative algorithms. We also use a weighted version of UNO method introduced recently in Reference [13]. The UNO or WUNO differencing is used in conjunction with the piecewise linear method. The ENO or WENO method is applied to determine edge values that are used to define a piecewise parabolic method. In our implementation of the ENO method, the stencils are precomputed and then hierarchically chosen, $\mathbf{w}_{j+1/2}^1 = \mathbf{w}_j$

$$\mathbf{w}_{j+1/2}^2 = \frac{\mathbf{w}_j + \mathbf{w}_{j+1}}{2}; \frac{3\mathbf{w}_j - \mathbf{w}_{j-1}}{2}$$

and

$$\mathbf{w}_{j+1/2}^3 = \frac{2\mathbf{w}_{j-2} - 7\mathbf{w}_{j-1} + 11\mathbf{w}_j}{6}; \frac{-\mathbf{w}_{j-1} + 5\mathbf{w}_j + 2\mathbf{w}_{j+1}}{6}; \frac{2\mathbf{w}_j + 5\mathbf{w}_{j+1} - \mathbf{w}_{j+2}}{6}$$

These are chosen on the basis of the stencil that has the smallest difference between it and the lower order edge value.

As described next, the ENO method is only used when the base high-order method is not monotone.

2.5. Method hybridization

High-resolution methods have usually utilized the hybridization of low-order monotone methods with high-order (non-monotone) schemes. Here, we apply principles in which we merge the monotone high-resolution methods with W(ENO) methods [13]. Our principle is the following: use the high-order approximation as much as possible. If the high-order approximation

produces a potential violation of monotonicity, then select the approximation that is bounded by two of the estimates provided by the monotonicity limit, the high-order approximation, and an essentially non-oscillatory approximation.

One can then compose all aspects of these elements to produce optimal methods. These methods combine the robustness of monotone methods without reducing the accuracy to first order at extrema and discontinuities. This is accomplished by utilizing the W(UNO) or W(ENO) methodology when monotonicity is violated, in order to test whether higher accuracy is still a viable and nonlinearly stable approximation. The first-order approach is only used as a last resort when the flow is grossly under-resolved and high-order stencils of any sort are not viable. As the next section will clearly demonstrate, this approach yields great improvements in solution accuracy and method efficiency.

To summarize, the algorithm used to select the differencing has the following steps:

1. Start with a high-order difference approximation;
2. Check whether this approximation is monotone preserving;
3. If it is monotone, use the high-order approximation;
4. Form a UNO or ENO approximation as appropriate for the method;
5. The new monotone limit is based on the ENO method for PPM;
6. From the triple (high-order, monotone limit, and ENO or UNO) use the value that is bounded by the other two (the median); in the simplest case, this is accomplished by $w_{j\pm 1/2} := \text{median}(w_{j\pm 1/2}^M, w_{j\pm 1/2}, w_{j\pm 1/2}^{\text{ENO}})$. We note that the median function has the following property, i.e. two entries are $\mathcal{O}(h^n)$ and $\mathcal{O}(h^m)$, where $m \leq n$ and then the function returns a $\mathcal{O}(h^m)$ value.

3. RESULTS

We show results for several cases: Sod's shock tube, the interacting blast wave problem and the Shu–Osher entropy wave. These results are shown in Table I. In each case, the new methods xPPM are more accurate than either of the monotone methods (cPPM or WENO5). The ultimate arbiter of the solution quality is the efficiency of a method, which compares the amount of effort for a method to achieve comparable errors. The new methods can be as much as three times the efficiency of the monotone methods, but much more efficient than the classical WENO method. This is greatly impacted by the convergence rate, which is observed to be about 0.8. This convergence rate is expected for a problem with a discontinuity [14].

We have also examined a simple steepening Riemann invariant to understand the details of the dissipation and resolution of the algorithm. Prior to the formation of a shock, the PPM method produces third-order solutions when the CFL number is near one, but higher order solutions defined by the order of the estimate of the edge values as the CFL number goes to zero. The new methods commit far lower errors in the spectrum of solution and produces far smaller unphysical side-effects at longer wavelengths. In three dimensions, we have compared solutions for the Taylor–Green vortex. Here we have found that these methods produce errors comparable to fifth-order WENO with 100–1000 times less computational effort. Our present implementation uses dimensional splitting, but nothing precludes applying these concepts in a more genuinely multidimensional fashion.

Table I. The relative accuracy, cost and efficiency of a set of modern algorithms for the 1D test problems.

Scheme	Sod' shock tube	Interacting blast waves	Shu–Osher entropy wave
sPLM2	1.00/1.00/1.00	1.00/1.00/1.00	1.00/1.00/1.00
cPPM6	0.70/1.41/0.58	0.63/1.36/0.44	0.78/1.42/0.75
xENO-PPM6	0.72/1.51/0.67	0.57/1.43/0.35	0.71/1.41/0.60
xENO-PPM7	0.70/1.48/0.60	0.56/1.45/0.34	0.69/1.43/0.57
xENO-PPM7p	0.66/1.47/0.53	0.36/1.47/0.12	0.79/1.56/0.86
xENO-PPM6o	0.53/1.71/0.35	0.45/1.52/0.21	1.32/1.43/2.87
xWENO-PPM6	0.71/1.59/0.67	0.58/1.43/0.37	0.77/1.43/0.75
xWENO-PPM7	0.69/1.62/0.63	0.65/1.43/0.48	0.78/1.45/0.78
xWENO-PPM7p	0.65/1.68/0.58	0.62/1.48/0.45	0.78/1.50/0.80
xWENO-PPM6o	0.64/1.60/0.54	0.47/1.39/0.21	0.84/1.48/0.95
WENO5	1.44/9.22/23.09	0.96/6.16/5.59	0.76/8.77/4.47

These are reported in triples (accuracy/cost/efficiency), where the efficiency is computed as $\text{cost}(\text{error})^{d/n}$, where d is the dimension (1, 2 or 3) and n is the convergence rate. sPLM = simple PLM, cPPM = characteristic PPM, xENO-PPM = extreme ENO PPM, xWENO-PPM = extreme WENO PPM, 6 = sixth-order difference or edge, 7 = seventh-order, 7p = 7 point parabolic, 6o = six point optimal.

ACKNOWLEDGEMENTS

This work was supported by the Los Alamos National Laboratory and Lawrence Livermore National Laboratory, by Accelerated Strategic Computing Program under Contract W-7405-ENG-36. This paper is also available as Los Alamos Report LA-UR-04-1860.

REFERENCES

1. Van Leer B. Towards the ultimate conservative difference scheme. V. A second-order sequel to Godunov's method. *Journal of Computational Physics* 1979; **32**:101–136. (Reprinted in 1997; **135**(2):229–248.)
2. Colella P, Woodward PR. The piecewise parabolic method (PPM) for gas-dynamical simulations. *Journal of Computational Physics* 1984; **54**:174–201.
3. Harten A, Engquist B, Osher S, Chakravarthy S. Uniformly high order accurate essentially non-oscillatory schemes, III. *Journal of Computational Physics* 1987; **71**:231–301.
4. Harten A, Osher S. Uniformly high-order accurate nonoscillatory schemes. I. *SIAM Journal on Numerical Analysis* 1987; **24**:1565–1619.
5. Jiang G-S, Shu C-W. Efficient implementation of weighted ENO schemes. *Journal of Computational Physics* 1996; **126**:202–228.
6. Huynh HT. Accurate upwind methods for the Euler equations. *SIAM Journal on Numerical Analysis* 1995; **32**:279–309.
7. Suresh A, Huynh HT. Accurate monotonicity-preserving schemes with Runge–Kutta time stepping. *Journal of Computational Physics* 1997; **136**:83–99.
8. Boris JP. A fluid transport algorithm that works. *Computing as a Language for Physics*. International Atomic Energy Commission: Trieste, 1971; 171–189.
9. Van Leer B. Towards the ultimate conservative differencing scheme I: The quest of monotonicity. *Lecture Notes in Physics* 1973; 163–168.
10. Tam CKW, Webb JC. Dispersion-relation-preserving schemes for computational acoustics. *Journal of Computational Physics* 1993; **107**:262–281.

11. Rider WJ. An adaptive Riemann solver using a two-shock approximation. *Computers and Fluids* 1999; **28**:741–777.
12. Greenough JA, Rider WJ. A quantitative comparison of numerical methods for the compressible Euler equations. *Journal of Computational Physics* 2004; **196**(1):281–296.
13. Rider WJ, Greenough JA, Kamm JR. Extrema, accuracy and monotonicity preserving methods through adaptive nonlinear hybridizations. *Journal of Computational Physics* 2004, submitted. Also *Los Alamos Report LA-UR-04-0593*.
14. Majda A, Osher S. Propagation of error into regions of smoothness for accurate difference approximations to hyperbolic equations. *Communications on Pure and Applied Mathematics* 1977; **30**:671–705.