High Order Schemes in BATS-R-US: Is it OK to Simplify Them?

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Abstract. We describe a number of high order schemes and their simplified variants that have been implemented into the University of Michigan global magnetohydrodynamics code BATS-R-US. We compare the various schemes with each other and the legacy 2nd order TVD scheme for various test problems and two space physics applications. We find that the simplified schemes are often quite competitive with the more complex and expensive full versions, despite the fact that the simplified versions are only high order accurate for linear systems of equations. We find that all the high order schemes require some fixes to ensure positivity in the space physics applications. On the other hand, they produce superior results as compared with the second order scheme and/or produce the same quality of solution at a much reduced computational cost.

1. Introduction

The University of Michigan global magnetohydrodynamics code BATS-R-US (Powell et al. 1999; Tóth et al. 2012) has employed second-order accurate total variation diminishing (TVD) schemes for a long time. It relies on block-adaptive mesh refinement (AMR) to increase numerical accuracy in regions of interest. While in principle grid refinement can achieve arbitrary accuracy, in practice computational resources are limited. To further improve the accuracy of the code without a significant increase in computational time or memory requirements, we have recently implemented a number of high order methods into BATS-R-US: the 4th order finite volume (FV4, McCrorquodale & Colella 2011) and the 5th order Monotonicity Preserving (MP5, Suresh & Huynh 1997) schemes. Since BATS-R-US can solve several different equation sets, we tried to avoid the conversion to characteristic variables. We also tried to simplify the schemes so that they require smaller stencils and the grid blocks do not need an excessive number of ghost cells. We carefully evaluated the impact of these simplifications and we report here some of the main findings.

Currently, all high order methods are implemented for the uniform parts of the grid only, and we revert back to the TVD scheme at grid resolution changes. Although the new schemes can be used on non-Cartesian grids too, the current implementation is not truly high order accurate in that case. Despite these limitations and restrictions, the new schemes can achieve great improvement in accuracy and/or efficiency relative to the TVD scheme.

Section 2 describes the basic ingredients of the high order schemes and their simplified variants. Section 3 reports the results of some verifications tests and illustrates the performance of the high order schemes for two space physics applications. We conclude with section 5.
2. High Order Schemes and their Simplified Versions

Since high order schemes require a larger stencil and more ghost cells than the second order TVD scheme that needs 2 ghost cells only, the first step was to completely replace the original AMR code in BATS-R-US with the Block Adaptive Tree Library (BATL, Tóth et al. 2012)), so that we can use arbitrary number of ghost cells around the grid blocks. We also implemented the classical 4th order Runge–Kutta (RK4) and the strong stability-preserving 3rd order Runge–Kutta (RK3) time integration schemes so that we can match the spatial accuracy of the high order schemes.

2.1. 4th Order Finite Volume Scheme: FV4

The 4th order finite volume scheme by McCorquodale & Colella (2011) is based on an improved version of the PPM limiter that requires 4 instead of 3 ghost cells. In addition, it uses a 4th order accurate conversion between cell averaged and cell centered state values, also between face averaged and face centered fluxes. The conversions involve the addition or substraction of the 3D/2D Laplacian of the variable/flux, respectively. These conversion steps increase the stencil of the scheme to 5 ghost cells. There is also a shock flattening algorithm for strong shocks and an artificial viscosity to suppress some oscillations. A nice feature of FV4 that it does not require the use of characteristic variables or fluxes.

Although we implemented the full FV4 scheme (with the exception of the artificial viscosity) we also experimented with a simplified version that has a smaller stencil and requires 3 ghost cells only. The simplified algorithm is essentially a finite difference scheme, as it uses the cell center values of the state variables. We also dropped the third-derivative based limiting of the limiter as it requires an extra ghost cell. The resulting algorithm is just like our usual TVD scheme but with a much fancier limiter requiring 3 ghost cells. It is a finite difference scheme that is 4th order accurate for linear equations (FD4) except for some special circumstances that would require the 3rd derivative-based part of the limiter. Both FV4 and FD4 rely on the RK4 scheme for time integration, although we have also experimented with RK3 and even RK2.

There is no formal mechanism in the FV4 and FD4 schemes that would ensure positivity of pressure and density. The PPM-type limiter avoids major oscillations, but it does not enforce positivity. We found that it was necessary to implement minimum floor values both for pressure and density. In addition, we modified the limiter so that it switches back to a second order scheme if the face value would become negative, i.e. if $U_{i+1/2} < 0$ then $U_{i+1/2} = (U_i + U_{i+1})/2$. Here $U$ is one of the positive variables, e.g. density or pressure. For the FV4 scheme, it is also necessary to check and fix positivity after the conversions between cell average and cell centered variables.

2.2. 5th Order Monotonicity Preserving Scheme: MP5

The MP5 scheme by Suresh & Huynh (1997) is a 5th order finite difference scheme. In its simplest form the primitive variables are limited one-by-one with the sophisticated MP5 limiter that requires 3 ghost cells only. For non-linear equations one has to limit the fluxes instead of the state variables to retain the full 5th order accuracy. This is achieved by using cell centered fluxes that are split with a simple global Lax-Friedrich flux into $F^\pm_i = (F_i \pm c_{\text{max}} U_i)/2$ where $F$ is the flux function for variable $U$ and $c_{\text{max}}$ is the largest wave speed over the whole domain. The fluxes $F^\pm_i$ are then interpolated to the faces with the MP5 limiter and combined into the high order face flux as $F_{i+1/2} = \ldots$
For systems of equations it is recommended to limit the characteristic fluxes (see Li & Jaberí 2012, for details). The recommended time integration scheme for MP5 is RK3.

We have implemented both the primitive variable and the cell centered flux based versions of the MP5 scheme, but we did not implement the conversions to characteristic variables/fluxes and back, as this is difficult to generalize to the various equation sets solved by BATS-R-US, and it is also a rather expensive operation.

Although the MP5 limiter is monotonicity (and therefore positivity) preserving for linear equations, it does not guarantee the positivity of pressure and density for the non-linear MHD equations. We found that the pressure and density can be pushed towards zero (or the floor value) in some parts of the computational domain even if it does not become negative. To avoid this problem, we modified the MP5 limiter so that it switches back to a first order scheme if the face value of a positive variable would drop below a fraction of the cell center value, i.e. if \( U_{i+1/2}^L < C U_i \) then \( U_{i+1/2}^L = U_i \) and the same for \( U_{i-1/2}^R \). Here \( L \) and \( R \) refer to the left and right face values and \( C \) is an adjustable constant. We typically use \( C = 0.6 \) so that this fix only switches on when the variable changes rapidly towards zero.

3. Verification Tests and Space Physics Applications

The primary use of verification tests is to check various properties of the implemented schemes, such as order of accuracy for smooth linear and non-linear problems in 1D and 2D, and the oscillation free property for discontinuous problems. In addition, we used these tests to compare the full and simplified versions of the schemes and quantitatively evaluate their relative accuracy at various resolutions. For example, we compared our schemes on smooth but non-linear wave propagation tests. Due to the non-linearity, only the FV4 scheme and the flux-based MP5 schemes are truly 4th and 5th order accurate, nevertheless the simplified versions of these schemes performed almost as well as the full versions. The differences do show up eventually at very high resolutions, but in real applications these small differences are not important.

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We discuss the results for the Shu-Osher shock tube problem in some detail. This test involves the interaction of a strong shock with a sinusoidal perturbation in the density. It tests the schemes both for oscillatory and dissipative errors. Table 1 shows the L1 norm of the error in the density for \( n = 200, 400 \) and 800 grid cells for several schemes. We tested both the local Lax-Friedrichs (LLF) and the Godunov (Godu.) flux functions with the 2nd order TVD scheme with Koren’s limiter, the FD4, the FV4 and the primitive variable based MP5 scheme. The final column contains the results from the cell-centered flux based MP5 scheme that only works with the global Lax-Friedrichs flux splitting.
All schemes are about equally inaccurate for \( n = 200 \) grid cells. The 2nd order TVD scheme (first two columns) is significantly less accurate than the high order schemes for \( n \geq 400 \). On the other hand the FD4 and FV4 schemes produce essentially identical results, despite the fact that only the FV4 scheme is truly 4th order accurate for this non-linear problem. The non-linearly 5th order accurate flux-based MP5 scheme is actually less accurate than the linearly 5th order primitive variable based version. This is due to the fact that the flux-based MP5 scheme uses the most dissipative global Lax-Friedrich flux, while the variable based versions use the less dissipative local LF or Godunov flux functions. For this particular problem the Godunov flux gives significantly smaller errors than the LLF flux, unlike in smooth problems where the difference becomes insignificant for the high order schemes. It is also interesting to note that the MP5 schemes do not produce any spurious oscillations eventhough we do not employ characteristic variables or fluxes.

3.1. Magnetosphere Simulation

![Diagram](image)

Figure 1. The thermal pressure in a 2D cut in the \( Z = 0 \) plane near the planet. Solution obtained with \( 1/4 \) (left column), \( 1/8 \) (middle column) and \( 1/16R_E \) (right column) resolution with the TVD (top) and the simplified MP5 scheme (bottom).

We model the 3D magnetosphere on an adaptive Cartesian grid with BATS-R-US. The inner boundary is a sphere of radius \( 2.5R_E \) where the density is 28 amu/cm\(^3\), the pressure floats, the velocity is zero, and the analytic part of the magnetic field \( \mathbf{B}_0 \) is set to a dipole field aligned with the \( Z \) axis. The solar wind enters at the inflow boundary at \( x = 32R_E \) with \( \rho = 5 \) amu/cm\(^3\), \( u_x = -400 \) km/s, \( T = 10^5 \) K and \( B_z = -5 \) nT. At the other boundaries at \( x = -224 \) \( R_E \) and \( Y, Z = \pm 128 \) \( R_E \) a zero gradient condition is applied. We solve the resistive MHD equations with a magnetic diffusivity of \( 10^{11} \) m\(^2\)/s. This small amount of uniform resistivity improves the solution when the numerical diffusion...
is very small. The grid resolution is kept uniform within the $-10 \, R_E < x, y, z < 10 \, R_E$ cube so that the high order scheme can be fully employed in this region. We use local time stepping for 10,000 steps and then switch to time accurate mode.

Figure 1 shows the pressure in the $Z = 0$ plane near the body obtained with the TVD (top) and the MP5 (bottom) schemes, respectively. One can see the characteristic signatures of the Kelvin-Helmholtz instability as long as the numerical diffusion is small enough. For the TVD scheme this requires $1/16 \, R_E$ resolution, while the MP5 scheme can obtain essentially the same result with $1/8 \, R_E$ resolution. For coarser grids the instability is suppressed by the numerical diffusion.

### 3.2. Heliosphere Simulation

![Image of synthetic and observed EUV images](image)

**Figure 2.** Comparison of synthetic and observed EUV images in three different wavelength (171, 195 and 284 Å) obtained with the TVD scheme (top row), MP5 limiter (middle row) and observations (bottom row)
We used the Alfvén Wave Solar Model (AWSoM, van der Holst et al. 2014) implemented in BATS-R-US to model the solar wind for Carrington rotation 2107. The stretched spherical grid extends from the transition region all the way to 24 R⊙ (solar radii). Near the inner boundary the resolution is about 1° in the latitude and longitude directions and Δr = 0.001 R⊙ in the radial direction. AMR is used to better resolve the current sheet. At the inner boundary the density and temperature are constant, the velocity is zero, the magnetic field is set by a synoptic magnetogram, and the Alfvén wave energy density inflow is based on the magnetic field strength. At the outer boundary zero gradient condition is applied. We obtain a steady state solution in the heliographic rotating frame with about 60,000 iterations using local time stepping.

Figure 2 shows the synthetic EUV images obtained from the model using the TVD scheme or the MP5 limiter as well as the actual observations from the Stereo B spacecraft. Although our implementation of the MP5 limiter is formally only 2nd order accurate for spherical grids, it still has much less numerical diffusion than the 2nd order TVD limiter, as clearly demonstrated by the amount of detail shown in the figure. The solution obtained with the MP5 limiter agrees much better with the observed images than the solution from the TVD scheme: one needs good physics as well as good numerics for a good model.

4. Conclusion

Based on a large number of standard numerical tests, we find that full non-linear high order accuracy is not an absolute requirement for an accurate scheme. The most important attribute of a good scheme is small amount of numerical diffusion, no spurious oscillations and high order accuracy for linear equations in 1D at least. The simplified schemes are much easier to implement and require less computational resources than their original fully high order versions.

When applied to challenging magnetospheric and heliospheric problems, the high order schemes often produced negative pressures and/or densities. We have implemented some simple fixes that improved the robustness of the schemes. When the high order schemes work, however, we find that in most cases they can obtain similar or better results than the TVD scheme on twice finer grids. The high order schemes are about twice as expensive as the TVD scheme on the same grid. This means that the high order schemes are about 8 times faster and require 8 times less storage than the second order method for three dimensional time dependent simulations.

References