On Taylor-Series Approximations of Residual Stress[1]

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Abstract

Although subgrid-scale models of similarity type are insufficiently dissipative for practical applications to large-eddy simulation, in recently published *a priori* analyses, they perform remarkably well in the sense of correlating highly against exact residual stresses. Here, Taylor-series expansions of residual stress are exploited to explain the observed behavior and "success" of similarity models. Until very recently, little attention has been given to issues related to the convergence of such expansions. Here, we re-express the convergence criterion of Vasilyev et al. [*J. Comput. Phys.*, **146** (1998)] in terms of the transfer function and the wavenumber cutoff of the grid filter.

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1 Introduction

In contrast to direct numerical simulation (DNS), in which all energetic scales of motion are resolved on a fine grid, in large-eddy simulation (LES), the spatially filtered Navier-Stokes equations (FNSE) are solved numerically on a relatively coarse grid. For incompressible flow, and in tensor notation, the FNSE are given by

$$\frac{\partial \overline{u}_k}{\partial x_k} = 0 \tag{1}$$

$$\frac{\partial \overline{u}_k}{\partial t} + \frac{\partial(\overline{u}_k\overline{u}_l)}{\partial x_l} = -\frac{\partial \overline{p}}{\partial x_k} + \frac{1}{Re}\frac{\partial^2 \overline{u}_k}{\partial x_l \partial x_l} + \frac{\partial \tau_{kl}}{\partial x_l} \tag{2}$$

where u_k is the velocity vector, p is the pressure, and τ_{kl} is the subgrid-scale (SGS) stress tensor (or residual-stress tensor) defined exactly as

$$\tau_{kl} \equiv \overline{u}_k\overline{u}_l - \overline{u_k u_l} \tag{3}$$

Here overlines denote grid-filtered quantities, and Re is the Reynolds number.

The residual-stress tensor incorporates the effects of the unresolved scales of motion upon the resolved scales. It is customary in LES to model these effects, for which there exists a variety of possible models. In 1991, Germano et al. [1] introduced the concept of dynamic modeling, which exploits the resolved-turbulent-stress tensor $\mathcal{L}_{ij}$, a computable quantity that is extracted by applying an explicit secondary filter–the test filter–to the resolved velocity fields as follows:

$$\mathcal{L}_{kl} \equiv \hat{\overline{u}}_k\hat{\overline{u}}_l - \widehat{\overline{u}_k\overline{u}_l} \tag{4}$$

Here hats denote test-filtered quantities. In general, the test- and grid-filter widths, $\hat{\Delta}$ and Δ respectively, may differ. For later convenience, we denote their ratio by $r = \hat{\Delta}/\Delta$.

Recently, interest in SGS models of similarity type (e.g., Liu et al. [2], Stolz and Adams [3], and Pruett and Adams [4]) has revived (despite the fact that these models are typically insufficiently dissipative for stand-alone applications to LES). Under certain conditions, remarkably high correlations between τ_{kl} and $\mathcal{L}_{kl}$ have been observed in *a priori* analyses based on experimental (Liu et al. [2]) and computational (Pruett and Adams [4]) data. On the basis of their observations, Liu et al. [2] propose the stress-similarity model

$$\tau_{kl} \approx c_L \mathcal{L}_{kl} \tag{5}$$

where c_L is simply a constant.

In this paper, we exploit Taylor-series expansions of the grid- and test-filter operators to analyze the relationship between the tensors τ_{kl} and $\mathcal{L}_{kl}$ and to optimize the value of c_L in Eq. 5. The convergence properties of such expansions are subtle, and attention is devoted herein to establish a criterion for convergence. For simplicity, we apply filtering only in the x direction and suppress the y and z coordinates and the time t. However, numerical experiments (Pruett and Adams [4]) suggest that the results carry over to multi-dimensional filters.

2 Taylor-Series Analyses

Although the use of fixed-width filters is common in LES, in our judgment, this is an ill-advised practice that usually leads to the contamination of the SGS dissipation by the truncation error of the numerical scheme. Recently, the utility of tunable (one-parameter) filters has been recognized (e.g., Vasilyev et al. [6] and Pruett and Adams [4]). One-parameter filters permit the filter width Δ (or preferably for this work, the wavenumber cutoff k_c) to be specified independently of the grid increment Δx. In our view, k_c should be specified on the basis of physical considerations; that is, the cutoff should lie in the inertial range of the Kolmogorov spectrum. On the other hand, Δx should be determined by numerical considerations; that is, by the grid resolution necessary to resolve the smallest eddies for the numerical scheme of choice. The dimensionless product $\alpha_c \equiv k_c \Delta x$ defines the cutoff parameter to remove the degree of arbitrariness. To this end, we exploit one-parameter filters of Pade type, the details of which are relegated to the Appendix.

The following discussion applies to *a priori* analyses, in which DNS data are filtered to extract the exact residual stresses and their modeled counterparts. By implication, in this section $\Delta x = \Delta x_{\text{DNS}}$. As discussed in the Appendix, a discrete filter can be represented by a Taylor-series expansion in the grid increment Δx. For example, if $\bar{u}_k$ is a filtered velocity field, then

$$\bar{u}_k(x) = u_k(x) + a_1 u_k'(x)\Delta x + a_2 u_k''(x)\Delta x^2 + a_3 u_k'''(x)\Delta x^3 + \ldots \tag{6}$$

Here, primes denote (partial) derivatives with respect to x. For notational simplicity, the factorials associated with the Taylor expansion have been absorbed into the coefficients a_j. As shown in the Appendix, the Taylor series of a filter implies its transfer function and *vice versa*. In general, a filter is said to be of order m if the first non-vanishing coefficient of its Taylor series is a_m. By applying Eq. 6 to Eq. 3, we obtain a Taylor series for the residual stress, namely

$$\tau_{kl} = (a_1^2 - 2a_2)u_k'u_l'\Delta x^2 + (a_1 a_2 - 3a_3)(u_k'u_l'' + u_l'u_k'')\Delta x^3 + \ldots \tag{7}$$

Because the coefficients a_j depend implicitly upon α_c, it is useful to regard $\tau_{kl} = \tau_{kl}(\alpha_c)$. As the tensor τ_{kl} arises solely from the quadratic nonlinearity of the Navier-Stokes equations, it is quadratic at leading order in Δx, *provided that the filter is of either first- or second-order.* On the other hand, if the filter is of order $m > 2$, then τ_{kl} is of leading order m.

With the help of *Mathematica*, a similar expansion of $\mathcal{L}_{kl}$ leads to

$$\mathcal{L}_{kl} = (a_1^2 - 2a_2)u_k'u_l'r^2\Delta x^2 + (a_1^3 r^2 - 2a_1a_2r^2 + a_1a_2r^3 - 3a_3r^3)(u_k'u_l'' + u_l'u_k'')\Delta x^3 + \ldots \tag{8}$$

where the test and grid filters differ only in their respective widths, whose ratio is r. In (preferred) terms of grid- and test-filter cutoffs, $(k_c)_{\text{G}}$ and $(k_c)_{\text{T}}$, respectively, $r = (k_c)_{\text{G}}/(k_c)_{\text{T}}$. Clearly, $\mathcal{L}_{kl} = \mathcal{L}_{kl}(\alpha_c, r)$. By comparing Eq. 7 and Eq. 8, we conclude that the SGS stresses are approximated to leading order by

$$\tau_{kl} \approx \frac{\mathcal{L}_{kl}}{r^2} \tag{9}$$

whereby $c_L = 1/r^2$ in Eq. 5. How good is the approximation? From Eqs. 7 and 8, we obtain the approximation error

$$E_{kl}(\alpha_c, r) \equiv \tau_{kl} - \frac{\mathcal{L}_{kl}}{r^2} = \left[3a_3(r-1) + a_1a_2(3-r) - a_1^3\right](u_k'u_l'' + u_l'u_k'')\Delta x^3 + \ldots \tag{10}$$

from which we conclude the following:

1. If the filter is of either first- or second-order in Δx, then the approximation error (Eq. 10) is of higher order ($O(\Delta x^3)$) than is the subgrid-scale stress ($O(\Delta x^2)$), and the approximation could be accurate provided that there is separation between the contributions at various orders (a topic discussed shortly).

2. If the filter is of order two ($a_1 = 0$, $a_2 \neq 0$) then

$$E_{kl} = 3a_3(r-1)(u'_k u''_l + u'_l u''_k)\Delta x^3 + ... \tag{11}$$

3. Although $r = 1$ is precluded in LES for reasons to be addressed shortly, $r = 1$ is *optimal* for *a priori* analyses because, for second-order filters, the leading-order error vanishes.

4. The approximation that results from the optimality condition $r = 1$ is simply the scale-similarity model proposed by Bardina et al. [5], namely $\tau_{kl} \approx \overline{\bar{u}}_k \overline{\bar{u}}_l - \overline{\bar{u}_k \bar{u}_l}$.

Whenever the grid and test filters differ in their Taylor coefficients, the situation is somewhat more complicated. Here, we presume that the grid and test filters are each of second order and symmetric, in which case

$$\begin{aligned} \bar{u}_k(x) &= u_k(x) + a_2 u''_k(x)\Delta x^2 + a_4 u^{(4)}_k(x)\Delta x^4 + ... \\ \hat{u}_k(x) &= u_k(x) + b_2 u''_k(x)\Delta x^2 + b_4 u^{(4)}_k(x)\Delta x^4 + ... \end{aligned} \tag{12}$$

Applying Eq. 12 to Eq. 3, we obtain

$$\tau_{kl} = -2a_2 u'_k u'_l \Delta x^2 + [(a_2^2 - 6a_4)(u''_k u''_l) - 4a_4(u'_k u^{(3)}_l + u'_l u^{(3)}_k)]\Delta x^4 + O(\Delta x^6) \tag{13}$$

Similarly, from Eqs. 12 and 4, we derive

$$\mathcal{L}_{kl} = -2b_2 u'_k u'_l \Delta x^2 + [(b_2^2 - 6b_4)(u''_k u''_l) - (4b_4 + 2a_2 b_2)(u'_k u^{(3)}_l + u'_l u^{(3)}_k)\Delta x^4 + O(\Delta x^6) \tag{14}$$

A comparison of Eqs. 14 and 13 reveals the following approximation to be correct to leading order:

$$\tau_{kl} \approx \frac{a_2}{b_2}\mathcal{L}_{kl} \tag{15}$$

If the grid and test filters are identical ($b_j = a_j$) then $a_2/b_2 = 1$, in which case most of the leading-order error drops out to yield

$$E_{kl} = \tau_{kl} - \mathcal{L}_{kl} = 2a_2^2(u_k' u_l^{(3)} + u_l' u_k^{(3)})\Delta x^4 + O(\Delta x^6) \tag{16}$$

By either approach, we conclude that the use of identical grid and test filters should produce optimal results in *a priori* analyses.

The present analysis corroborates and provides an explanation for the observations of Liu et al. [2] and Pruett and Adams [4], whose *a priori* analyses were based on experimental and computational data, respectively. To be specific, Liu et al. [2] observe negligible correlations between the residual stresses and their Smagorinsky-modeled counterparts when using spectral filters, which act with exponential order. Our results suggest that, because the Smagorinsky model is of second-order in Δx, the model is appropriate only in the context of first- or second-order grid filters. Moreover, for spatial top-hat filters (which are of second order), Liu et al. [2] observe the highest correlations between τ_{kl} and $\mathcal{L}_{kl}$ for $r = 1$, which we have shown to be optimal. In *a priori* analyses from DNS of isotropic turbulence, Pruett and Adams [4] observe correlations of the form $C(\tau_{kl}, \mathcal{L}_{kl})$ of nearly unity whenever the filter is weakly to moderately dissipative ($\pi/2 \le \alpha_c < \pi$) and $r = 1$. As the dissipation increases, the correlation coefficient diminishes gradually, but it remains surprisingly high ($C > 0.8$) even for quite dissipative filters ($\alpha_c \approx 0.45$). Furthermore, they observe correlations to degrade somewhat as r deviates substantially from unity.

3 Taylor-Series Convergence

Although Taylor-series analysis is frequently exploited to develop or analyze SGS-stress models (e.g., Rogallo and Moin [7] and Horiuti [8]), the approach has sometimes been criticized because of uncertain convergence, an issue that has received little attention until the recent work of Vasilyev et al. [6]. In practice, Taylor-series approximation is most useful if the leading-order error is relatively small, which in turn requires that the series converges fairly rapidly. Here, for completeness, we draw on the work of Vasilyev et al. [6] and re-express their convergence criterion in terms of the transfer function and wavenumber cutoff of the grid filter.

Let u denote one of the three velocity components, and, for simplicity, presume that u is periodic on $[-\pi, \pi]$ and contains no wavenumbers higher than $k_{\max}$, a finite integer such that $k_{\max} > k_\eta$, the Kolmogorov wavenumber. It will be useful in later discussion to think of $k_{\max}$ as the wavenumber cutoff for full resolution of quadratic nonlinearities in DNS, in which case, for a spectral numerical scheme

$$k_{\max}\Delta x_{\text{DNS}} = \pi \tag{17}$$

Equation 17 is simply the Nyquist criterion of signal processing. Given the assumptions above, the velocity field and its derivatives may be expanded as finite Fourier series; that is,

$$u(x) = \sum_{k=-k_{\max}}^{k_{\max}} U_k e^{\iota kx} \quad \text{and} \quad u^{(m)}(x) = \sum_{k=-k_{\max}}^{k_{\max}} (\iota k)^m U_k e^{\iota kx} \tag{18}$$

where $\iota = \sqrt{-1}$, and U_k is the k-th (complex) Fourier coefficient of u. Slightly adapting Vasilyev et al. [6] (who also assume finite $k_{\max}$), we obtain a bound on the magnitude of the m-th derivative of u, namely

$$\begin{aligned}
|u^{(m)}(x)| &\leq \sum_{k=-k_{\max}}^{k_{\max}} |k|^m |U_k| \\
&\leq \left(\sum_{k=-k_{\max}}^{k_{\max}} k^{2m}\right)^{1/2} \left(\sum_{k=-k_{\max}}^{k_{\max}} |U_k|^2\right)^{1/2} \\
&= \sqrt{E}\left(2\sum_{k=1}^{k_{\max}} k^{2m}\right)^{1/2} \\
&\leq \sqrt{2E}\left(\int_0^{k_{\max}} k^{2m} dk\right)^{1/2} \\
&= \sqrt{2E}\left(\frac{k_{\max}^{2m+1}}{2m+1}\right)^{1/2} = k_{\max}^m \sqrt{\frac{Ek_{\max}}{m+1/2}}
\end{aligned} \tag{19}$$

where Hölder's inequality is used to proceed from the first to the second step of Eq. 19, and where $E = \sum_{k=-k_{\max}}^{k_{\max}} |U_k|^2$ is the total "energy" as per Vasilyev et al. [6]. Recall from Eq. 6 that

$$\overline{u}(x) = \sum_{m=0}^{\infty} a_m u^{(m)}(x) \Delta x^m \quad (a_0 = 1) \tag{20}$$

By Eq. 19

$$\sum_{m=0}^{\infty} |a_m u^{(m)}(x)\Delta x^m| \leq \sum_{m=0}^{\infty} |a_m| \sqrt{\frac{Ek_{\max}}{m+1/2}} (k_{\max}\Delta x)^m \tag{21}$$

Thus, the series in Eq. 20 is absolutely convergent provided that the series on the right-hand side above (Eq. 21) converges. By the ratio test, the power series in $k_{\max}\Delta x$ above converges provided that

$$\lim_{m\to\infty} \frac{|a_{m+1}|}{|a_m|} k_{\max}\Delta x < 1 \tag{22}$$

As discussed in the Appendix, the coefficients a_m depend on derivatives of the transfer function $H(\alpha, \alpha_c)$ of the filter as follows:

$$a_m(\alpha_c) = \frac{H^{(m)}(0, \alpha_c)}{(m!)\iota^m} \tag{23}$$

From Eqs. 17, 22, and 23, we obtain the following convergence criterion in terms of the filter's transfer function and its cutoff:

$$\lim_{m\to\infty} \frac{\pi}{(m+1)} \frac{|H^{(m+1)}(0, \alpha_c)|}{|H^{(m)}(0, \alpha_c)|} < 1 \tag{24}$$

For filters whose stencils and coefficients are symmetric, the appropriate criteria are

$$\lim_{m\to\infty} \frac{\pi^2 |a_{2m+2}|}{|a_m|} < 1 \quad \text{or} \quad \lim_{m\to\infty} \frac{\pi^2}{(2m+2)(2m+1)} \frac{|H^{(2m+2)}(0, \alpha_c)|}{|H^{(2m)}(0, \alpha_c)|} < 1 \tag{25}$$

By the Cauchy product theorem, if the convergence of the Taylor series for $\overline{u}_k$ is guaranteed by Eq. 24 or Eq. 25, then the series for $\overline{u}_k\overline{u}_l$ also converges. Moreover, by definition, $k_{\max}$ is sufficiently large so that quadratic nonlinearities are well-resolved in DNS. It follows that if the series for $\overline{u}_k$ converges, so must that for $\overline{u_k u_l}$. These two additional considerations guarantee that the Taylor series for τ_{kl} (Eq. 3) converges provided Eq. 24 or Eq. 25 is satisfied. For symmetric, fully explicit filters (see the terminology in the Appendix), Eq. 25 holds for all values of the cutoff parameter such that the off-center weights remain of the same sign.

We now specialize the analysis to the symmetric, second-order Pade filter, whose transfer function $H(\alpha, \alpha_c)$ is given in Eq. 34 and Fig. 1 of the Appendix. For this class of filters, the dependence upon α_c of the convergence criterion is subtle. Originally, we conjectured that

m	0	1	2	3	4	5
a_{2m}	1	0.75	0.4375	0.2521	0.1453	0.0838
$\|a_{2m+2}\|/\|a_{2m}\|$	NA	0.75	0.5833	0.5762	0.5766	0.5766

Table 1: Taylor-series coefficients for Pade filter with $\alpha_c = \pi/3$.

Eq. 25 holds at least for all $\pi/2 \leq \alpha_c \leq \pi$. However, attempts at formal proof failed. Subsequent numerical experimentation over a range of cutoffs suggests (but does not guarantee) that Eq. 25 is satisfied approximately for $-0.1 < \zeta = -\cos(\alpha_c) \leq 1$, and, as a general rule of thumb, the more dissipative the filter (the smaller α_c), the slower the convergence. (This is not entirely accurate, but a truer statement is too detailed for the present forum.)

Here, we will be content to consider three specific cutoff values, two for which the convergence criterion Eq. 25 is satisfied, and one for which it is not. First, for DNS, $\alpha_c = \pi$. From Eq. 34, $H(\alpha, \pi) = 1$, independently of α. Consequently, $\overline{u}_k = u_k$ and $\tau_{kl}(\pi) = \overline{u}_k\overline{u}_l - \overline{u_k u_l} = u_k u_l - u_k u_l = 0$. Similarly, for $r = 1$, $\mathcal{L}_{kl}(\pi, 1) = \overline{\overline{u}}_k\overline{\overline{u}}_l - \overline{\overline{u}_k\overline{u}_l} = \overline{u}_k\overline{u}_l - \overline{u_k u_l} = u_k u_l - u_k u_l = 0$. As expected, in the DNS limit, the filters turn off, the residual stress vanishes, the resolved turbulent stress also vanishes (for $r = 1$), and the resulting Bardina model is trivially exact. Second, for the special case $\alpha_c = \pi/2$, $|H^{(2m)}(0, \pi/2)| = 1/2$ for all $m > 0$, in which case Eq. 25 is clearly satisfied. Third, we consider $\alpha_c = \pi/3$ ($\zeta = -0.5$), for which Table 1 presents the first few coefficients a_{2m} and their ratios. Although the coefficients eventually diminish at an apparently constant rate, that rate is too slow to satisfy Eq. 25. For sufficiently dissipative Pade filters, the Taylor coefficients apparently grow at an asymptotically constant rate.

Returning briefly to the (convergent) case for which $\alpha_c = \pi/2$, we have

$$\tau_{kl}(\pi/2) = -\frac{1}{2}u'_k u'_l \Delta x^2 - \left[\frac{1}{16}u''_k u''_l + \frac{1}{12}\left(u'_k u^{(3)}_l + u'_l u^{(3)}_k\right)\right]\Delta x^4 + ... \tag{26}$$

and

$$E_{kl}(\pi/2, 1) = \tau_{kl} - \mathcal{L}_{kl} = \frac{1}{8}\left(u'_k u^{(3)}_l + u'_l u^{(3)}_k\right)\Delta x^4 + ... \tag{27}$$

Careful examination of Eqs. 26 and 27 reveals that the leading order error term above *could* be large relative to the magnitude of the residual stress. Indeed, criterion Eq. 25

guarantees only that the terms of Taylor expansions *eventually* diminish, not necessarily that the leading order approximation error is small. One might expect that higher order corrections to the expansion for $\mathcal{L}_{kl}$ would be necessary before the similarity model (Eq. 5) is even approximately valid. (See, for example, the generalized similarity model of Stolz and Adams [3].) In this light, that correlations $C(\tau_{kl}, \mathcal{L}_{kl})$ are typically observed to be high (Pruett and Adams [4]) even for quite dissipative filters (whose Taylor series may even diverge) is at first intriguing. With regard to LES, there are three ameliorating factors. First, in the inertial subrange, the Fourier coefficients U_k decay as $k^{-5/6}$ in amplitude. Second, for $k_{\max} \geq k \geq k_\eta$, the Fourier coefficients decay even more rapidly due to the effectiveness of viscosity. Neither factor has been taken into account. Third and dominant, the bound expressed by Eq. 19 is extremely pessimistic; equality holds only when all Fourier components align in phase, an unlikely scenario in a turbulent flow.

4 LES

Finally, we turn to an implication of our analysis to LES. For *a priori* analyses, there is no prohibition on the use of identical test and grid filters. However, $r = 1$ is disallowed in LES with secondary filtering, as the following line of reasoning suggests (and as also noted in Liu et al. [2]). For LES, $\Delta x = \Delta x_{\rm LES}$. Recall that $(k_c)_{\rm G}$ and $(k_c)_{\rm T}$ denote the grid- and test-filter cutoffs, respectively, where we now presume $(k_c)_{\rm T} \leq (k_c)_{\rm G}$. By design, once $(k_c)_{\rm G}$ is established from physical considerations, then (for a spectral numerical scheme) the Nyquist criterion $(k_c)_{\rm G}\Delta x_{\rm LES} \equiv (\alpha_c)_{\rm G} \approx \pi$ establishes the appropriate grid increment $\Delta x_{\rm LES}$. By definition, $(k_c)_{\rm T}\Delta x_{\rm LES} \equiv (\alpha_c)_{\rm T}$. Thus,

$$r_{\rm LES} \equiv \frac{(k_c)_{\rm G}}{(k_c)_{\rm T}} = \frac{\pi}{(\alpha_c)_{\rm T}} \geq 1 \tag{28}$$

In LES, it is common to use $r_{\rm LES} = 2$. Attempts to use $r_{\rm LES} = 1$ yield $(\alpha_c)_{\rm T} = \pi$, which turns off the secondary filter. However, at least in theory, there is no reason why similarity models with $r > 1$ are not viable for LES.

5 Conclusions

In conclusion, Taylor-series expansions of residual stress are useful for developing and analyzing SGS models for LES. In particular, Taylor-series analysis reveals the explicit dependence of the residual stress on the grid filter, and thereby reveals potential model-filter inconsistencies. Moreover, such analysis underscores the desirability of one-parameter filters, whose cutoffs can be tuned independently of grid resolution. The degree of usefulness of Taylor-series expansions, however, depends ultimately on how rapidly the series converge. A rigorous convergence criterion has been developed that is expressed in terms of the transfer function and wavenumber cutoff of the grid filter. As a rule of thumb, the more (less) dissipative the filter, the slower (faster) the convergence. Taylor-series expansions have then been applied to the analysis of the similarity models of Bardina [5] and of Liu et al. [2]. The analysis corroborates and appears to explain a number of observations regarding such models (e.g., Liu et al. [2] and Pruett and Adams [4]). In *a priori* analyses, similarity models typically perform far better than expected based on the mathematical analysis herein, which suggests that a refined analysis is both desirable and possible.

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Appendix: One-Parameter Pade Filters

Following Lele [9], a discrete, second-order, one-parameter (ζ) Pade filter is constructed by considering the symmetric pointwise scheme

$$\zeta \bar{f}_{i-1} + \bar{f}_i + \zeta \bar{f}_{i+1} = a f_i + \frac{b}{2}(f_{i-1} + f_{i+1}) \quad ; \quad (i = 1, 2, ...n-1) \tag{29}$$

Various treatments are possible for the boundary nodes $i = 0$ and $i = n$. However, the simplest tack is to impose no filtering at the boundaries. In matrix form $M\bar{\mathbf{f}} = E\mathbf{f}$, where M and E are tridiagonal.

The action of the filter above on the single Fourier mode $\exp(\iota kx)$ yields the complex *transfer function*

$$H(\alpha) = \frac{a + b\cos(\alpha)}{1 + 2\zeta\cos(\alpha)} \tag{30}$$

where $\alpha = k\Delta x$. For applications to LES, we consider only *low-pass* filters, for which $H(0) = 1$ and $H(\pi) = 0$. In combination, these constraints imply $b = a = 0.5 + \zeta$. Admissible values of the parameter are $-\frac{1}{2} < \zeta \leq \frac{1}{2}$. Whenever $\zeta = 0$, M is the identity matrix, and the filter is *fully explicit*. The fully explicit case corresponds to a discrete *top-hat* filter with weights at adjacent nodes of [1/4, 1/2, 1/4]. Otherwise, the filter is *implicit*. The value $\zeta = \frac{1}{2}$ yields $M = E$, which turns off the filter. For all admissible parameter values, the matrices M and E are diagonally dominant with positive diagonal elements, in which case the filter operator $L = M^{-1}E$ is positive semidefinite.

By analogy to discrete differentiation operators, to each discrete filter is associated a Taylor-series expansion of the form

$$\bar{f}(x_i) = f(x_i) + a_1 f'(x_i)\Delta x + a_2 f''(x_i)\Delta x^2 + a_3 f'''(x_i)\Delta x^3 + ... \tag{31}$$

Here, for notational simplicity, the factorials in the Taylor series have been absorbed into the coefficients a_j. By applying the Taylor-series representation of the filter to $\exp(\iota k x_i)$, we obtain the corresponding Taylor series of the transfer function, namely

$$H(\alpha) \;=\; 1 + a_1(\iota\alpha) + a_2(\iota\alpha)^2 + a_3(\iota\alpha)^3 + ... \tag{32}$$

Evaluating successive derivatives of Eq. 32 at $\alpha = 0$ yields

$$a_m = \frac{H^{(m)}(0)}{(m!)\iota^m} \tag{33}$$

Thus, the Taylor series implies the transfer function and *vice versa*. In general, a filter is of order m if its first non-vanishing Taylor coefficient is a_m. Filters associated with symmetric stencils are of even order with purely real transfer functions. In particular, the Pade scheme above is of second order (provided $\zeta \neq 0.5$).

The coefficients of the Taylor series of Eq. 31 are functions of the parameter. To quantify this dependence for the Pade filter, we (unconventionally) define α_c, the dimensionless wavenumber cutoff, such that $\frac{1}{2} = H(\alpha_c)$, whereby

$$H(\alpha, \alpha_c) = \frac{(1 - \cos\alpha_c)(1 + \cos\alpha)}{2(1 - \cos\alpha_c \cos\alpha)} \tag{34}$$

Figure 1 compares the transfer functions of the Pade filter for selected values of α_c.

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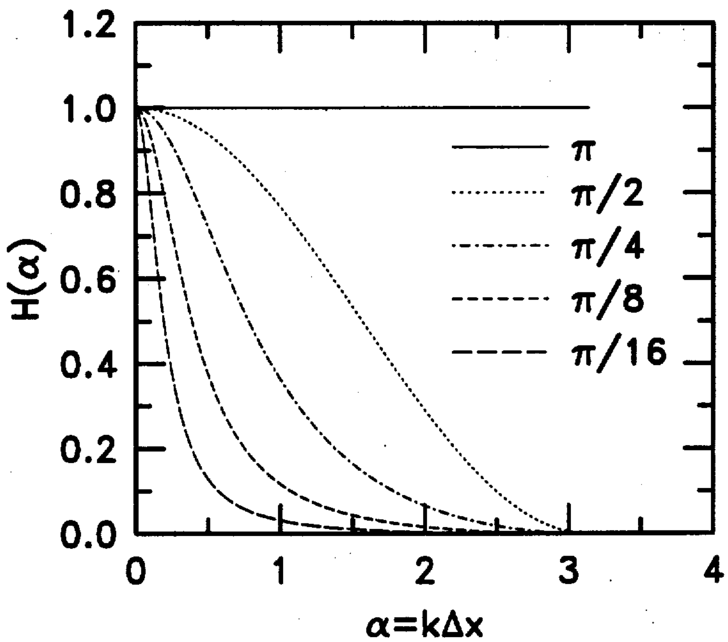

Figure 1: Transfer function of one-parameter family of second-order low-pass filters of Pade type for selected values of dimensionless wavenumber cutoff α_c.