SPECTRAL METHODS FOR TIME-DEPENDENT STUDIES OF ACCRETION FLOWS. III. THREE-DIMENSIONAL, SELF-GRAVITATING, MAGNETOHYDRODYNAMIC DISKS

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ABSTRACT

Accretion disks are three-dimensional, turbulent, often self-gravitating, magnetohydrodynamic (MHD) flows, which can be modeled with numerical simulations. In this paper, we present a new algorithm that is based on a spectral decomposition method to simulate such flows. Because of the high order of the method, we can solve the induction equation in terms of the magnetic vector potential and, therefore, ensure trivially that the magnetic fields in the numerical solution are divergence free. The spectral method also suffers minimally from numerical dissipation and allows for an easy implementation of models for subgrid physics. Both properties make our method ideal for studying MHD turbulent flows such as those found in accretion disks around compact objects. We verify our algorithm with a series of standard tests and use it to show the development of MHD turbulence in a simulation of an accretion disk. Finally, we study the evolution and saturation of the power spectrum of MHD turbulence driven by the magnetorotational instability.

Key words: accretion, accretion disks – black hole physics – hydrodynamics – MHD

1. INTRODUCTION

Although the standard accretion disk model was proposed more than 30 years ago (Shakura & Sunyaev 1973), the properties of turbulent angular momentum transport in accretion disks are still not well understood. Shakura & Sunyaev (1973) hypothesized in their original work that magnetic fields may be important in mediating the required angular momentum transport. However, it was not until the last decade that Balbus & Hawley (1991a, 1991b) pointed out that the magnetorotational instability (MRI) can generate turbulence and lead to transport of angular momentum in accretion disks.

The nonlinear evolution of the MRI and the generation of turbulence was studied numerically by Balbus & Hawley (1991b), following the earlier linear analysis of the instability. Later, local numerical simulations were performed in the shearing box approximation (e.g., Hawley et al. 1995; Brandenburg et al. 1995; Hawley et al. 1996), aimed to study further the local properties of three-dimensional MRI, with and without stratification (Stone et al. 1996). The natural extension of shearing box calculations, namely the cylindrical disks with vanishing vertical gravitational force, were simulated by Hawley (2001) and Armitage et al. (2001) to illustrate some important aspects of the turbulent transport, especially in the vicinity of the inner-most stable circular orbit around a black hole. Finally, global numerical simulations of magnetohydrodynamic (MHD) disks have also been carried out for a variety of settings and physical conditions.

All of the codes that have been used to study the properties of MRI-driven turbulence have been based on two types of schemes. The first class of studies make use of the very successful scheme developed originally for the ZEUS code (e.g., Stone & Pringle 2001; Armitage et al. 2001; see Stone & Norman 1992a, 1992b for the ZEUS code) or schemes based on it (e.g., Hawley 2000; De Villiers & Hawley 2003; Steinacker & Papaloizou 2002; Igumenshchev et al. 2003). The other class of studies have used different conservative schemes (e.g., Koide et al. 1999; Gammie et al. 2003; Machida & Matsumoto 2003).

Both types of methods allow for a stable and efficient implementation of solvers of the MHD equations. However, they also introduce a considerable amount of numerical dissipation to the problem. This is significant because most calculations have been performed for ideal MHD and, hence, it is this numerical dissipation that allows for the MRI instability to saturate and the resulting turbulence to reach a dynamical steady state (see however, Fleming et al. 2000; Fromang et al. 2007; Lesur & Longaretti 2007, where the assumption of ideal MHD is relaxed). As a result, the kinetic and magnetic energies of different simulations saturate at different levels depending on the resolution and the scheme (Hawley et al. 1999). The effect of this shortcoming can be reduced, e.g., by increasing the resolution, by increasing the discretization order, or by using numerical schemes that reduce numerical diffusion (see, e.g., Gardiner & Stone 2005; Stone et al. 2008, for an unsplit Godunov MHD code Athena).

In this third paper of the series, we address this issue by developing a version of our pseudo-spectral numerical algorithm to simulate three-dimensional MHD disks. Spectral algorithms are high order numerical methods, in which dynamical variables are evolved along orthogonal modes. For smooth functions, they require only $\sim \pi$ grid points to accurately resolve one wavelength, compared to $\sim 16$ grid points for finite difference schemes to reach the same accuracy. Moreover, the MHD equations can be evolved in time in terms of the magnetic vector potential $\mathbf{A}$, preserving thus trivially the divergenceless character of the magnetic field.

The high order of spectral methods makes them ideal for studying problems of MHD turbulence, since they do not suffer from serious numerical dissipation. Moreover, spectral methods can easily incorporate models of subgrid physics, such as the those involved in large-eddy simulation (LES, see, e.g., Berselli et al. 2005; John 2003; Lesieur et al. 2005; Sagaut 2004). The idea of LES is to model approximately the small-scale structures, instead of resolving all features of a turbulent flow, with subgrid models that are based either on experiments or phenomenological descriptions of the small-scale turbulence.
2. EQUATIONS AND ASSUMPTIONS

Magnetohydrodynamics. We consider three dimensional viscous, compressible, MHD flows. The MHD equations contain four equations, namely, the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$  

(1)

the momentum equation

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho (\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla \mathbf{P} + \frac{1}{4\pi} (\mathbf{B} \cdot \nabla) \mathbf{B} + \nabla \tau + \rho \mathbf{g},$$

(2)

the energy equation

$$\frac{\partial E}{\partial t} + \nabla \cdot (E \mathbf{v}) = -P \nabla \cdot \mathbf{v} + \Phi_v + \Phi_B - \nabla \cdot \mathbf{q} - \nabla \cdot \mathbf{F},$$

(3)

and the induction equation

$$\frac{\partial \mathbf{A}}{\partial t} = \mathbf{v} \times (\nabla \times \mathbf{A}) + \frac{c^2}{4\pi \sigma} \nabla^2 \mathbf{A} + \nabla \dot{\Lambda}.$$  

(4)

We denote by $\rho$ the density, by $\mathbf{v}$ the velocity, and by $E$ the thermal energy. In the momentum equation, $\mathbf{P}$ is the thermal pressure, $\tau$ is the viscosity tensor, and $\mathbf{g}$ is the gravitational acceleration. In the energy equation, there are two dissipative terms, namely, the Ohmic dissipation $\Phi_v$, and the viscous dissipation $\Phi_B$. We use $\mathbf{q}$ to denote the heat flux vector and $\mathbf{F}$ to denote the radiation flux.

We write the induction equation in terms of the vector potential $\mathbf{A}$, so that the magnetic field is given by $\mathbf{B} \equiv \nabla \times \mathbf{A}$. The symbol $\sigma$ here represents the electrical conductivity and we define the microscopic resistance by $\eta \equiv c^2/4\pi \sigma$. The last term, $\nabla \dot{\Lambda}$, in the induction equation is a gauge source/sink term, the purpose of which we explain below.

It is straightforward to show that Equation (4) leads to the standard induction equation

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}) + (\nabla \cdot \eta \nabla) \mathbf{B}.$$  

(5)

Because $\nabla \times (\nabla \dot{\Lambda}) \equiv 0$, $\nabla \dot{\Lambda}$ does not affect the magnetic field. However, we retain this gauge term because, by proper choice, it can be used to suspend a nonphysical linear growth in $\mathbf{A}$ and hence improve the numerical accuracy of the scheme. To illustrate this, we consider a Keplerian disk with a constant vertical magnetic field so that the vector $\mathbf{v} \times \mathbf{B}$ has a nonzero $r$-component. By assuming $\eta = 0$, the potential form of the induction equation reduces to

$$\frac{\partial \mathbf{A}_r}{\partial t} = B_z \sqrt{\frac{GM}{r}} + \frac{\partial \dot{\Lambda}}{\partial r},$$  

(6)

where $G$ and $M$ are the gravitational constant and the mass of the central object, respectively. The first term on the right-hand side leads to a linear growth of $A_r$ in time. This growth will never saturate, because the mean of the product $v_k B_z$ is always positive. Although the actual value of the magnetic field will not be affected, this growth will lead to a large round-off error in $A_r$ if the MHD equations are integrated for a long time. This difficulty can be overcome by setting

$$\dot{\Lambda} \equiv -B_z \int dr \sqrt{\frac{GM}{r}} \equiv -2B_z \sqrt{GMr},$$  

(7)

which suppresses the linear growth of the vector potential. In our algorithm, $\dot{\Lambda}$ is calculated dynamically from the values of $\dot{B}_z(t, r)$ and $\dot{v}_k(t, r)$, where the over-bars indicate averages over the azimuthal and vertical directions of the disk, respectively.

The analytical forms of the various physical quantities in Equations (1)–(3) were given in Chan et al. (2005). Here, we generalize them to three dimensions. The viscosity tensor (in Cartesian coordinates) is

$$\tau_{ij} = 2(\mu_\tau + \mu_s) e_{ij} + \left( -\frac{4}{3} \mu_s \right) (\nabla \cdot \mathbf{v}) \delta_{ij},$$

(8)

where the strain-rate tensor $e_{ij}$ is

$$e_{ij} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right).$$

(9)

The viscous dissipation rate is, therefore,

$$\Phi_v = 2(\mu_\tau + \mu_s) e_{ij}^2 + \left( -\frac{4}{3} \mu_s \right) (\nabla \cdot \mathbf{v})^2.$$  

(10)

Finally, the Ohmic dissipation rate, $\Phi_\eta$, is given by

$$\Phi_\eta = \frac{J^2}{\sigma} = \frac{\eta}{4\pi} ||\nabla \times \mathbf{B}||^2.$$  

(11)

We again assume an ideal gas law so that

$$E = \frac{\rho k_B T}{2 \mu_m H},$$

(12)

$$P = \frac{\rho k_B T}{\mu_m H}.$$  

(13)

For the induction equation, we typically set the resistance $\eta$ to zero so that the diffusion term in the induction equation vanishes.

Gravity. We solve for the gravitational acceleration, $\mathbf{g}$, in a similar way as in Chan et al. (2006). We first define the gravitational potential $\Psi$ by

$$\mathbf{g} \equiv -\nabla \Psi,$$  

(14)

which is given by the volume integral

$$\Psi(t, \mathbf{x}) = -G \int \frac{\rho(t, \mathbf{x}^\prime)}{||\mathbf{x} - \mathbf{x}^\prime||^3} d^3 x^\prime.$$  

(15)
over all space. Rewriting Equation (15) in differential form, we obtain Poisson’s equation

\[ \nabla^2 \Psi = 4\pi G \rho, \]  

(16)

with \( \Psi \) satisfying the boundary condition \( \Psi(t, \infty) = 0 \) at all times. When simulating accretion flows, the computational domain \( D^3 \) is usually finite. Based on its linearity, we can decompose Poisson’s equation into two parts, i.e.,

\[ \nabla^2 \Psi_{\text{int}} = 4\pi G \rho_{\text{int}}, \]  

(17)

and

\[ \nabla^2 \Psi_{\text{ext}} = 4\pi G \rho_{\text{ext}}, \]  

(18)

where \( \rho_{\text{int}} \) denotes the mass density within the computational domain, which in our case is the disk density, and \( \rho_{\text{ext}} \) refers to external sources such as the central object and/or a companion star. The gravitational field is then given by

\[ g = g_{\text{ext}} + g_{\text{ext}} = -\nabla(\Psi_{\text{int}} + \Psi_{\text{ext}}). \]  

(19)

For the gravitational field of the central object, we use the pseudo-Newtonian approximation of Mukhopadhyay (2002) for \( g_{\text{ext}} \), which takes the form

\[ g_{\text{ext}} = -\frac{c^2}{r^3} \left( \frac{GM}{c^2} \right)^2 \left[ \frac{r^2 - 2(a/c)^2GMr/c^2 + (a/c)^2}{\sqrt{GMr/c^2}} + a/c \right]^2 \hat{r}. \]  

(20)

Here, \( r_s \equiv 2GM/c^2 \) is the Schwarzschild radius and \( a \) is a parameter related to the spin of the central object.

In order to solve for self-gravity using Equation (17) within \( D^3 \), we compute the integral

\[ \Psi_{\text{int}}(t, x) = -G \int_{D^3} \rho_{\text{int}}(t, x') |x - x'|^3 \]  

(21)

as in Chan et al. (2006). We then use Equation (19) to obtain the total gravitational field and use it in the momentum equation.

**Subgrid Physics.** For homogeneous and isotropic turbulence, the ratio between the most energetic scale to the viscous length scale is proportional to \( \mathcal{O}(Re^{5/4}) \), where \( Re \) is the Reynolds number. This scaling law suggests that the computational cost is proportional to \( \mathcal{O}(Re^3) \) for three-dimensional, time-dependent simulations. Although spectral methods offer efficient ways to capture small-scale features, they are still unable to resolve the expected dynamical range in accretion disks down to the molecular viscous length scale.

In order to reduce the computational cost, we need to introduce an artificial cutoff to the problem. Following the LES approach (see Sagaut 2004, for a very informative introduction), we will use our numerical algorithm to solve the MHD equations for scales larger than this cutoff scale and introduce an approximate model for the smaller scales. Introducing such a model is required by the nonlinear character of the MHD equations, which allow for coupling between the simulated large scales and the unresolved small scales.

For any physical quantity \( f \), we denote by \( \hat{f} \) the filtered (i.e., resolved) function and define the subgrid fluctuation by

\[ f' \equiv f - \hat{f}. \]  

(22)

We can then formally decompose any nonlinear product of two physical quantities \( fg \) in physical space as

\[ \overline{fg} = (\overline{f'} + \overline{g})(\overline{f} + \overline{g}) \]

\[ = \overline{ff'} + L_{ij} + C_{ij} + R_{ij}. \]  

(23)

where \( L_{ij} = \overline{f'g'} - \overline{f}\overline{g} \), \( C_{ij} = \overline{fg'} + \overline{f'g} \), and \( R_{ij} = \overline{fg'}. \)

If the quantities \( f \) and \( g \) are different components of the velocity, these higher order correlations are the Leonard tensor, the cross-stress tensor, and the Reynolds subgrid tensor, respectively (Sagaut 2004). Note that the Reynolds subgrid tensor is different from the physical viscosity tensor. It appears because of the presence of the artificial cutoff and is independent of the molecular viscosity.

The basic idea of LES is to devise a model for the three tensors (24) that captures the physics of subgrid turbulence. This is beyond the scope of the current paper. Here, we will approximate the effect of \( L_{ij} + C_{ij} + R_{ij} \) by applying the following spectral filter (see Chan et al. 2005, and references therein) in spectral space,

\[ \sigma_\beta \left( \frac{n}{N} \right) = \exp \left( -\frac{|\ln \epsilon|}{N} \right), \]  

(25)

where \( \beta \) is the order of the filter; \( \epsilon \) is the machine accuracy, which is of order \( 10^{-15} \) for double precision floating point numbers; and \( n \) and \( N \) are the point index and number of points in spectral space, respectively. Applying this filter once after every time step is equivalent to adding a high-order (super)diffusion term in the dynamic equations.

Although this approach is not based on any physical model, it has been known to reproduce the large-scale properties of turbulent flows reasonably well (see, for example, Karamanos & Karniadakis 2000; Pasquetti 2005). Moreover, such filtering process is equivalent to the so-called super vanishing viscosity (Ma 1998a, 1998b). By setting the order of the filter, \( \beta \), proportional to the number of grid point \( N \), super vanishing viscosity is able to stabilize the pseudo-spectral method even though discontinuities may be present. Its effect is similar to artificial viscosity used in finite difference methods but it preserves the spectral accuracy for the resolved scales.

3. IMPLEMENTATION OF THE PSEUDO-SPECTRAL METHODS

**Spatial Discretization.** In our current implementation of the pseudo-spectral method in three-dimensions we use cylindrical coordinates because we are interested in the study of geometrically thin accretion disks. It is trivial, however, to alter the geometry of the domain of solution, when necessary, and use spherical-polar coordinates.

Along the radial direction, we use a Chebyshev collocation method, whereas, for the azimuthal and vertical directions, we choose the Fourier basis. This implies periodic boundary conditions for both the azimuthal direction (which is natural) and the vertical direction (which needs to be justified for each specific application). The computational domain is \( D^3 = [r_{\text{min}}, r_{\text{max}}] \times [-\pi, \pi] \times [-Z, Z] \) and we require \( r_{\text{min}} > 0 \) to avoid the coordinate singularity at the origin.

Formally, we expand any physical quantity \( f(t, r, \phi, z) \) as

\[ f(t, r, \phi, z) = \sum_{n,m,l} \tilde{f}_{nm}(t)T_n(\phi)e^{im\phi}e^{inlZ/Z}. \]  

(26)
Here, $T_n$ is the $n$th order Chebyshev polynomial and $F \in [-1, 1]$ is the standardized coordinate in the radial direction (Chan et al. 2005). Note that the frequently used Chebyshev–Gauss–Lobatto grid

$$\tilde{r}_k = \cos\left(\frac{\pi k}{N}\right), \text{ for } 0 \leq k \leq N$$

has the property that

$$\tilde{r}_0 - \tilde{r}_1 = \tilde{r}_{N-1} - \tilde{r}_N \propto N^{-2}.$$  \hspace{1cm} (28)

This gives the time-stepping constrain $\Delta t \propto N^{-2}$ for hyperbolic (wave-like) equations and $\Delta t \propto N^{-4}$ for parabolic (diffusion-like) equations. To overcome this restriction, we use instead the Kosloff–Tal-Ezer mapping (Kosloff & Tal-Ezer 1993)

$$r = \frac{r_{\max}}{2} \left[ \frac{\arcsin(\alpha \tilde{r}) + 1}{\arcsin(\alpha)} + 1 \right] - \frac{r_{\min}}{2} \left[ \frac{\arcsin(\alpha \tilde{r}) - 1}{\arcsin(\alpha)} + 1 \right].$$  \hspace{1cm} (29)

We compute the parameter $\alpha$, which controls the regularity of the grid spacing, to be $\alpha = \text{sech}\left[\ln(\epsilon)/N\right]$, where $\epsilon$ is the machine accuracy, in order to optimize the accuracy of the spatial derivatives (Don & Solomonoff 1997).

We compute the numerical derivatives along the $r$- and $\phi$-directions as in Chan et al. (2005, 2006). Hence, the radial derivative is given by the chain rule

$$\frac{\partial f}{\partial r} = \frac{1}{dr/d\tilde{r}} \frac{\partial f}{\partial \tilde{r}},$$

where the derivative in the standardized coordinate is

$$\frac{\partial f}{\partial \tilde{r}} = \sum_{n,m,l} f^{(1)}_{nml}(t) T_n(\tilde{r}) e^{im\phi} e^{in\tilde{r}/Z}.$$  \hspace{1cm} (31)

We precompute analytically the derivative of the mapping, $dr/d\tilde{r}$. Here, we use $f^{(1)}$ to denote the Chebyshev coefficient of the radial derivative and compute it using the following three-term recursive relation

$$f^{(1)}_{N,m,l} = 0,$$

$$f^{(1)}_{N-1,m,l} = 2N f^{(1)}_{N,m,l},$$

$$c_n f^{(1)}_{n,m,l} = f^{(1)}_{n+2,m,l} + (2n + 1) f^{(1)}_{n+1,m,l},$$

where $c_0 = 2$ and $c_n = 1$ for $n = 1, 2, \ldots, N$. The azimuthal derivative is given by

$$\frac{\partial f}{\partial \phi} = \sum_{n,m,l} f^{(1)}_{nml}(t) T_n(\tilde{r}) e^{im\phi} e^{in\tilde{r}/Z}.$$  \hspace{1cm} (35)

Finally, the derivative along the $z$-direction is similar to the azimuthal derivative except for the extra normalization $\pi/Z$, i.e.,

$$\frac{\partial f}{\partial z} = \sum_{n,m,l} \frac{i\pi l}{Z} f^{(1)}_{nml}(t) T_n(\tilde{r}) e^{im\phi} e^{in\tilde{r}/Z}.$$  \hspace{1cm} (36)

Temporal Discretization. In accretion disk simulations, the dominant velocity component is $v_\phi \approx r \Omega_K$, where $\Omega_K$ is the Keplerian angular velocity. Because the azimuthal grid size $r d\phi$ is proportional to $r$, the CFL stability criterion is a function of the radius. This suggests that the time step is bounded by the angular velocity at the inner boundary, i.e., that

$$\Delta t_{\text{CFL},v_\phi} \propto r_{\text{in}}^{3/2}.$$  \hspace{1cm} (37)

Therefore, the whole disk has to evolve with very small time steps even though a large part of the flow rotates slowly. In order to overcome the CFL constraint, we use a spectral based semi-Lagrangian technique, which allows for a much larger time step for thin accretion disk simulations.

The hydrodynamic part of the algorithm is the same as the one used by Masset (2000) in the two-dimensional hydrodynamic code, FARGO, to simulate planet–disk tidal interactions. Gammie (2001) and Johnson & Gammie (2003, 2005) used the same approach to study gravitational instability and vortices in unmagnetized disks. Recently, Johnson et al. (2008) extended this algorithm to work with constraint transport MHD in the shearing box approximation. An algorithm based on the same idea is already implemented in the Athena Code (Stone et al. 2008) in order to simulate large shearing boxes more efficiently.

We split the advective terms into two parts, namely, a background and a fluctuation. We define the background (azimuthal) velocity by

$$\mathbf{V} = V_\phi(r, z) \hat{\phi} = \frac{\dot{\phi}}{2\pi} \int v_\phi(r, \phi, z) d\phi,$$

and the fluctuating by

$$\mathbf{v}'(r, \phi, z) = \mathbf{v}(r, \phi, z) - V_\phi(r, z) \hat{\phi}.$$  \hspace{1cm} (39)

Because $\nabla \cdot \mathbf{V} = 0$, we can easily rewrite the MHD equations in term of a semi-Lagrangian derivative

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \frac{V_\phi}{r} \frac{\partial}{\partial \phi},$$

which describes how the dynamic variables move with the background flow. Specifically, the continuity equation becomes

$$\frac{D\rho}{Dt} + \nabla \cdot (\rho \mathbf{v}') = 0,$$

while the Navier–Stokes equation becomes

$$\rho \frac{D\mathbf{v}}{Dt} + \rho (\mathbf{v}' \cdot \nabla) \mathbf{v} = -\nabla \left( P + \frac{B^2}{8\pi} \right) + \frac{1}{4\pi} (\mathbf{B} \cdot \nabla) \mathbf{B} + \nabla \tau + \rho \mathbf{g},$$

and the thermal energy equation becomes

$$\frac{D E}{Dt} + \nabla \cdot (E \mathbf{v}') = -P \nabla \cdot \mathbf{v} + \Phi_v + \Phi_B - \nabla \cdot \mathbf{q} - \nabla \cdot \mathbf{F}.$$  \hspace{1cm} (43)

The induction equation is less trivial. Considering only the advective terms, the different components of the vector potential evolve as

$$\frac{\partial A_r}{\partial t} = -v_\phi \frac{\partial A_r}{\partial \phi} - v_z \frac{\partial A_r}{\partial z} + \cdots$$  \hspace{1cm} (44)

$$\frac{\partial A_\phi}{\partial t} = -v_z \frac{\partial A_\phi}{\partial z} - v_r \frac{\partial (r A_\phi)}{r \partial r} + \cdots$$  \hspace{1cm} (45)
\[
\frac{\partial A_z}{\partial t} = -v_r \frac{\partial A_z}{\partial r} - v_\phi \frac{\partial A_z}{\partial \phi} + \cdots \tag{46}
\]

Note that the component \( A_i \) is not advected in the \( i \)-direction. Therefore, we obtain
\[
\frac{\partial A_z}{\partial t} = -v_r \frac{\partial A_z}{\partial r} - v_\phi \frac{\partial A_z}{\partial \phi} + \cdots \tag{47}
\]
\[
\frac{\partial A_\phi}{\partial t} = -v_z \frac{\partial A_\phi}{\partial z} - v_r \frac{\partial (r A_\phi)}{\partial r} + \cdots \tag{48}
\]
\[
\frac{\partial A_z}{\partial t} = -v_r \frac{\partial A_z}{\partial r} - v_\phi \frac{\partial A_z}{\partial \phi} + \cdots . \tag{49}
\]

There is no semi-Lagrangian derivative in Equation (48) because \( A_\phi \) is not frozen in \( V_\phi \).

Assuming that \( V_\phi \) is independent of time, and considering only the Lagrangian step in the continuity Equation (41), the solution is simply
\[
\rho(t, r, \phi, z) = \rho(t_0, r, \phi - V_\phi(t - t_0), z). \tag{50}
\]

Taking the Fourier transform along the azimuthal direction, we then find
\[
\sum_m \hat{\rho}_m(t_0, r, z)e^{im\phi} = \sum_m \hat{\rho}_m(t_0, r, z)e^{i(m\phi-V_\phi(t-t_0))}. \tag{51}
\]

It is clear that advection (due to the background \( V_\phi \)) is equivalent to phase-shifting the Fourier coefficients in the complex plane,
\[
\hat{\rho}_m(t, r, z) = \hat{\rho}_m(t_0, r, z)e^{-imV_\phi(t-t_0)}. \tag{52}
\]

We also handle the other dynamic variables in the MHD equations in a similar way, which is trivial to implement in our pseudo-spectral algorithm.

4. CODE VERIFICATION

We have verified our numerical algorithm using a suit of test problems, some of which we present in this section. For a test particular to the three-dimensional hydrodynamics, we adopt the free-falling dust ring test from Chan et al. (2005). In order to test the semi-Lagrangian method, we present a simple hydrodynamic problem with both the standard and semi-Lagrangian implementation of our pseudo-spectral code. Finally, for MHD, we study the magnetic braking of a rotating slab, following Stone et al. (1992).

4.1. An Advection Test: Free Fall of a Dust Ring

Following Chan et al. (2005), we use a free falling dust ring as an advection test of our three-dimensional algorithm. The computational domain is \([0.2, 1.8] \times [-\pi, \pi] \times [-1, 1]\) with \(65 \times 32 \times 65\) collocation points. The initial density is the Gaussian
\[
\rho_0 = \exp[-20(r-1)^2 - 20z^2]. \tag{53}
\]

In order to also test the advection along the \( z \)-direction, we set the initial velocity to \( v = (0, 0, 1) \), which is equivalent with performing this test on a nonstationary Galilean frame. We assume that the gravitational acceleration is Newtonian and that of an external central object, i.e., that \( g = (-1/r^2, 0, 0) \). (Note that, for a cylindrically symmetric central object, the gravitational field should have been proportional to \( 1/r \).) We also neglect pressure and magnetic fields in this test.

An analytical solution exists for this testing problem. It is derived in the same way as in Chan et al. (2005). Because the initial vertical velocity is nonzero, we have to replace \( z \) by \( z - v_z t \) in order to capture the vertical motion. The solution, therefore, reads
\[
\Sigma(t, r, \phi, z) = \Sigma_0(r_0, z - v_z t) r_0^2 \left[ \frac{3t}{2} \sqrt{\frac{2}{r_0^2}} \left( \frac{r_0}{r} - 1 \right) + r \right]^{-1}, \tag{54}
\]
where \( r_0 \), which is the location of a fluid element at \( t = 0 \), is given by solving implicitly the equation
\[
\sqrt{\frac{2}{r_0^2}} - 1 = \frac{1}{2} \sin \left( 2 \arccos \sqrt{\frac{r}{r_0}} \right) + \arccos \sqrt{\frac{r}{r_0}}. \tag{55}
\]

In Figure 1, we plot the numerical density at \( \phi = 0 \) as grayscale contours for different times. The difference between the numerical solution and the analytical solution is overplotted as a set of contour lines. The maximum error throughout the simulation is of order \( 10^{-4} \). Note that our implementation of the inner boundary condition, described in Chan et al. (2006), which is also known as the buffer zone method, does not introduce any significant errors.

4.2. Test for Semi-Lagrangian Method: A Centrifugally Supported Torus

We study here the accuracy and stability of the semi-Lagrangian method we described in the previous section. In order to demonstrate the advantage of this method in disk simulations, we use a Keplerian velocity profile in the same gravitational law as in the previous test, i.e., we use \( g = (-1/r^2, 0, 0) \) so the background velocity is given by \( V_\phi(t = 0, r, \phi, z) = r^{-1/2} \). The initial density is constant \( \rho(t = 0, r, \phi, z) = 1 \) and the vertical velocity is zero. We perturb the radial velocity by a doubly Gaussian function
\[
v_r(t = 0, r, \phi, z) = 0.01 \exp[-20(r-1)^2 - 20z^2] \sin(\phi). \tag{56}
\]
so the initial condition now depends on all spatial variables. For simplicity, we set the thermal energy and the magnetic field to zero. The computational domain is also the same as Section 4.1 and the resolution is \( 65 \times 64 \times 64 \).

We let the simulation evolve to \( t = 10 \), which corresponds to about 18 orbits at the inner boundary, and measure the computational time it takes. The standard method takes 3 hr 39 minutes, where the semi-Lagrangian method takes only 12 minutes 35 s on the same machine. This corresponds to a speed up of 17.4. Of course, this demonstration is in an extreme setup. Because we choose both \( B = 0 \) and \( K = 0 \), the time step size is completely determined by the velocity. In the standard scheme, \( \Delta t \) is controlled by \( r_0^{5/2} \approx 0.03 \), while in the semi-Lagrangian scheme it is controlled by \( \Delta t/\max(v_r) \approx 3 \). In Figure 2, we study the maximum difference between the standard and semi-Lagrangian schemes. We plot the maximum difference as a solid line. The difference is less than 0.5% at \( t = 10 \).
4.3. A Test of Alfvén Wave Propagation: Magnetic Breaking of an Aligned Rotator

The problem of magnetic breaking of an aligned rotator via the emission of nonlinear, incompressible Alfvén waves was solved analytically by Mouschovias & Paleologou (1980). It was then used by Stone et al. (1992) to verify the ability of MHD algorithms to propagate transverse Alfvén waves. In this test, we use the same initial conditions as those described by Stone et al. (1992), namely, the discontinuous initial condition (DIC) and the continuous initial condition (CIC). Because our algorithm is designed for compressible MHD flows, we discard the radial and vertical components of the momentum equation and set \( \partial P/\partial \phi = 0 \) in the azimuthal component.

We use the computational domain \([0.2, 1.8] \times [-\pi, \pi] \times [-16, 16]\) with \(33 \times 32 \times 512\) collocation points. We set the initial density to

\[
\rho_0 = \begin{cases} 
1, & |z| > 1 \\
10, & \text{otherwise,}
\end{cases} \quad (57)
\]

the initial magnetic field to \(\mathbf{B} = (0, 0, 1)\), and the initial velocity to \(\mathbf{v} = (0, r\Omega_0, 0)\), where \(\Omega_0\) is the initial angular velocity. For the discontinuous case (DIC), we set the angular velocity to

\[
\Omega_0 = \begin{cases} 
0, & |z| > 1 \\
1, & \text{otherwise.}
\end{cases} \quad (58)
\]

whereas for the continuous case (CIC) we set it to

\[
\Omega_0 = \begin{cases} 
0, & |z| > 1 \\
\frac{1}{2}(1 + \cos \pi z), & \text{otherwise.}
\end{cases} \quad (59)
\]

The analytic solutions are given in Mouschovias & Paleologou (1980).

In Figure 3, we compare the numerical to the analytical solutions for the two initial conditions at \(t = 50\), right before the wave front passes \(z = 16\). Our pseudo-spectral scheme is stable even though discontinuity is present because of our usage of spectral filtering (or super vanishing viscosity, see Ma 1998a, 1998b). The numerical solution for the discontinuous problem shows oscillations around the discontinuity (the Gibbs phenomenon), which are inherent to all spectral methods. However, the properties of the shock as well as those of the fluid around it are captured correctly in our numerical solutions. For the continuous problem, the numerical and analytical solutions are indistinguishable.

5. TURBULENT MHD DISKS DRIVEN BY THE MAGNETOROTATIONAL INSTABILITY

One of the advantages of spectral methods is the fact that they allow for an accurate control of numerical dissipation and hence they can be used to track accurately the stability of a flow. In Chan et al. (2005) we used our two-dimensional, hydrodynamic spectral algorithm to successfully reproduce the Rayleigh stability criterion in a Couette flow, even near the
separatrix between stability and instability. In Chan et al. (2006), we applied our spectral algorithm to self-gravitating disks and studied Toomre’s criterion. In this section, we use our MHD spectral algorithm to study the properties of accretion disks driven by the MRI (Balbus & Hawley 1991a).

Any ionized and magnetized accretion disk is unstable to the MRI as long as the angular velocity of the flow is a decreasing function of radius. If a cylindrical disk is threaded by a mean vertical magnetic field \( B_z \), all the waves along the vertical direction with wavenumbers less than

\[
k_{MRI} = \sqrt{2q} \left( \frac{\Omega}{v_A} \right),
\]

are unstable. Here, \( \Omega \) is the angular frequency,

\[
q \equiv -\frac{d \ln \Omega}{d \ln r}
\]

is a measure of the shear, and \( v_A = B_z/\sqrt{4\pi\rho} \) is the Alfvén velocity for the background field. The growth rate of the instability depends strongly on the wavenumber and is given by (Balbus & Hawley 1991a; Pessah et al. 2006a)

\[
\gamma = \left[ -2 - q - k^2 + \sqrt{(2 - q)^2 + 4k^2} \right]^{1/2} .
\]

The fastest growing mode has a wavenumber given by

\[
k_{\text{peak}} = \frac{q}{2} \left( \frac{4}{q} - 1 \right)^{1/2} \left( \frac{\Omega}{v_A} \right).
\]

We use our numerical algorithm to simulate the evolution of a Keplerian disk in a pseudo-Newtonian potential around a non-rotating object of mass \( M \). For this calculation, we set \( G = c = 1 \) and express all the distances and times in gravitational units. We solve the MHD equations in the computational domain \([-3, 43] \times [-\pi, \pi] \times [-2, 2]\) using \( 257 \times 64 \times 32 \) grid points.

In order to justify the periodic boundary conditions along the vertical direction and to avoid numerical problems around the innermost stable circular orbit, we set the sound speed to \( c^2_s \approx 0.2 \). We set the initial density to unity everywhere in the disk and thread the flow with a vertical magnetic field with a corresponding Alfvén velocity equal to \( 2 \times 10^{-3} \). In our dimensionless units, it takes a time of \( t \approx 60 \) and of \( t \approx 500 \), respectively, for the fluid elements to complete one orbit at \( r = 6 \) and \( r = 20 \).

The initial exponential growth of the MRI offers another possibility to test the ability of our numerical method to capture the properties of an MHD instability. For this reason, we first discuss the initial stages of the simulation and then the properties of the final state of saturated MHD turbulence.

In Figure 4, we show the power spectrum of the magnetic and kinetic energies in the simulation, at a radius \( r = 20 \), during the initial linear regime of the instability. The similarity of the peak of the numerical power spectrum to the wavenumber of the most unstable mode of the linear MRI demonstrates that our numerical algorithm can reproduce, with an uncertainty comparable to the resolution, the wavenumber of the mode that shows the fastest growth rate (Equation (63)).

The Maxwell and Reynolds stresses are amplified exponentially during the initial growth of the instability, with their ratios determined only by the value of local shear (Pessah et al. 2006a). In Figure 5, we plot the ratio of the Maxwell to Reynolds stresses as a function of radius in the accretion disk at time \( t = 200 \) and compare it to the analytical solution of Pessah et al. (2006a). The numerical and analytical ratios agree well, within the uncertainties of estimating appropriate averages.
After a few orbital periods, turbulence is generated and the solution of the system of MHD equations becomes highly non-linear. Figure 6 shows the evolution of the density and magnetic energy in the accretion flow from the initial laminar state (first panel), through the time of the exponential growth of the MRI (second panel), to the final saturated state of MHD turbulence (last two panels). As also found in previous simulations of MRI-driven turbulent accretion disks, the solution is highly variable, with large fluctuations in the various physical quantities. Moreover, the magnetic and material stresses are not consistent with the prediction of the alpha model and are non-vanishing inside the innermost stable circular orbit. In this paper, we are particularly interested in the evolution and properties of the power spectrum of turbulence, which is a statistic that spectral methods are primarily suited to calculate.

Figure 7 shows the evolution of the power spectrum along the vertical direction of the magnetic energy at cylindrical radius \( r = 20 \). At early times, the magnetic energy increases exponentially because of the growth of the MRI, generating a spectrum of fluctuations that peaks around the wavenumber of maximum growth. At later times, interactions between different modes lead to spreading of turbulent energy to nearby modes, generating a power-law spectrum of fluctuations. The index of the power spectrum of magnetic energy fluctuations is comparable to that of a Kolmogorov spectrum, even though the MHD turbulence is highly anisotropic.
The power-law spectrum of magnetic energy fluctuations extends from the largest vertical scale of the simulation (which is the vertical extent of the domain of solution) to the smallest vertical scale (which is equal to the numerical resolution). Moreover, because of the flatness of the power spectrum, its integral is equal to the total variance, depends on both scales. This is consistent with the fact that the saturation predictor found in numerical simulations of shearing boxes depends on both the vertical size of the box and the numerical resolution (Hawley et al. 1995, 1996; Pessah et al. 2006b). It is, however, a result of two simplifying assumptions in our simulation. The power spectrum extends to the largest vertical scale because we have neglected the vertical component of gravity and, therefore, the disk is not stratified. At the same time, the power spectrum extends to the smallest resolved scale because we have neglected Ohmic dissipation. Obtaining a realistic saturation predictor of MRI-driven turbulence in accretion disks will require numerical simulations of stratified flows with the largest possible dynamical range and an accurate model of subgrid physics.

6. CONCLUSIONS

In this paper, we present a parallel, three-dimensional pseudo-spectral MHD algorithm based on the two-dimensional hydrodynamic algorithm we had previously developed. We use a vector potential instead of magnetic field in the induction equation to ensure the lack of divergence in the magnetic fields up to machine accuracy. We also describe a new method to apply existing libraries to perform parallel fast Fourier transforms (FFT). We discuss briefly a semi-Lagrangian scheme, which can potentially speed up simulations for thin accretion disks. We also give an overview of the approach required to perform LES, and treat the spectral filtering as a minimal subgrid model.

In additional to the detail description of the numerical method and implementation, we also carry out a series of standard test. The results demonstrate the ability of our pseudo-spectral to use less grid points to resolve the same accuracy compared to low-order methods. This is an important advantage in three dimensional since it can save up to 99% of the required memory. The semi-Lagrangian scheme shows significant performance boost for the particular problems we choose. As an application, we apply our algorithm to MHD flow in cylindrical coordinate under pseudo-Newtonian gravity. The MRI kicks in and generate turbulence. We plot the power spectrum $B_\theta$ and demonstrate that the result agrees with the Balbus & Hawley (1991a, 1991b) dispersion relation.

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APPENDIX A

ADVECTIVE–CONSERVATIVE MIXED FORMALISM FOR MHD

As in Chan et al. (2005), we use the nonlinear terms $(\mathbf{v} \cdot \nabla) \mathbf{v}$ in their advective forms, whereas we use the terms that involve the density, $\rho$, and the energy, $E$, in their conservative forms. For the vector potential, we use an advective form in order to increase stability. In detail:

$$D_t \rho = -\frac{\partial_r (\rho \mathbf{v}_r)}{r} - \frac{\partial_\phi (\rho \mathbf{v}_\phi)}{r} - \partial_z (\rho \mathbf{v}_z), \quad (A1)$$

$$D_t \mathbf{v}_r = -v_r \partial_r v_r - \frac{v'_r}{r} \partial_\phi v_r - \frac{v^2_r}{r} - v_z \partial_z v_r + \frac{\partial_r (r \tau_{rr})}{r} P - r B^2 / (8 \pi) + \frac{\partial_\phi (r \tau_{r\phi})}{r \rho} + \frac{\partial_z (r \tau_{rz})}{\rho}, \quad (A2)$$

$$D_t \mathbf{v}_\phi = -v_r \partial_r v_\phi - \frac{v'_r}{r} \partial_\phi v_\phi - \frac{v^2_r}{r} v_z - v_z \partial_z v_\phi + \frac{\partial_r (r \tau_{r\phi})}{r} + \frac{\partial_\phi (r \tau_{r\phi})}{r \rho} - P - r B^2 / (8 \pi) + \frac{\partial_z (r \tau_{rz})}{\rho}, \quad (A3)$$

$$D_t \mathbf{v}_z = -v_r \partial_r v_z - \frac{v'_r}{r} \partial_\phi v_z - v_z \partial_z v_z + \frac{\partial_r (r \tau_{rz})}{r} + \frac{\partial_\phi (r \tau_{r\phi})}{r \rho} + \frac{\partial_z (r \tau_{rz})}{\rho}, \quad (A4)$$

$$D_t E = -\frac{\partial_r (r E v_r + r q_r + r F_r)}{r} - \frac{\partial_\phi (E \mathbf{v}_\phi + q_\phi + F_\phi)}{r} - \partial_z (E v_z + q_z + F_z) - P \left( \partial_r v_r + \frac{\partial_\phi v_\phi + v_z}{r} + \partial_z v_z \right) + \Phi_\kappa + \Phi_\eta, \quad (A5)$$

$$D_t A_r = v'_r B_z - v_z B_\phi - \eta \left[ \frac{1}{r} \partial_r (r \partial_r A_r) + \frac{1}{r^2} \partial_\phi^2 A_r + \partial_z^2 A_r - \frac{A_r}{r^2} \right] - \partial_\phi \hat{A}, \quad (A6)$$
\[ \partial_t A_\phi = v_z B_r - v_r B_z + \eta 
\times \left[ \partial_z^2 A_\phi - \frac{A_\phi}{r^2} + \frac{1}{r} \partial_r (r \partial_r A_\phi) + \frac{1}{r^2} \partial_\phi^2 A_\phi \right] - \frac{1}{r} \partial_\phi A, \]

\[ (A7) \]

\[ D_t A_z = v_r B_\phi - v_\phi B_r + \eta \left[ \frac{1}{r} \partial_r (r \partial_r A_z) + \frac{1}{r^2} \partial_\phi^2 A_z + \partial_z^2 A_z \right] - \partial_z A, \]

\[ (A8) \]

where \( D_t \equiv \partial_t + (V_\phi/r) \partial_\phi \) is the “semi-Lagrangian derivative” with \( V_\phi \) being some background azimuthal velocity. The fluctuation \( v_\phi \) is defined by \( v_\phi = V_\phi \) as we describe in Section 3. We integrate these equations forward in time using a low storage, third-order Runge–Kutta scheme (see Chan et al. 2005, 2006, for detail).

We compute the magnetic field from the vector potential as

\[ B_r = \frac{\partial_\phi A_z}{r} - \partial_z A_\phi, \]

\[ (A9) \]

\[ B_\phi = \partial_z A_r - \partial_r A_z, \]

\[ (A10) \]

\[ B_z = \frac{\partial_r (r A_\phi)}{r} - \frac{\partial_\phi A_r}{r}. \]

\[ (A11) \]

The only nontrivial term here is \( \partial_r (r A_\phi) \), which is in conservative form.

The viscosity tensor \( \tau_{ij} \) in the above equation has the following general form

\[ \tau_{ij} = 2(\mu_r + \mu_s) \delta_{ij} + \left( \mu_r + \mu_b - \frac{2}{3} \mu_s \right) (\nabla \cdot \mathbf{v}) \delta_{ij}. \]

\[ (A12) \]

As we describe before, \( \mu_r, \mu_b, \) and \( \mu_s \) are the coefficients of radiative, bulk, and shearing viscosity. The strain rate tensor \( e_{ij} \) written in cylindrical coordinate becomes

\[ e_{rr} = \partial_r v_r, \]

\[ (A13) \]

\[ e_{\phi\phi} = \frac{\partial_\phi v_\phi + v_r}{r}, \]

\[ (A14) \]

\[ e_{zz} = \partial_z v_z, \]

\[ (A15) \]

\[ e_{r\phi} = e_{\phi r} = \frac{1}{2} \left( \partial_r v_\phi - \frac{v_\phi}{r} + \frac{1}{r} \partial_\phi v_r \right), \]

\[ (A16) \]

\[ e_{\phi z} = e_{z\phi} = \frac{1}{2} \left( \frac{\partial_\phi v_z + v_r}{r} \right), \]

\[ (A17) \]

\[ e_{zr} = e_{rz} = \frac{1}{2} (\partial_r v_r + \partial_r v_z). \]

\[ (A18) \]

The viscous dissipation is

\[ \Phi_v = 2(\mu_r + \mu_s)(e_{ij})^2 + \left( \mu_r + \mu_b - \frac{2}{3} \mu_s \right) (\nabla \cdot \mathbf{v})^2, \]

\[ (A19) \]

and the Ohmic dissipation rate \( \Phi_\eta \) is given by

\[ \Phi_\eta = \frac{\eta}{4\pi} \left[ \left( \frac{\partial_\phi B_x}{r} - \partial_z B_\phi \right)^2 + \left( \partial_z B_r - \partial_\phi B_z \right)^2 \right]. \]

\[ (A20) \]

**APPENDIX B**

**CODE PARALLELIZATION**

If the MHD equations were linear, the parallelization of the spectral algorithm would be trivial because each spectral coefficient evolves independently of the others. However, the nonlinear terms in the equations necessitate cross-processor communication. As we discussed in Chan et al. (2005), we handle the nonlinear terms by taking the derivatives in spectral space and the product in coordinate space. The efficient parallelization of our algorithm, therefore, relies on efficiently implementing a parallel version of the FFT algorithm for a multidimensional set of grid points. We use the Message Passing Interface (MPI) standard to parallelize our algorithm (see Gropp et al. 1999a, 1999b).

In Figure 8, we illustrate the FFT algorithm for transforming the values of a physical quantity on a two-dimensional grid along the \( x_1 \) and \( x_2 \) directions. The standard algorithm for parallel FFT starts with an one-dimensional ("slab") decomposition, which distributes the data across different processors. We use solid lines in the figure to denote the distribution of grid points on different processors, which are labeled by P0, P1, P2, etc. It is clear from the upper left panel of the figure that applying spectral methods along the \( x_2 \) direction is straightforward. We can simply use the ordinary FFT for each row locally. However, for the \( x_1 \) direction, communication between the various processors is necessary. The standard method requires taking first a parallel transpose (PT), exchanging data between processors, and then carrying out a local transpose (LT) per processor. This is showed in the upper panels of Figure 8. PT and LT exchange the
directions of $x_1$ and $x_2$ and FFTs are then applied on each row separately.

We developed an alternate (“flip-flop”) procedure to increase the performance of parallel multidimensional FFT by avoiding the local transpose on each processor. The lower row of Figure 8 illustrates the flipping procedure, which involves a block transpose (BT) and a PT operation. “EQ” in the figure indicates that the two panels are equivalent because the C arrays are row-major. Instead of transposing the data as in the standard algorithm, the flipping procedure effectively changes the decomposition direction. This makes other parts of our spectral algorithm easier to be implemented. Moreover, we can take advantage of the resulting memory layout and use the cache more efficiently. Depending on the domain size and the number of processors we use, this approach can speed up the parallel FFT as well as the spectral algorithm in our 32 processor Beowulf cluster. The flopping algorithm is exactly the opposite procedure.

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