A COMPARISON BETWEEN DIVERGENCE-CLEANING AND STAGGERED-MESH FORMULATIONS FOR NUMERICAL MAGNETOHYDRODYNAMICS

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ABSTRACT

In recent years, several different strategies have emerged for evolving the magnetic field in numerical MHD. Some of these methods can be classified as divergence-cleaning schemes, in which one evolves the magnetic field components just like any other variable in a higher order Godunov scheme. The fact that the magnetic field is divergence-free is imposed post facto via a divergence-cleaning step. Other schemes for evolving the magnetic field rely on a staggered-mesh formulation that is inherently divergence-free. The claim has been made that the two approaches are equivalent. In this paper we compare three divergence-cleaning schemes based on scalar and vector divergence-cleaning and a popular divergence-free scheme. All schemes are applied to the same stringent test problem. Several deficiencies in all the divergence-cleaning schemes become clearly apparent, with the scalar divergence-cleaning schemes performing worse than the vector divergence-cleaning scheme. The vector divergence-cleaning scheme also shows some deficiencies relative to the staggered-mesh divergence-free scheme. The differences can be explained by realizing that all the divergence-cleaning schemes are based on a Poisson solver that introduces a nonlocality into the scheme, although other, subtler points of difference are also cataloged. By using several diagnostics that are routinely used in the study of turbulence, it is shown that the differences in the schemes produce measurable differences in physical quantities that are of interest in such studies.

Subject headings: methods: numerical — MHD

1. INTRODUCTION

In recent years there has been substantial progress in numerical magnetohydrodynamics (MHD). This progress has been spurred by the great utility of this system of equations in the modeling of problems in astrophysics and space physics. A key advance in the field has come from the application of higher order Godunov methodology to numerical MHD. These higher order Godunov schemes were first developed for Euler flows by van Leer (1979), ushering in a new era of robust, accurate, and reliable simulation techniques. In order to enjoy the same advantages of accuracy, reliability, and robustness in numerical MHD, several groups have developed higher order Godunov schemes for MHD. A brief list includes Brio & Wu (1988), Zachary, Malagoli, & Colella (1994), Powell (1994), Dai & Woodward (1994), Ryu & Jones (1995), Roe & Balsara (1996), and Balsara (1998a, 1998b, 2004). Viewed on a dimension-by-dimension basis, the MHD equations do lend themselves to an interpretation as a system of conservation laws. Since much of the higher order Godunov scheme methodology works best for a system of conservation laws, it is therefore natural that early efforts focused entirely on the formulation of numerical MHD as yet another system of conservation laws that is amenable to treatment by higher order Godunov methods. In keeping with that view, early efforts also treated the magnetic fields as zone-centered variables.

The above plan seems like an elegant one until one takes a multidimensional view of the induction equation. It has the form

$$\frac{\partial \mathbf{B}}{\partial t} + \mathbf{c} \nabla \times \mathbf{E} = 0,$$

(1.1)

where $\mathbf{B}$ is the magnetic field, $\mathbf{E}$ is the electric field, and $c$ is the speed of light. In the specific case of ideal MHD, the electric field is given by

$$\mathbf{E} = -\frac{1}{c} \mathbf{v} \times \mathbf{B},$$

(1.2)

where $\mathbf{v}$ is the fluid velocity. Equation (1.1) is fundamentally different from a conservation law. It does not require the components of the magnetic field to be conserved in a volume-averaged sense. Equation (1.1) does predict, via application of Stoke’s law, that the magnetic field remains divergence-free. Brackbill & Barnes (1980) and Brackbill (1985) have shown that violating the $\nabla \cdot \mathbf{B} = 0$ constraint leads to unphysical plasma transport orthogonal to the magnetic field, as well as a loss of momentum and energy conservation. For that reason, almost all the groups that initially presented higher order schemes for MHD showed at least some awareness of the fact that it is important to preserve the divergence-free aspect of the magnetic field. Thus, Zachary et al. (1994), Balsara (1998b), Ryu, Jones, & Frank (1995), and Kim et al. (1999) all suggested that a divergence-cleaning step be used in conjunction with their early higher order Godunov-based MHD schemes. (It might be pointed out that the divergence-cleaning step also destroys strict conservation of magnetic field components, which is the very attribute we sought to preserve via application of conservation laws.) In an effort to accommodate the fact that the early higher order Godunov MHD schemes built up divergence in the magnetic field, Powell (1994) took an alternative approach in which he tried to modify the MHD equations. He did so by including source terms in the MHD equations that were proportional to $\nabla \cdot \mathbf{B}$. Recently, Dedner et al. (2002) extended the so-called divergence wave scheme of Powell (1994). The advantage of their method is that the divergence correction part, which is obtained by evaluating a Riemann problem for a $2 \times 2$ system and using a scalar source term, can be completely decoupled from the usual MHD
solver. The basic idea of the latter two schemes is to propagate any nonzero divergence out of the computational domain or to damp it. We did not include the latter two schemes in our tests.

An alternative line of thought for dealing with the $\nabla \cdot \mathbf{B} = 0$ problem stems from the work of Yee (1966), who built up these ideas for the transport of electromagnetic fields. The basic idea consists of having a “staggered-mesh magnetic field transport algorithm,” in which the magnetic field components are collocated at the face centers of each zone and the electric field components are collocated at the edge centers of the zones. Stoke’s law is then applied to equation (1.1) to yield a discrete time-update strategy for the face-centered magnetic fields. Because it follows from a discrete version of Stoke’s law, the resulting discrete time-update strategy clearly shows that if the magnetic field is divergence-free at the beginning of a time step, it will remain so at the end of the time step. Yee’s idea was extended to numerical MHD by Brecht et al. (1981). Evans & Hawley (1988) then implemented the staggered-mesh (SM) algorithm developed by Brecht et al. (1981) in their code, coining the term “constrained transport.” DeVore (1991) applied the SM algorithm of Brecht et al. (1981) to his flux-corrected transport scheme, albeit with a more accurate acknowledgement of its antecedents. Similar schemes were developed for higher order Godunov scheme–based MHD by Dai & Woodward (1998), Ryu et al. (1998), Balsara & Spicer (1999b), Londrillo & Del Zanna (2000), and Balsara (2004). There are different ways to construct the electric field, but perhaps the most elegant and economical strategy consists of utilizing the dualism between the components of the Godunov flux and the electric fields, as shown by Balsara & Spicer (1999b). Londrillo & Del Zanna (2000) have shown that a (SM) formulation of the type used by the references cited in the previous sentence is fundamental to divergence-free evolution of the magnetic field. Tóth (2000) made a comparative study of such schemes and found the scheme of Balsara & Spicer (1999b) to be one of the most accurate second-order schemes that he tested. However, Tóth (2000) found that using a zone-centered approach with divergence cleaning yielded results that were comparable to the (SM) formulations for the simple test problems that he used. One is therefore led to wonder whether there might be stringent enough test problems for which the differences between divergence-cleaning and (SM) formulations may become more apparent. After all, an analysis of the different forms of divergence-cleaning algorithms, which we catalog in §2, shows that one should expect differences between them. Furthermore, a comparison of divergence-cleaning algorithms and (SM) formulations, which we also undertake in §2, shows that we should expect differences. The purpose of this paper is to make the differences apparent by applying all the formulations to the same stringent test problem. The test problem does provide radiative cooling, along with the interplay of strong shocks. Such problems are shown to be especially pernicious for certain kinds of schemes for numerical MHD because the colliding, radiative shocks tend to form persistent, converging flows that result in a rapid, local buildup of error in the divergence of the magnetic field. Self-gravitating astrophysical flows also produce persistent, converging flows and should therefore be susceptible to the same problems described here.

In §2 we catalog a few different divergence-cleaning schemes, as well as provide a brief recapitulation of the (SM) scheme of Balsara & Spicer (1999b). In doing so, we also provide comparisons between them, cataloging insights about these schemes that we have not seen cataloged in a comprehensive way in the literature. In §3 we introduce the test problem and compare numerical results. In §4 we provide some conclusions.

2. DIVERGENCE-CLEANING SCHEMES AND THE STAGGERED-MESH SCHEME OF BALSARA & SPICER (1999b)

The MHD equations can be written in an explicitly conservative form as

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho v_z \\ \rho B_x \\ \rho B_y \\ \rho B_z \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho v_x \\ \rho v_y \\ \rho v_z \\ \rho B_x \\ \rho B_y \\ \rho B_z \end{pmatrix} = 0,$$

where $E = \rho v^2/2 + P/\gamma + B^2/8\pi$ is the total energy of the plasma. We assume a Cartesian mesh with edges of size $\Delta x$, $\Delta y$, and $\Delta z$. In addition, let the time step be denoted by $\Delta t$. We describe the different schemes for enforcing divergence-free evolution of the magnetic field in the ensuing subsections.
2.1. Scalar Divergence Cleaning

The scalar divergence cleaning scheme that is cataloged in this subsection (SDC1) exactly clears the discrete divergence in physical space after one application but is susceptible to even-odd decoupling. It has been cataloged by several authors. We follow the prescription in Kim et al. (1999). In that strategy, at the end of every time step we make the assignments

\[
\begin{align*}
B_{x,i,j,k}^{i+1,j,k} & = B_{x,i,j,k} - \frac{\Phi_{i+1,j,k} - \Phi_{i-1,j,k}}{2\Delta x}, \\
B_{y,i,j,k}^{i,j+1,k} & = B_{y,i,j,k} - \frac{\Phi_{i,j+1,k} - \Phi_{i,j-1,k}}{2\Delta y}, \\
B_{z,i,j,k}^{i,j,k+1} & = B_{z,i,j,k} - \frac{\Phi_{i,j,k+1} - \Phi_{i,j,k-1}}{2\Delta z}.
\end{align*}
\]  

(2.2)

The vector with components given by \((B_{x,i,j,k}, B_{y,i,j,k}, B_{z,i,j,k})\) satisfies the discrete divergence condition

\[
\frac{B_{x,i+1,j,k} - B_{x,i-1,j,k}}{2\Delta x} + \frac{B_{y,i,j+1,k} - B_{y,i,j-1,k}}{2\Delta y} + \frac{B_{z,i,j,k+1} - B_{z,i,j,k-1}}{2\Delta z} = 0,
\]  

(2.3)

if the scalar \(\Phi\) satisfies the condition

\[
\begin{align*}
\Phi_{i+2,j,k} - 2\Phi_{i,j,k} + \Phi_{i-2,j,k} & = \frac{4\Delta x^2}{\Phi_{i+2,j,k} - 2\Phi_{i,j,k} + \Phi_{i-2,j,k}} \\
& + \frac{4\Delta y^2}{\Phi_{i,j+2,k} - 2\Phi_{i,j,k} + \Phi_{i,j-2,k}} \\
& + \frac{4\Delta z^2}{\Phi_{i,j,k+2} - 2\Phi_{i,j,k} + \Phi_{i,j,k-2}}
\end{align*}
\]

\[
= \frac{B_{x,i+1,j,k} - B_{x,i-1,j,k}}{2\Delta x} + \frac{B_{y,i,j+1,k} - B_{y,i,j-1,k}}{2\Delta y} + \frac{B_{z,i,j,k+1} - B_{z,i,j,k-1}}{2\Delta z}.
\]  

(2.4)

The scheme has the following advantages:

1. It is exact in physical space. The discrete divergence in equation (2.3), measured after a single application of the scheme cataloged in this subsection, will be exactly zero.
2. A spectral method is fast because one needs only to evaluate fast Fourier transforms (FFTs) for a single scalar field.

The scheme also has the following disadvantages:

1. In equation (2.4) each \(\Phi_{i,j,k}\) is coupled with those at every other cell in the \(x, y,\) and \(z\)-directions. Therefore, an original computational domain is divided into eight subdomains, and \(\Phi\) is computed in those subdomains separately, which is called even-odd decoupling. In other words, the divergence-cleaning step applied to a mesh with \(N^3\) zones requires us to make eight independent solutions of the Poisson problem on meshes with \((N/2)^3\) zones each. Equation (2.4) is susceptible to even-odd decoupling. (For narrative simplicity we assume for the rest of this paper that we are dealing with a cubic mesh with \(N\) zones on each side. The present comments are, however, more generally applicable to any cubic mesh.) It is true that the decoupling enables one to reduce the amount of calculations. However, the solution with the decoupling is more susceptible to aliasing due to the reduced sampling.

2. It can accommodate a few different kinds of boundary conditions. In that sense, it is somewhat flexible. However, for general boundary conditions, one does not know whether the boundary conditions on \(\Phi\) in equation (2.4) should be Dirichlet, Neumann, or mixed. In that sense, the scheme is not exactly specifiable for all manner of boundary conditions. Using this method, we can only resolve the question of boundary conditions unambiguously for periodic domains.
3. For anything other than periodic domains, and especially for problems with complicated, nonperiodic boundaries, it is not possible to use FFTs. In such situations, the method might become slow.
4. When using FFTs, aliasing errors cannot be avoided.
5. When solving the problem on a parallel machine, one cannot escape the need for all-to-all communication.
6. With a lot of effort, this method may perhaps take well to adaptive mesh refinement (AMR), as was done in Powell et al. (1999). In that situation, it would certainly be hobbled by the elliptic solution step. As the depth of the AMR hierarchy increases, the divergence-cleaning step progressively becomes more computationally expensive.
7. The emergence of a nonzero divergence in one local region in a simulation produces local source terms on the right-hand side of equation (2.4). The divergence cleaning involves a Poisson solver, i.e., the solution of an elliptic equation. As a result, the local divergence provides corrections, via equation (2.2), to all parts of physical space. Ignoring the effects of periodicity, the corrections are directly proportional to the right-hand side of equation (2.4) and inversely proportional to the square of the distance from the region with nonzero divergence. The use of periodic boundaries only introduces more image sources in the problem, thereby degrading the quality of the solution even further. As a result, even though the MHD system is hyperbolic and propagates information locally, the inclusion of the divergence-cleaning step is nonlocal and produces action at a distance. This can become especially pernicious if persistent divergence-producing structures develop in lines, sheets, or volumes (see Jackson 1975), in which the fall-off with distance from the source of divergence is even slower.
8. The divergence cleaning is applied at every time step, and as a result, the damaging effects mentioned above can build up over thousands of time steps.

2.2. Scalar Divergence Cleaning (Not Exact but without Even-Odd Decoupling)

This method (SDC2) is a variant of the method in § 2.1 and has been cataloged in Balsara (1998b). It does not completely clean the discrete divergence in physical space after one application but is not susceptible to the even-odd decoupling described above. This is done by replacing equation (2.4) with

\[
\begin{align*}
\frac{\Phi_{i+1,j,k} - 2\Phi_{i,j,k} + \Phi_{i-1,j,k}}{\Delta x^2} & \Delta x^2 \\
& + \frac{\Phi_{i,j+1,k} - 2\Phi_{i,j,k} + \Phi_{i,j-1,k}}{\Delta y^2} \\
& + \frac{\Phi_{i,j,k+1} - 2\Phi_{i,j,k} + \Phi_{i,j,k-1}}{\Delta z^2}
\end{align*}
\]

\[
= \frac{B_{x,i+1,j,k} - B_{x,i-1,j,k}}{2\Delta x} + \frac{B_{y,i,j+1,k} - B_{y,i,j-1,k}}{2\Delta y} + \frac{B_{z,i,j,k+1} - B_{z,i,j,k-1}}{2\Delta z}.
\]  

(2.5)
The remaining equations in § 2.1 are unchanged. The Poisson problem in equation (2.5) is solved on a single mesh with \( N^3 \) zones.

The scheme has the same advantages and disadvantages as the scheme in § 2.1 with the following exceptions:

1. It has the advantage that it is not susceptible to even-odd decoupling.
2. It has the disadvantage that it is not exact in physical space. In fact, successive application of this scheme causes a different nonzero divergence to be evaluated at each point in real space at the end of each application.

2.3. Vector Divergence Cleaning

Vector divergence cleaning (VDC) is not exact in real (physical) space, but it is exact in Fourier space. It was cataloged in Balsara (1998b). It consists of transforming the vector field componentwise into spectral space. Thus, given the three components \( B_{y,j,k}, B_{x,j,k}, B_{z,j,k} \) at each spatial point \((i,j,k)\) on the mesh, we carry out three three-dimensional FFTs to obtain the field \([B_y(k), B_x(k), B_z(k)]\) in spectral space. Here \( k \) is the vector of wavenumbers in Fourier space. The field \([B_y(k), B_x(k), B_z(k)]\) is not divergence-free in Fourier space. However, once we know the \( B\)-field in Fourier space, it is easy to correct for a nonzero divergence in Fourier space because the divergence operator in real space transforms to a dot product between \( k \) and \([B_y(k), B_x(k), B_z(k)]\) in Fourier space. This fact enables one to derive

\[
B_i(k) = \sum_{j=1}^{3} \left( \delta_{i,j} - \frac{k_j k_i}{k^2} \right) B_j(k)
\]  

(see Balsara 1998b). The second term in the parentheses is the component parallel to the wavenumber. The resulting field on the left-hand side of equation (2.6) has a zero scalar product with \( k \). We therefore refer to the magnetic field on the left-hand side of equation (2.6) as being divergence-free in Fourier space. Balsara (1998b) considers further variants of this scheme that are more relevant to the discrete form of the divergence operator, but those variants do not produce results that are any different from equation (2.6). Thus, equation (2.6) suffices for our purposes in this work. Therefore, transforming equation (2.6) back to real space completes the divergence-cleaning step.

The scheme has the following advantages:

1. It is not susceptible to even-odd decoupling. This is a major advantage over the SDC1 scheme cataloged in § 2.1.
2. It is exact up to machine accuracy in Fourier space. In fact, for a mesh with \( N^3 \) zones, equation (2.6) provides \( N^3 \) divergence-free conditions that hold in Fourier space. Thus, there is an equivalence between the information content in real and Fourier space.
3. Because of the above two points, this scheme has a major advantage over the SDC2 scheme cataloged in § 2.2. The SDC2 scheme avoids the problem of even-odd decoupling, but it is exactly divergence-free in neither physical space nor Fourier space.

The scheme also has the following disadvantages:

1. It is not exact in real space. However, unlike the SDC2 scheme in § 2.2, successive application of this scheme does not cause the divergence in physical space to change after every application. In that sense, it is unambiguous.
2. It is only applicable to uniform meshes that cover rectangular domains. It cannot be extended to non-Cartesian domains.
3. One has to resort to three FFTs instead of one. As a result, it is slower than SDC1 and SDC2.
4. When solving the problem on a parallel machine, one cannot escape the need for all-to-all communication. The all-to-all communication needed for the present scheme is 3 times as large as the amount of communication needed for SDC1 and SDC2.
5. This method cannot be used for AMR.
6. It might seem that the VDC scheme does not involve a Poisson solver. However, that feeling is illusory. The \(1/k^2\) term in equation (2.6) implicitly involves a Poisson solver step. As a result, the VDC scheme also introduces a nonlocal component into the MHD equations.
7. As for the SDC1 and SDC2 schemes, when using FFTs, aliasing errors cannot be avoided.

2.4. Divergence-Free Staggered-Mesh Scheme

The divergence-free SM scheme is exact in real space. It was described in Balsara & Spicer (1999b). On comparing equation (2.1) with a formal conservation law of the form

\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = 0,
\]

(7.2)

where \( F, G, \) and \( H \) are the fluxes in the \( x-, y-\), and \( z\)-directions, we notice that the flux terms obey the symmetries

\[
F_y = -G_x, \quad F_z = -H_y, \quad G_x = -H_z.
\]

(2.8)

The Balsara & Spicer (1999b) scheme is based on realizing that there is a duality between the fluxes that are produced by a higher order Godunov scheme and the electric fields that are needed in equation (1.1). The duality is put to use by capitalizing on the symmetries in equation (2.8). In a straightforward higher order Godunov scheme that is spatially and temporally second-order accurate, the flux variables are available at the center of each zone’s face. The last three components of the \( F, G, \) and \( H \) fluxes can also be reinterpreted as electric fields in our dual approach. The electric fields are needed at the edge centers, as shown in Figure 1, and are to be used to update the face-centered magnetic fields. Thus, the Godunov fluxes are directly assigned to the edge centers as follows (eqs. [2.9]–[2.14] should not be viewed as matrix equations):

\[
E_{x,j+1/2,k+1/2}^{\pi+1/2} = \frac{1}{4c} \left( H_{x,j+1/2,k+1/2} + H_{x,j+1/2,k+1/2} - G_{y,j+1/2,k+1/2} - G_{y,j+1/2,k+1/2} \right),
\]

(2.9)

\[
E_{y,j+1/2,k+1/2}^{\pi+1/2} = \frac{1}{4c} \left( F_{x,j+1/2,k+1/2} + F_{x,j+1/2,k+1/2} - H_{y,j+1/2,k+1/2} - H_{y,j+1/2,k+1/2} \right),
\]

(2.10)

\[
E_{z,j+1/2,k+1/2}^{\pi+1/2} = \frac{1}{4c} \left( G_{z,j+1/2,k+1/2} + G_{z,j+1/2,k+1/2} - F_{z,j+1/2,k+1/2} - F_{z,j+1/2,k+1/2} \right).
\]

(2.11)
The magnetic fields are updated by applying a discrete version of Stok’s law to equation (1.1), which yields

\[
B_{x,i+1/2,j,k}^{n+1} = B_{x,i+1/2,j,k}^{n} - \frac{\epsilon \Delta t}{\Delta y \Delta z} \left( \Delta z E_{z,i+1/2,j,k+1/2}^{n+1/2} - \Delta z E_{z,i+1/2,j,k-1/2}^{n+1/2} - \Delta y E_{y,i+1/2,j,k+1/2}^{n+1/2} + \Delta y E_{y,i+1/2,j,k-1/2}^{n+1/2} \right),
\]

\[
B_{y,i,j+1/2,k}^{n+1} = B_{y,i,j+1/2,k}^{n} - \frac{\epsilon \Delta t}{\Delta z \Delta x} \left( \Delta x E_{x,i,j+1/2,k}^{n+1/2} - \Delta x E_{x,i,j-1/2,k}^{n+1/2} - \Delta z E_{z,i,j+1/2,k}^{n+1/2} + \Delta z E_{z,i,j-1/2,k}^{n+1/2} \right),
\]

\[
B_{z,i,j+1/2,k}^{n+1} = B_{z,i,j+1/2,k}^{n} - \frac{\epsilon \Delta t}{\Delta y \Delta x} \left( \Delta x E_{x,i,j+1/2,k}^{n+1/2} - \Delta x E_{x,i,j-1/2,k}^{n+1/2} - \Delta y E_{y,i,j+1/2,k}^{n+1/2} + \Delta y E_{y,i,j-1/2,k}^{n+1/2} \right).
\]

This scheme has the following advantages:

1. It is exactly divergence-free in real space. This exactness holds true in a very strong sense. Thus, if the method is exactly divergence-free in a discrete sense in each zone in physical space, then it can be shown that the method is divergence-free at every point in physical space. This is true because one can use the divergence-free reconstruction of vector fields that has been presented in Balsara (2001) to reconstruct the divergence-free magnetic field at all points in space. Balsara (2004) amplifies this point much further, showing that an MHD scheme that relies on divergence-free reconstruction of vector fields has several advantages over one that does not use these concepts.

2. One can assert that on a mesh with \(N^3\) zones, this scheme corresponds to naturally imposing \(N^3\) divergence-free conditions in physical space. The VDC scheme in § 2.3 can be viewed as imposing \(N^3\) divergence-free discrete conditions in Fourier space. However, because of the previous point, we realize that the present scheme furnishes a divergence-free representation of the magnetic field at all points in the computational domain in a continuous sense. Thus, the SM scheme can be made to yield a stronger divergence-free constraint, i.e., one that is valid at any point in the computational domain, as shown by Balsara (2004). The VDC scheme only constrains the magnetic field to be divergence-free at discrete points in Fourier space. Thus, there is indeed a real difference between the two schemes. As a result, for sufficiently difficult problems, we do expect to see differences.

3. The SM scheme has been shown to extend naturally to AMR in Balsara (2001).

4. On parallel machines, it requires minimal interprocessor communication.

5. There are no even-odd decoupling issues to deal with.

6. The issue of aliasing does not arise, because the method does not use FFTs. In that sense, this scheme has an advantage over the VDC scheme in § 2.3.

7. Unlike the SDC schemes, this method does not involve Poisson solvers, and so it is totally local in its influence.

Table 1 provides a comparative synopsis of the points made in this section.

### 3. TEST PROBLEM

#### 3.1. Description of the Test Problem

This present test problem derives from attempts to study the evolution of the turbulent interstellar medium (ISM). It has been studied in Mac Low et al. (2003) and subsequent papers in that series (see D. S. Balsara et al. 2004, in preparation, and J. S. Kim, D. S. Balsara, & M.-M. Mac Low 2004, in preparation). It simulates a patch of the turbulent ISM of a galaxy. Because the ISM is rendered turbulent by strong supernova explosions, the problem consists of having strong pointwise explosions in the medium. To a first approximation, these explosions occur at random points in the galaxy. As a result, we initiate supernova explosions at random points in the computational domain. The physics of the problem is described in the papers cited above. In this paper we describe the problem in its computational aspects and units. The three-dimensional computational domain grows \([-0.1, 0.1] \times [-0.1, 0.1] \times [-0.1, 0.1]\], and 128\(^3\) zones are used in the simulation. Periodic boundary conditions are used. The medium is initially static and has \(\rho = 1.0\), \(P = 0.3\), and \(B_x = 0.056117\). The remaining components of the magnetic field and all three components of the velocity are initially 0. The ratio of the specific heats in the gas is 5/3. Our procedure for initializing supernovae consists of first identifying a random location in the computational domain and then resetting the pressure to 13649.6 in the zones that are within a radial distance of 0.005 from the chosen point. Supernovae are initialized every 0.00125 units of simulation time. The sequence of \((x, y, z)\) positions at which supernovae are initialized is listed in Table 2 for the first 0.035688 units of simulation time, by which time interesting differences arise between the schemes being tested. Interstellar heating and cooling are incorporated, and a detailed description of the physical processes is given in Mac Low et al. (2003) and
references therein. Because of the energetic input in the supernovae explosions, the heating and cooling are needed to help the system maintain temperature equilibrium over long intervals of time. The results presented here were verified to be independent of the details of the heating and cooling processes.

The magnetic field that is initialized in this problem has a magnetic pressure that is much smaller than the gas pressure. Successive explosions generate vorticity and helicity as they interact with the turbulence left behind by the prior set of explosions, as shown in Balsara, Benjamin, & Cox (2001). This builds up helicity, which in turn causes an increase in the magnetic energy. Because of the significant changes in field topology and field energy, this is a stringent test problem for the schemes being tested. We therefore focus on the evolution of the magnetic energy as a function of time through images of the magnetic pressure at different representative times, as well as on the histograms and spectra of turbulence simulations. These are very standard diagnostics used in the turbulence community for analyzing the results of turbulence simulations.

The problem was simulated using an algorithm that is second-order accurate in space and time. Temporal accuracy is obtained by using a two-stage, i.e., predictor-corrector-type, scheme. Each stage uses piecewise-linear interpolation on the primitive variables. The van Leer (1979) limiter is used for interpolation of the density and magnetic field variables. Pressure and velocity variables are interpolated using a minmod limiter. Through extensive experimentation, Balsara has found that this provides rather nice results in MHD calculations at a very low cost (see Balsara 2004). The interpolation scheme is coupled with an HLL-type (Harten, Lax, & van Leer 1983) Riemann solver to yield a spatially second-order accurate scheme. Pressure positivity is ensured using the formulation in Balsara & Spicer (1999a). The algorithm described here is one of several algorithms implemented in Balsara’s RIEMANN framework for computational astrophysics. While it is not as accurate as the method described in Balsara (1998b), its twin advantages are robustness and speed without relinquishing second-order accuracy. The second-order accuracy of the present algorithm is cataloged in D. S. Balsara et al. (2004, in preparation).

3.2. Description of the Results

3.2.1. Energy Evolution of the Magnetic Field

Figure 2 shows the evolution of the magnetic energy as a function of time for the four different schemes that are compared. The divergence-cleaning schemes, SDC1, SDC2, and VDC, were applied to the simulation at every time step, and the results are shown in Figures 2a, 2b, and 2c, respectively. The result from the SM scheme is shown in Figure 2d. From

| Number | X       | Y       | Z       |
|--------|---------|---------|---------|
| 1....... | 7.825E−07 | 1.315E−02 | 7.556E−02 |
| 2....... | −5.413E−02 | −4.672E−02 | −7.810E−02 |
| 3....... | −3.211E−02 | 6.793E−02 | 9.346E−02 |
| 4....... | −6.165E−02 | 5.194E−02 | −1.690E−02 |
| 5....... | 5.346E−03 | 5.297E−02 | 6.711E−02 |
| 6....... | 7.698E−04 | −6.165E−02 | −9.331E−02 |
| 7....... | 4.174E−02 | 6.867E−02 | 5.889E−02 |
| 8....... | 9.304E−02 | −1.538E−02 | 5.269E−02 |
| 9....... | 9.196E−03 | −3.460E−02 | −5.840E−02 |
| 10...... | 7.011E−02 | 9.103E−02 | −2.378E−02 |
| 11...... | −7.375E−02 | 4.746E−03 | −2.639E−02 |
| 12...... | 3.653E−02 | 2.470E−02 | −1.745E−03 |
| 13...... | 7.268E−03 | −3.683E−02 | 8.847E−02 |
| 14...... | −7.272E−02 | 4.364E−02 | 7.664E−02 |
| 15...... | 4.777E−02 | −7.622E−02 | −7.250E−02 |

| Number | X       | Y       | Z       |
|--------|---------|---------|---------|
| 16...... | −1.023E−02 | −9.079E−03 | 6.056E−03 |
| 17...... | −9.534E−03 | −4.954E−02 | 5.162E−02 |
| 18...... | −9.092E−02 | −5.223E−03 | 7.374E−03 |
| 19...... | 9.138E−02 | 5.297E−02 | −5.355E−02 |
| 20...... | 9.409E−02 | −9.499E−02 | 7.615E−02 |
| 21...... | 7.702E−02 | 8.278E−02 | −8.746E−02 |
| 22...... | −7.306E−02 | −5.846E−02 | 5.373E−02 |
| 23...... | 4.679E−02 | 2.872E−02 | −8.216E−02 |
| 24...... | 7.482E−02 | 5.545E−02 | 8.907E−02 |
| 25...... | 6.248E−02 | −1.579E−02 | −8.402E−02 |
| 26...... | −9.090E−02 | 2.745E−02 | 5.857E−02 |
| 27...... | −1.130E−02 | 6.520E−02 | 8.496E−02 |
| 28...... | −3.186E−02 | 3.858E−02 | 3.877E−02 |
| 29...... | 4.997E−02 | −8.524E−02 | 5.871E−02 |
| 30...... | 8.455E−02 | −4.098E−02 | −4.438E−02 |
Figure 2a we see that the SDC1 scheme shows a chaotic and very rapid rise in the magnetic energy. Even after the first few supernova explosions, there is a dramatic increase in the magnetic energy. This increase sets in as soon as we have a situation in which one explosion interacts with the complicated magnetic field structure left behind by a prior explosion. This point is made graphically in Figure 3, which shows an illustrative slice plane at a time of 0.005948 for the four schemes being tested. The SDC1 scheme is applied after every time step and does cause the magnetic field to be restored to its divergence-free state after each application of equation (2.2). However, SDC1 is also susceptible to even-odd decoupling. As a result, even though the divergence is zero in each zone in the sense of equation (2.3), each zone is decoupled from the zones that surround it in the divergence-cleaning step. For that reason, even though the scheme treats isolated explosions just fine (as shown by Balsara 1998b and Tóth 2000), when explosions interact and generate small-scale structure in the process, there is a dramatic increase in the magnetic energy. At late times, the supernovae inevitably explode in a field of relic turbulence left behind by prior explosions. Each of the spikes in Figure 2a at late times corresponds to the interaction of a new supernova explosion with the ambient turbulence. From Figure 2b we see that the SDC2 scheme also shows a chaotic and rather rapid rise in the magnetic energy. From Figure 2c we see that the VDC scheme also shows some fluctuations. The SM scheme, for which the temporal evolution of the magnetic energy is shown in Figure 2d, is the only scheme for which the magnetic energy grows in a monotonically increasing fashion without any strong fluctuations. When two remnants collide, they produce a converging flow that stagnates at the point of collision. Cooling tends to abet the formation of very persistent, converging flows over very small length scales (as does gravity in self-gravitating flows). Because of the formation of persistent, converging flows, we have rapid, localized buildup of nonzero divergence that the SDC1, SDC2, and VDC schemes are incapable of removing. Even the SDC1 scheme, which makes the discrete divergence mathematically zero in real space, is not without aliasing errors due to even-odd decoupling. The SM scheme, which does not rely on divergence cleaning, faithfully describes the field evolution in such situations.

It is worth pointing out that the fluctuations in the VDC scheme are small enough that one could perhaps have
extracted the rate of growth of the magnetic field by averaging over the fluctuations. Furthermore, once the fluctuations subside, the scheme produces the same amount of growth in magnetic energy as the SM scheme. We have also run all four schemes for a length of time that is almost 7 times longer than the times reported here. The magnetic energy in the VDC and SM schemes reaches the same final level once the fluctuations in the VDC scheme have subsided. This provides an important cross-check for the two schemes. The cross-check is important because spectral schemes (see, e.g., Zeinecke, Politano, & Pouquet 1998) invariably use the VDC scheme and have been successfully applied to incompressible dynamo simulations. The magnetic energy in the SDC1 and SDC2 schemes undergoes explosive growth and saturates at a level that is an order of magnitude larger than that in the VDC and SM schemes. We therefore identify the SDC1 and SDC2 schemes as being unsuitable for dynamo applications. It must also be noted that had the problem not been so severe, as is the case for incompressible and moderately compressible dynamo simulations, the VDC scheme would have performed just fine.

3.2.2. Magnetic Structures

The evolution of magnetic energy that was discussed in the previous two paragraphs gives us a clue that something may be wrong with the SDC1/2 schemes and the VDC scheme. However, it does not make the reason for the fluctuations graphically clear. That is done in Figures 3 and 4. Figure 3 (top left) shows the logarithm of the magnetic pressure in a selected slice plane of the shells a brief time after they have interacted, i.e., at a simulation time of 0.005948, for the SDC1 scheme. Figure 3 (top right, bottom left, bottom right) shows the logarithm of the magnetic pressure in the same slice plane at the same time for the SDC2, VDC, and SM schemes, respectively. (Taking the logarithm of the magnetic pressure only helps in bringing out the contrasts that would otherwise be missed.) From Figure 3 (top left) we expect the interacting shells in the three-dimensional simulation to intersect in a plane, which is shown as a line in the slice plane. We can also see that the spurious fluctuations are most prominent in the portion of the interior of each interacting shell that is closest to the plane of interaction and decrease with distance from that
plane. Since the plane in which the shells intersect is also the region where the nonlocal divergence cleaning is maximally applied (see disadvantage 7 in §2.1), we expect that the zones around that region will be maximally influenced by the divergence-cleaning step in equation (2.2). This expectation is exactly borne out in Figure 3 (top left). We can also see that the interior of the isolated shell has small fluctuations in it. However, the fluctuations are not so pronounced that one would focus on them, unless one anticipated them in advance. Figure 3 (top right) shows that SDC2 shares many of the same traits as SDC1. We do, however, see that the pronounced banded structure that is visible in the lower interacting shell of Figure 3 (top left) is not present in Figure 3 (top right). This is symptomatic of the fact that SDC2 is free of even-odd decoupling, while SDC1 is not. Thus, we see that even though SDC2 does not clean the divergence entirely in one step, it has some advantages because it does not suffer from some of the other limitations of SDC1. Figure 3 (bottom left) shows the same slice plane from the VDC scheme. We see that it, too, has unphysical fluctuations in the magnetic energy around the plane where the two shells interact. We see from Figure 3 (bottom left) that spurious fluctuations in the VDC scheme are most prominent in the portion of the interior of each interacting shell that is closest to the plane of interaction and decrease with distance from that plane. Thus, VDC, SDC1, and SDC2 all display the same kinds of spurious fluctuations. This clearly bears out the point made in disadvantage 6 of §2.3, where we pointed out that the VDC scheme also has a nonlocal character implicitly built into it because of the use of a Poisson solver. Thus, even though the VDC scheme exactly imposed $N^3$ divergence-free conditions in spectral space (just as the SDC1 scheme imposes $N^3$ divergence-free conditions in real space), that is still not sufficient to ensure that it obtains a physical result. The reason invariably stems from the nonlocal aspect of the SDC1, SDC2, and VDC schemes. The above three schemes are also not free of aliasing effects. Figure 3 (bottom right) shows the same slice plane for the SM scheme. The SM scheme is free of the unphysical fluctuations in the magnetic energy that emerged in the SDC1, SDC2, and VDC schemes. Moreover, we see that the interior of the isolated supernova shell in Figure 3 (bottom right) is entirely free of small-scale fluctuations, illustrating the usefulness of a divergence-free scheme that is totally local. We also remind the reader of advantages 1 and 2 in §2.4, which show that a scheme that is divergence-free in a discrete sense has the special property that its magnetic field can be reconstructed in
a divergence-free fashion at every point in physical space. This is a property that does not hold true for the VDC scheme.

It is also interesting to ask what happens at a somewhat later time, when several supernova shells have begun to intersect. Figure 4 (top left, top right, bottom left, bottom right) shows the same slice plane as in Figure 3 at a later time of 0.0011896 for the SDC1, SDC2, VDC, and SM schemes, respectively. We see that the fluctuations in Figure 4 (top left) for the SDC1 scheme have grown to the point at which they are on par with the compressed field in the individual supernova shells! The fluctuations in Figure 4 (top right) for the SDC2 scheme are also unacceptably large, but not so large as to swamp the shell boundaries. From Figure 4 (bottom left) we see that the magnetic field fluctuations in the VDC scheme are also quite large. They are, however, better localized and, for the most part, do not exceed the strength of the magnetic field in the shells. From Figure 4 (bottom right) we see that the SM scheme is the only scheme that produces interacting shells with clean interiors.

3.2.3. Statistics of the Magnetic Field

In the previous two paragraphs we showed that the turbulent structures that are produced by the SDC1, SDC2, and VDC schemes can have some faulty elements. In turbulence simulations it is also of interest to study statistics and spectra. It is therefore worthwhile to ask whether differences show up in the statistical measures that are traditionally used in turbulence studies. In view of the computational focus of this paper, we focus on the histogram of the magnitude of the magnetic field, which is but one of many popular diagnostics that are used in turbulence research. Figure 5a shows the histograms for the SDC1 scheme at times of 0.004758, 0.005948, and 0.008327. The times are also shown by the vertical lines in Figure 2a and straddle the first strong fluctuation in magnetic energy, which sets in when the first two shells interact. The horizontal axis in the histogram shows the strength of the magnetic field, and the vertical axis shows the fraction of the computational volume that has that field strength. Figure 5b shows the histograms for the SDC1 scheme at times of 0.03093, 0.03212, and 0.03331. The times are also shown by the vertical lines in Figure 2a and straddle a strong fluctuation in magnetic energy that occurs much later. Figure 5c shows the same times as Figure 5a for the SM scheme. Figure 5d shows the same times as Figure 5b for the SM scheme. From Figure 5a we see that when the magnetic

![Figure 5: Histograms of the magnitude of the magnetic field for the SDC1 scheme at times of 0.004758, 0.005948, and 0.008327. (b) Histograms for the SDC1 scheme at times of 0.03093, 0.03212, and 0.03331. (c, d) Same as (a, b) but for the SM scheme.](attachment:image.png)
energy spikes upward in Figure 2a at a time of 0.005948, the histogram undergoes a shift to the right, indicating that when the shells intersect, several zones in the computation acquire strong magnetic fields. From Figure 2a we also see that when the magnetic energy subsides in Figure 2a at a time of 0.0035688, the histogram has resumed a shape quite similar to its original shape at the time of 0.004758. From Figure 5c we see that the SM scheme does not suffer from this deficiency. Figure 5b corresponds to the SDC1 scheme at a later time, when the magnetic energy in Figure 2a undergoes a similar, albeit smaller, spike. Again we observe that the histogram of the magnetic field for the SDC1 scheme undergoes a substantial shift. The histogram for the SM scheme in Figure 5d does not undergo a similar shift. The shift of the histograms is clearly a consequence of the FFT-based elliptic solver, which causes local information to propagate globally. We also see from Figure 5 that the histograms broaden with increasing time. This is an expected result for the present class of turbulence simulations. Since histograms are one of the most popular ways of gathering statistics from a turbulent simulation, we have convincingly demonstrated in this paragraph that one is apt to extract spurious results from an inadequate scheme for numerical MHD.

3.2.4. Spectra of the Magnetic Field

Spectral analysis is another very powerful and well-used strategy for extracting diagnostics from a turbulence simulation. In Figure 6 we show power spectra for the magnetic field at the simulation time of 0.035688 for all four schemes. By this time, all points in the simulation have been processed at least once by the supernova explosions. We see that the SDC1 and SDC2 schemes produce a considerable amount of small-scale power. This is consistent with the spurious structures they produced in Figures 3 and 4 and the peculiar shifts in the histograms in Figure 5. From Figure 6 we see that SDC1 produces the worst spectrum because of its susceptibility to even-odd decoupling. The spectrum from SDC2 is marginally better, although the SDC2 scheme also suffers from the deficiency that it is not exact in real space. The spectrum from the VDC scheme is quite good, although it, too, shows some spurious energy on the smallest scales. The SM scheme alone produces spectra with well-tempered dissipation characteristics on the smallest scales.

4. CONCLUSIONS

Based on the work presented here, we offer the following conclusions:

1. We have cross-tested the SDC1, SDC2, and VDC (divergence-cleaning) schemes and the SM (divergence-free) scheme for numerical MHD. We have found that there are important differences in the results if one looks closely enough with a rich enough set of diagnostic tools. The differences become quite pronounced when the physical problem becomes rather stringent. This has been demonstrated by applying the four schemes to the same test problem of supernova-induced MHD turbulence in the ISM.

2. The scalar divergence-cleaning strategies, such as those examined by Tóth (2000), show spikes in the magnetic energy on stringent enough problems. The physical reason for these spikes is explained. The vector divergence-cleaning method also shows some spurious energetic fluctuations, but it does, at least, converge to the right level of energy after the fluctuations have died out.

3. The problems with the SDC1, SDC2, and VDC schemes are properly explained as being a consequence of the non-locality introduced into numerical MHD by the divergence-cleaning strategy. The schemes also suffer from aliasing errors. The SDC1 scheme also suffers from even-odd decoupling.

4. Examination of the magnetic field structures shows that the differences between the divergence-cleaning and divergence-free schemes become especially pronounced when persistent linear, sheetlike, and volumetric structures form in the flow that have a tendency to generate divergence. The physical reasoning for that is given in the text.

5. Statistical and spectral analyses also show the deficiency of the divergence-cleaning schemes, thereby limiting their utility in any numerical study of MHD turbulence.

6. Spectral analysis of the SM scheme on some of the most stringent problems that we have been able to design shows that the method is not susceptible to unbounded growth of spurious oscillations.

7. We have shown that SDC1 and SDC2 produce spurious results for energetics, structures, statistics, and spectra, which are the four mainstays of turbulence studies. From this we conclude that the SDC1 and SDC2 schemes are really not suitable for turbulence studies. The VDC scheme shows some deficiencies. The SM scheme is the only scheme that does not show deficiencies on any of the fronts on which we tested, showing that it is uniquely well suited for turbulence studies.

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REFERENCES

Balsara, D. S. 1998a, ApJS, 116, 119
———, 1998b, ApJS, 116, 133
———, 2001, J. Comput. Phys., 174, 614
———, 2004, ApJS, 151, 149
Balsara, D. S., Benjamin, R. A., & Cox, D. P. 2001, ApJ, 563, 800
Balsara, D. S., & Spicer, D. S. 1999a, J. Comput. Phys., 148, 133
———, 1999b, J. Comput. Phys., 149, 270
Brackbill, J. 1985, Space Sci. Rev., 42, 153
Brackbill, J. U., & Barnes, D. C. 1980, J. Comput. Phys., 35, 426
Brecht, S. H., Lyon, J. G., Fedder, J. A., & Hain, K. 1981, Geophys. Res. Lett., 8, 397
Brio, M., & Wu, C. C. 1988, J. Comput. Phys., 75, 400
Dai, W., & Woodward, P. R. 1994, J. Comput. Phys., 111, 354
———, 1998, ApJ, 494, 317
Dedner, A., et al. 2002, J. Comput. Phys., 175, 645
DeVore, C. R. 1991, J. Comput. Phys., 92, 142
Evans, C. R., & Hawley, J. F. 1988, ApJ, 332, 659
Harten, A., Lax, P. D., & van Leer, B. 1983, SIAM Rev., 25, 35

Jackson, J. D. 1975, Classical Electrodynamics (New York: Wiley)
Kim, J. S., Ryu, D., Jones, T. W., & Hong, S. S. 1999, ApJ, 514, 506
Londrillo, P., & Del Zanna, L. 2000, ApJ, 530, 508
Mac Low, M.-M., Balsara, D. S., de Avillez, M. A., & Kim, J. S. 2003, ApJ, submitted
Powell, K. G. 1994, An Approximate Riemann Solver for MHD That Actually Works in More Than One Dimension, ICASE Rep. 94-24 (Langley: ICASE)
Powell, K. G., Roe, P. L., Linde, T. J., Gombosi, T. I., & DeZeeuw, D. L. 1999, J. Comput. Phys., 154, 284
Roe, P. L., & Balsara, D. S. 1996, SIAM J. Appl. Math., 56, 57
Ryu, D., & Jones, T. W. 1995, ApJ, 442, 228
Ryu, D., Jones, T. W., & Frank, A. 1995, ApJ, 452, 785
Ryu, D., Miniati, F., Jones, T. W., & Frank, A. 1998, ApJ, 599, 244
Toth, G. 2000, J. Comput. Phys., 161, 605
van Leer, B. 1979, J. Comput. Phys., 32, 101
Yee, K. S. 1966, IEEE Trans. Antenna Propagation, 14, 302
Zachary, A. L., Malagoli, A., & Colella, P. 1994, SIAM J. Sci. Comput., 15, 263
Zeinecke, E., Politano, H., & Pouquet, A. 1998, Phys. Rev. Lett., 81, 4640