

TUNED FINITE-DIFFERENCE DIFFUSION OPERATORS

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ABSTRACT

Finite-difference simulations of fluid dynamics and magnetohydrodynamics generally require an explicit diffusion operator, either to maintain stability by attenuating grid-scale structure, or to implement physical diffusivities such as viscosity or resistivity. If the goal is stability only, the diffusion must act at the grid scale, but should affect structure at larger scales as little as possible. For physical diffusivities the diffusion scale depends on the problem, and diffusion may act at larger scales as well. Diffusivity can undesirably limit the computational time step in both cases. We construct tuned finite-difference diffusion operators that minimally limit the time step while acting as desired near the diffusion scale. Such operators reach peak values at the diffusion scale rather than at the grid scale, but behave as standard operators at larger scales. These operators will be useful for simulations with high magnetic diffusivity or kinematic viscosity such as in the simulation of astrophysical dynamos with magnetic Prandtl number far from unity, or for numerical stabilization using hyperdiffusivity.

Key words: diffusion – hydrodynamics – methods: analytical – methods: numerical – MHD – turbulence

1. INTRODUCTION

Astrophysics is rich in phenomena where diffusivity poses an obstacle to simulation. The obstacle arises when diffusion poses a more stringent time step limit than other dynamics. This can happen either when its physical magnitude is large, when it is used to model effects such as viscosity, resistivity, conductivity, or the diffusion of passive scalars; or when hyperdiffusion is used to maintain numerical stability.

One significant example of such an obstacle occurs in modeling astrophysical dynamos. These generate magnetic fields in galaxies, stars, planets, and accretion disks. In such systems, the ratio of the kinematic viscosity ν to the magnetic diffusivity η , known as the magnetic Prandtl number $\text{Pr}_M = \nu/\eta$, normally takes on values far from unity. Maron et al. (2004) and Boldyrev & Cattaneo (2004) find that the dynamics of these dynamos depend on the value of Pr_M . Simulations of astrophysical dynamos such as those performed by Brandenburg (2001), Schekochihin et al. (2005), Iskakov et al. (2007), and Brandenburg (2008), therefore require implementation of diffusion operators with large magnitudes to capture the magnetohydrodynamical (MHD) behavior of interest. More generally, in any turbulent flow, reducing the diffusion scale increases the effective resolution of a simulation. It has been shown that this can be achieved through the use of fourth or sixth-order hyperdiffusivities ($\nu_4 \nabla^4$ or $\nu_6 \nabla^6$) to maintain numerical stability and dissipate turbulence (Brandenburg & Dobler 2002).

We here consider how to design diffusion and hyperdiffusion operators such that they have the desired behavior at the diffusion scale and larger scales, while still restricting the numerical time step as little as possible. The time step depends inversely on the strength of the diffusion

$$\Delta t = \Delta x^2 / 2\nu. \quad (1)$$

Classical diffusion operators such as Laplacian viscosity ($\nu \nabla^2$), or fourth or sixth-order hyperdiffusivities, reach their maximum values at the grid scale, but act at the larger diffusion scale where the effective diffusivity is lower. The operators designed here reach their maximum value at the diffusion scale rather than

at the grid scale, so that they limit the time step no more than necessary.

In a spectral code, the diffusive terms are linear and can thus be handled spectrally without limitation on the time step. For example, let a field evolve as $\partial_t \mathbf{V} = \mathbf{A} + \nu \nabla^2 \mathbf{V}$, where \mathbf{A} denotes the nondiffusive terms. In Fourier space, $\partial_t \hat{\mathbf{V}} = \mathbf{A} - \nu k^2 \hat{\mathbf{V}}$. The solution, with \mathbf{A} constant throughout the interval Δt , is

$$\hat{\mathbf{V}}(\Delta t) = \left[\hat{\mathbf{V}}(0) + \frac{\mathbf{A}}{\nu k^2} (e^{\nu k^2 \Delta t} - 1) \right] e^{-\nu k^2 \Delta t}. \quad (2)$$

When evolved in Fourier space, the diffusivity operator is stable for any value of $\nu k^2 \Delta t$, whereas in physical space, instability occurs if $\nu k^2 \Delta t > 2$ (restating Equation (1) in terms of wavenumber).

However, finite difference codes do have advantages that make them worth pursuing: they use fewer floating-point operations per grid point; they can be more easily parallelized without the all-to-all communications required for Fourier transforms; they are not restricted to periodic boundary conditions; and they handle discontinuous jumps more robustly.

The Navier–Stokes equation can include a number of different types of diffusion operators:

$$\begin{aligned} \partial_t \mathbf{V} = & -\mathbf{V} \cdot \nabla \mathbf{V} - \rho^{-1} \nabla P + \nu_2 \nabla^2 \mathbf{V} - \nu_4 \nabla^4 \mathbf{V} + \nu_6 \nabla^6 \mathbf{V} \\ & - \nu'_4 (\partial_x^4 + \partial_y^4 + \partial_z^4) \mathbf{V} + \nu'_6 (\partial_x^6 + \partial_y^6 + \partial_z^6) \mathbf{V} - \nu_D D[\mathbf{V}], \end{aligned} \quad (3)$$

where the ν_2 term is the usual Laplacian physical viscosity, the ν_n and ν'_n terms are n th-order hyperviscosities, the term $\nu_D D(\mathbf{V})$ is a customized diffusion operator.

Either the sixth-order hyperdiffusivity term or the physical diffusivity can maintain numerical stability. The hyperdiffusivity has been advocated (Brandenburg 2003) because it preferentially diminishes the high-wavenumber structure without modifying low-wavenumber structure. If the problem does require true physical diffusivities, we still want to consider the use of a customized operator. This would reduce excess diffusion at scales well below the diffusion scale. Such excess diffusion limits the time step without further modifying the solution as no structure exists at those scales.

To date the focus in the study of extensions to numerical diffusion has been on such hyperdiffusivities (e.g., Borue & Orszag 1995; Brandenburg 2003), as exemplified by the hyperviscosities described in Equation (3). However, the degrees of freedom available in the finite difference coefficients can be used instead for different goals.

In this paper, we describe methods for customizing diffusion operators that can be used to design operators that protect the time step while either minimizing diffusion or reproducing the physical diffusion operator at low wavenumber as well as possible. These methods can also be used to design different diffusion operators for other purposes. These methods rely on the tuning techniques used by Maron et al. (2008) for improving the high-wavenumber accuracy of finite-difference derivatives.

In Section 2, we summarize the constraints that lead to the need for tuning finite difference operators. We then describe operators suitable for implementing both numerical (Section 3) and physical (Section 4) diffusivities, and we summarize our results in Section 5.

2. TUNING FINITE-DIFFERENCE OPERATORS

Let us consider the question of how to tune a general, centered (symmetric) finite-difference operator, since all diffusion operators must be centered. We follow the treatment of the tuning of antisymmetric operators such as first derivatives given in Maron et al. (2008). Such tuning allows us to customize the wavenumber spectrum of the operator to meet the needs of the problem at hand, rather than relying on simple analytic forms. This allows us, for example, in a problem with large Laplacian diffusivity, to trade small deviations from Laplacian behavior at low wavenumber for large gains in the time step, by limiting the diffusion at high wavenumber. The deviations from Laplacian at low wavenumber can be maintained at levels small enough to not affect realistic simulations. We use both analytic solutions and numerical optimization to improve the spectral performance of the operators.

As an example of finite-difference representations of centered operators we examine second and fourth derivatives. Define a function $f_j(x_j)$ on a set of grid points $x_j = j$, with j being an integer. Then construct a finite-difference operator for the second derivative $f^{[2]}$ by sampling a stencil of grid points with radius S . Without loss of generality, we center the operator on $j = 0$ and use a grid interval of $\Delta x = 1$. The familiar result for a second derivative on a radius-1 stencil is

$$\partial_x^2 f(x)|_{x=0} = -2f_0 + f_1 + f_{-1}, \quad (4)$$

which is obtained from fitting a polynomial of degree 2 to f_j . For a fourth derivative, we can fit a degree 4 polynomial on a radius-2 stencil,

$$\partial_x^4 f(x)|_{x=0} = -6f_0 + 4(f_{-1} + f_1) - (f_{-2} + f_2). \quad (5)$$

In general, a centered operator on a stencil of order S can be represented as

$$m_0 f_0 + \sum_{j=1}^S m_j (f_{-j} + f_j). \quad (6)$$

Consider the value of the finite-difference operator at $x = 0$ for a Fourier mode $f = \cos(\pi k x)$. (Sine modes can be ignored because they do not contribute to the second derivative at $x = 0$.) The wavenumber k is scaled to grid units so that

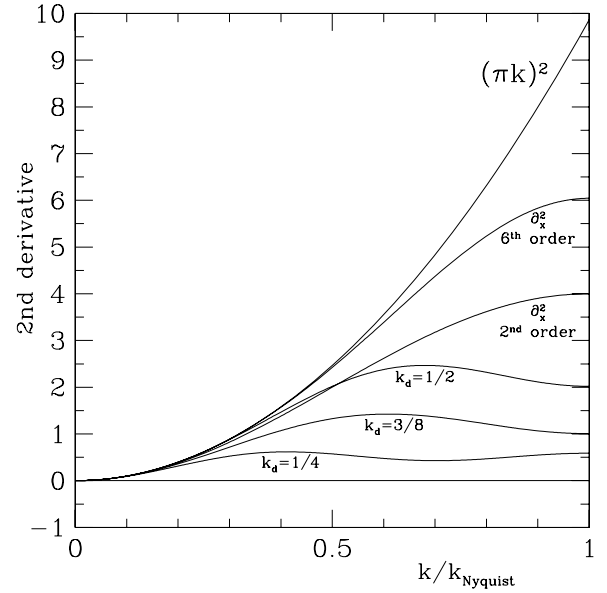


Figure 1. Values of $\partial_x^2 \cos(\pi k x) = (\pi k)^2$, evaluated at $x = 0$, and the different finite-difference operators having coefficients listed in Table 1. Two examples of polynomial-based difference operators with stencil radii $S = 1$ and highest order two and $S = 3$ and highest order six are shown, along with the three examples of operators tuned with different choices of the beginning of the diffusive range k_d .

$k = 1$ corresponds to the maximum (Nyquist) wavenumber $\pi(\Delta x)^{-1}$ expressible on the grid. The analytic value for the second derivative is $-\pi^2 k^2$ times the function value, whereas the finite difference operator (Equation (6)) gives

$$f^{[2]} \sim m_0 + 2 \sum_{j=1}^S m_j \cos(\pi j k) \equiv -D(k). \quad (7)$$

This defines a function $D(k)$ that, when positive, acts as a diffusion applied to $f(x)$, because the Fourier modes of f evolve as $\partial_t \hat{f} = -v_D D(k) \hat{f}$, where v_D is a viscositylike parameter that sets the level of diffusion. The maximum diffusive time step is given by the inverse of the maximum value of $D(k)$ over $0 < k < 1$:

$$\Delta t < \frac{1}{v_D \max[D(k)]}. \quad (8)$$

Ideally, $D(k)$ should scale as $(\pi k)^2$ for $k < k_d$ and should be constant for $k > k_d$. The focus of this work is on customizing the form of $D(k)$ so as to increase the maximum diffusive time step, and, in the case of hyperdiffusion, also minimize low- k diffusion.

Figure 1 shows $D(k)$ for finite-difference stencils of radius $S = 1$ (second order) and $S = 3$ (sixth order), in comparison to the analytic value, demonstrating how higher order more closely mimics the analytic function. The coefficients of these functions are listed in Table 1. The operator $D(k)$ can be Taylor expanded in the form

$$D(k) = D_0 + D_2 k^2 + D_4 k^4 + D_6 k^6 \dots \quad (9)$$

An operator that reproduces ∂^2 for all k would have $D_2 = \pi^2$ and all the rest of the coefficients $D_n = 0$ for $n \neq 2$. The radius-1 stencil (Equation (4)) has $D_0 = 0$ and $D_2 = \pi^2$, but the higher order coefficients are unconstrained, while the radius-2 stencil (Equation (4)) sets $D_0 = D_4 = 0$ and $D_2 = \pi^2$.

Table 1
Coefficients for Time-Step-Friendly Laplacian Diffusion Operators

	m_0	m_1	m_2	m_3	m_4	m_5
∂^2 , Second order	-2	1
∂^2 , Sixth order	-2.72222	1.5	-0.15	0.01111
$k_d = 1/2$	-1.514721	0.5692471	0.2524535	-0.0643401
$k_d = 3/8$	-0.9148711	0.2609054	0.2059354	-0.0094052
$k_d = 1/4$	-0.4334820	0.0752718	0.0696988	0.0717703
$k_d = 7/32$	-0.2733333	0.0179722	0.0172444	0.1014500
$k_d = 3/16$	-0.2679784	0.0393498	0.0283651	0.0304570	0.0358173	...
$k_d = 9/64$	-0.1317918	0.0097316	0.0094934	0.0088189	0.0081529	0.0296992
$k_d = 3/32$	-0.0585600	0.0029213	0.0030688	0.0029842	0.0027554	0.0026748

Notes. The coefficients for a finite-difference operator for ∂_x^2 . The second- and sixth-order entries are for a polynomial fit on a radius 1 and 3 stencil, respectively. The “ k_d ” entries are the tuned diffusion operators discussed in Section 4. These functions are shown in Figure 1. The last entry, for $k_d = 3/32$, additionally has $m_6 = 0.0024189$, $m_7 = 0.0024876$, and $m_8 = 0.0099690$.

The usual way to evaluate an operator for a function such as ∂^2 is to fit a maximal order polynomial to the points in the stencil. This yields equations that can be inverted to find the m_j coefficients in Equation (7) for stencil radius S :

$$D_0 = -m_0 - 2 \sum_{q=1}^S m_q, \quad (10)$$

$$D_p = -\frac{2\pi^p}{p!} (-1)^{p/2} \sum_{q=1}^S q^p m_q,$$

for even p . We call such operators polynomial-based operators. The form of these operators is shown in Figure 2. We may, however, use the available degrees of freedom in different ways. The goal of fitting a high-order polynomial to the derivative is to have high accuracy at high wavenumber. However, that may actually contradict the goal of protecting the time step while either minimizing diffusion or reproducing the physical diffusion operator at low wavenumber. Instead, we can use the available degrees of freedom to directly address these requirements.

As an example, for a Kolmogorov cascade, the diffusive scale λ_v and the viscosity ν scale as $\lambda_v \sim \nu^{3/4}$. The viscosity can be made sufficiently large that λ_v is substantially larger than the grid scale, and the velocity profile will be smooth at smaller scales. The cascading energy is eliminated at the diffusive scale, so there is no need for higher diffusivity at smaller scales, yet because of the form of the Laplacian diffusivity operator, the diffusivity increases all the way down to the grid scale. This excess diffusivity is unnecessary, and in fact is a liability because it restricts the time step.

Laplacian diffusion operators, or steeper operators such as hyperdiffusivities, rise in amplitude monotonically all the way to the Nyquist wavenumber $k = 1$. A large value of $D(1)$ requires a small time step, but is unnecessary because energy cascading from higher scales is removed earlier at the diffusion scale k_d . $D(k)$ need to only have enough presence above k_d to diffuse any Fourier modes that might arise there. For $k > k_d$, it can be as large as it is at k_d with no additional time step penalty.

This allows us to specify a strategically chosen diffusion operator that satisfies these requirements. Such an operator should rise through the diffusion range k_d , but then flatten out and merely remain positive at $k > k_d$. Since this constraint is much less critical than having controlled diffusion at low k , the low- k range of $D(k)$ should receive a higher priority in the optimization than the high- k range.

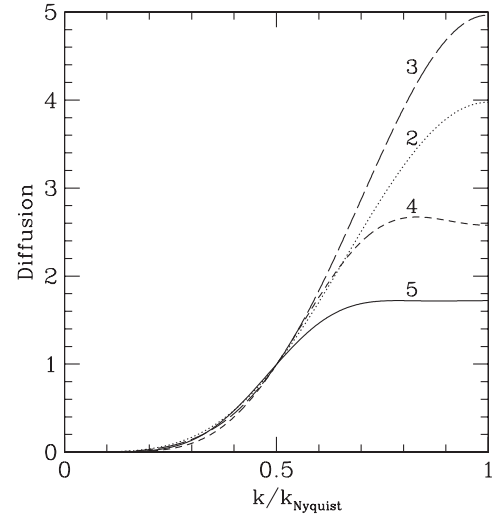


Figure 2. Time-step-protecting diffusion functions are compared to standard hyperdiffusivities. Each of these functions approaches $k = 0$ approximately as k^4 , and each has been normalized so that $D(1/2) = 1$. The function labeled “2” is the radius-2 stencil finite-difference formula for ∂^4 , or in other words, a ∇^4 hyperdiffusivity. The function labeled “3” is the radius-3 stencil finite-difference formula for ∂^4 . Since it is higher order, it more faithfully represents the function k^4 for large k . However, this is a liability for the time step because it is more vulnerable to a diffusive time step instability at $k = 1$ than the radius-2 function. The function labeled “4” has a different objective. It is a radius-4 stencil finite-difference formula for ∂^4 , but instead of using the extra degrees of freedom to represent k^4 at higher order, they are used to minimize $D(k)$ for $k > 1/2$. The function labeled “5” has the same goal as “4” implemented with a radius-5 stencil.

The behavior of the diffusion function at k_d critically determines its effect on the solution. The diffusion must act at both the Nyquist scale $k_{\text{NY}} = 1$, for stability, and at the resolution scale, to damp modes with wavenumbers too large to be accurately captured by the finite-difference scheme. The resolution scale depends on the details of the method. However, the common choice of radius-3 stencils for finite differences has a resolution scale $k = 1/2$ (Maron et al. 2008), so we choose in this work to use a diffusion scale $k_d = 1/2$, and examine diffusion functions normalized to $D(k_d) = 1$.

In situations where the cascade timescale is faster than the diffusion timescale, one can often get away with applying the diffusion operator only once every few time steps, rather than every time step, effectively removing diffusion from the computational load. One does this by simply increasing the magnitude of the diffusion coefficient by a factor of the time

step delay to compensate for its less frequent application. If this increased diffusivity is unstable, one then has the option of employing the flattened operators discussed in this paper to restabilize the diffusivity. Maron (2004) demonstrated that for a simulation of incompressible turbulence applying the diffusivity once every four time steps yielded indistinguishable results from applying it every time step.

In the next two sections, we describe how we perform the tuning and give some useful examples of operators for both hyperdiffusivity and Laplacian diffusivity.

3. TIME-STEP-FRIENDLY HYPERDIFFUSION

In situations where one wishes to maximize the scale range, and where the diffusion-scale dynamics do not affect larger scales, one can fruitfully use a diffusion operator that rises more rapidly with k than a Laplacian. Writing the diffusive terms from Equation (3) in Fourier space,

$$\begin{aligned} \partial_t \hat{\mathbf{V}} = & -\nu_2 k^2 \hat{\mathbf{V}} - \nu_4 k^4 \hat{\mathbf{V}} - \nu_6 k^6 \hat{\mathbf{V}} - \nu'_4 (k_x^4 + k_y^4 + k_z^4) \\ & \times \hat{\mathbf{V}} - \nu'_6 (k_x^6 + k_y^6 + k_z^6) \hat{\mathbf{V}} - \nu_d D(k) \hat{\mathbf{V}} \end{aligned} \quad (11)$$

one sees that hyperdiffusive terms such as those proportional to ν_4 and ν_6 have a steeper dependence on the wavenumber k than the Laplacian diffusivity proportional to ν_2 .

However, energy cascading from larger scales dissipates at the diffusion scale $k_d < 1$, so increasing the diffusion at $k > k_d$ further is unnecessary. A customized diffusion operator $D(k)$ can be constrained to have a similarly steep k dependence at low k , but to then flatten at the diffusion scale k_d , so that the value at the Nyquist wavenumber $D(1)$ is not markedly higher. Since the time step is limited by the maximum diffusivity on the grid at any scale, limiting the value of D at small wavenumber protects the time step.

We note in passing that the ν_4 term in Equation (11) contains two successive Laplacians and therefore two rounds of finite differences, whereas terms such as $(\partial_x^4 + \partial_y^4 + \partial_z^4)$ and $D(k)$ involve only one round of finite differences, and are therefore favored for their execution speed. Also, the diffusion function for ∇^4 has a greater value in the high- k “corners” of Fourier space than $(\partial_x^4 + \partial_y^4 + \partial_z^4)$, and hence a smaller maximum diffusive time step, and so for this reason as well, operators such as ∇^4 and ∇^6 are disfavored.

We begin by considering diffusion operators with a stencil radius $S = 3$, such as those used in the hyperdiffusion implemented in the Pencil code (Brandenburg & Dobler 2002). In this case, one can analytically construct a one-parameter family of functions parameterized by the degree of diffusivity $D(1)$ at $k = 1$. As before, we take $D(0) = 0$, the diffusion scale $k_d = 1/2$, and normalize $D(k)$ so that $D(1/2) = 1$. Inverting Equation (7) with these conditions yields

$$m_0 = -\frac{1}{2} - \frac{1}{4}D(1), \quad (12)$$

$$m_1 = \frac{1}{8} + \frac{7}{32}D(1), \quad (13)$$

$$m_2 = \frac{1}{4} - \frac{1}{8}D(1), \quad (14)$$

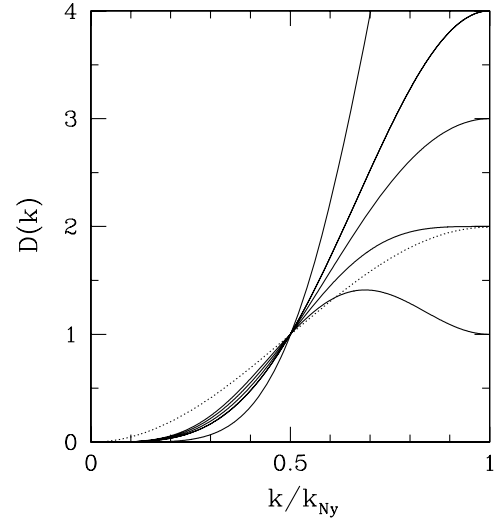


Figure 3. Family of diffusion functions $D(k)$ for $1 < D(1) < 8$ for a stencil with radius $S = 3$, represented with solid lines. The dotted line shows the $S = 1$ operator for ∂^2 ; the addition of the two additional parameters in the $S = 3$ operator allowed the reduction of diffusivity at both high and low wavenumber while maintaining the normalization at k_d . The $D(1) = 4$ line is identical to the standard $S = 2$ hyperdiffusivity. The functions are all continuous through $D(k_d)$, so the most diffusive above k_d are the least diffusive below it.

$$m_3 = -\frac{1}{8} + \frac{1}{32}D(1). \quad (15)$$

This also implies that

$$D_4 = \pi^4 \left(\frac{1}{8} - \frac{D(1)}{16} \right). \quad (16)$$

The magnitude of D_4 is inversely related to the sharpness of the hyperdiffusive operator. Sharpness of hyperdiffusivity is usually measured by giving the index of the scaling with wavenumber k at low k . In this example, however, all the functions we present have k^4 scaling at low k and are normalized at k_d , so the lower the value of the coefficient D_4 of the k^4 term, the sharper the hyperdiffusivity.

The free parameter $D(1)$ traces the maximum diffusivity, at least in the regime $D(1) > 2$, as shown in Figure 3, and thus determines the time step. This can be demonstrated by differentiating $D(k)$ (Equations (7) and (2)) and showing that in this regime, $D'(k) > 0$, so $D(k)$ monotonically increases between $0 < k < 1$. For $1 < D(1) < 2$, the maximum diffusivity is not much greater than the diffusivity at $k = 1$. For example, for $D(1) = 1.5$, the maximum diffusivity is $D = 1.63$ at $k = 0.762$. The useful range for $D(1)$ is $1 < D(1) < 8$ because the case $D(1) = 8$ corresponds to the operator for ∂^6 , which represents the $S = 3$ hyperdiffusivity operator that is least diffusive at low wavenumber. Choosing $D(1) > 8$ results in $D(k) < 0$ for some value of $k < k_d$. The choice $D(1) = 8$ corresponds to the standard hyperdiffusivity used in the Pencil code. We further find that the best choice to minimize diffusivity at low k is given by requiring that $D''(0) = 0$. If $D''(0) < 0$, then $D(k) < 0$ at low k , and hence unstable, while for $D''(0) > 0$, it is more diffusive at low k than it could be.

The goals of minimizing the low- k diffusivity and protecting the time step at high k are at odds if one normalizes the diffusion magnitude at the diffusion scale $D(k_d) = 1$. The tradeoffs can be seen by considering the behavior of $D(k)$ as $D(1)$ is increased

Table 2
Radius-3 Tuned Diffusion Values

$D(1/4)$	$D(1/3)$	$D(1)$
0.124	0.328	1.5
0.116	0.312	2.0
0.101	0.281	3.0
0.086	0.250	4.0
0.055	0.187	6.0
0.025	0.124	8.0

Notes. Values of the diffusion function $D(k)$ for $k = 1/4, k = 1/3$, and $k = 1$, for the sequence of radius-3 time-step-friendly hyperdiffusion functions with varying values of $D(1)$.

(Figure 3). Reducing the diffusion for $k < k_d$ requires increasing the diffusion for $k > k_d$, and vice versa. Although the values are much larger at high wavenumber, the percentage changes are actually similar in the two regimes (see Table 2 for the low wavenumber values).

Note that the function with $D(1) = 4$ is the standard hyperdiffusion with stencil radius $S = 2$, which is the most hyperdiffusive $S = 2$ operator. This is equivalent to Equation (5), with the additional normalization $D(1/2) = 1$. Adding one extra free parameter by moving to stencil size $S = 3$ allows both low- and high-wavenumber diffusivity to be tuned, but we cannot decrease both simultaneously. However, adding another free parameter by using stencil size $S = 4$ does allow both to be decreased (Figure 2). As an additional example, note that the dotted line in Figure 3 shows the $S = 1$ diffusivity, while the $S = 3$ result with $D(1) = 1.5$ has decreased diffusivity for both low and high k . Simultaneously decreasing the diffusion for $k < k_d$ and $k > k_d$ while maintaining a constant diffusion at $k = k_d$ thus clearly requires more than one free parameter. With two or more free parameters, we can simultaneously satisfy both goals.

Extending the stencil size to $S > 3$ allows us to further optimize the diffusion function. We now have multiple ways in which we could proceed. We choose to use numerical optimization to derive tuned $S > 3$ operators based on the following conditions: normalize the diffusion spectrum to $D(k_d) = 1$; insist that $0 < D(k) < \delta$ for some chosen value of the constant δ ; set $D(0) = 0$; and require that D monotonically increase for $k < k_d$. Within these constraints, we maximize $D'(k_d)$, which measures the sharpness of the operator at k_d .

To find the operator satisfying these conditions we use a multiparameter optimization of the coefficients m_j in order to maximize $D'(k_d)$ within the constraints. We have developed a novel Monte Carlo routine to perform the optimization. It evolves the solution by testing randomly selected nearby points, selecting the best among them and iterating with a search radius sensitive to the speed of improvement of the solution. Because different parameters have widely varying ranges, we use a logarithmic sampling distribution.

In Figure 2, we show the resulting optimized diffusivities for $S = 4$ and $S = 5$. The coefficients for these operators are given in Table 3. Comparing the $S = 2$ hyperdiffusivity to the optimized $S = 4$ operator gives another example of the benefit of taking advantage of two free parameters.

4. TIME-STEP-FRIENDLY LAPLACIAN DIFFUSION

Some applications require such large physical diffusivity that it becomes the dominant constraint on the time step. Examples include magnetized turbulent flows with separated viscous and resistive scales so that the magnetic Prandtl number

$$P_m = \frac{\nu}{\eta} \quad (17)$$

is far from unity, where η is the resistivity; and turbulence with a passive scalar such as temperature that diffuses at a scale different from the viscous scale so that the Schmidt number

$$S = \frac{\nu}{\kappa} \quad (18)$$

is far from unity, where κ is the diffusivity of the passive scalar. In this case, the physical diffusivity operators can also be adjusted so as to cause less harm to the time step.

The procedure that we used to generate coefficients for flat Lagrangian diffusion operators is to specify a value for k_d , and then constrain D so as to not further increase beyond its value at the diffusion scale. Specifically, we set $D(k) < (\pi k_d)^2$ for all k . Within this constraint, we minimize the value of $(\pi k_d)^2 - D(k)$ over $k > k_d$. For a radius $S = 3$ stencil, this procedure works for k_d as low as $7/32$. Any lower than that and $D(k) < (\pi k_d)^2$ cannot be satisfied without $D(k)$ taking on a dangerously small value for some $k > k_d$, or even worse, becoming negative. However, increasing the stencil size beyond $S = 3$ allows for flat diffusion operators with successively lower values of k_d . Such operators are shown in Table 1, and Figure 1 for $S = 3$.

5. SUMMARY

We have presented techniques for customizing diffusion operators with the goal of either decreasing low- k diffusion, or maximizing the time step, or some combination of both. We have given concrete examples that cover the commonly encountered cases, but since the requirements for diffusion can be problem dependent, we also emphasize techniques for customizing general diffusion operators.

Turbulent flows offer a major example of the need for careful choice of the magnitude of either physical diffusivity or hyperdiffusivity. The relevant magnitude is that at the diffusion scale $\nu D(k_d)$, where k_d is chosen to match the spectral resolution of the numerical scheme (Maron et al. 2008). There it must be large enough to absorb the energy from the turbulent cascade reaching that scale. The value of ν is generally set empirically to satisfy this requirement.

Table 3
Coefficients for Time-Step-Friendly Hyperdiffusion Operators

	m_0	m_1	m_2	m_3	m_4	m_5
∂^4 , Fourth order	1.500000	-1.	0.250000
∂^4 , Sixth order	1.750000	-1.218750	0.375000	-0.031250
Tuned, stencil 4	1.231682	-0.775549	0.074534	0.126481	-0.041307	...
Tuned, stencil 5	0.911455	-0.511864	-0.033699	0.094005	0.010574	-0.014743

The techniques developed here can also be applied to models with Prandtl and Schmidt numbers that are large or small compared to unity, as well as models with diffusive chemistry.

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