A systematic approach for obtaining and modeling a nonlocal eddy diffusivity

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Abstract

We consider nonlocal eddy diffusivities for passive scalar transport phenomena and show how to exactly obtain them using the macroscopic forcing method (MFM), a technique introduced by Mani and Park [1]. While for many flows the nonlocal eddy diffusivity is more accurate than the commonly used Boussinesq eddy diffusivity, the nonlocal eddy diffusivity is often too computationally cost-prohibitive to obtain and use in practice. We develop a systematic and more cost-effective approach for approximating the nonlocal eddy diffusivity using matched moment inverse (MMI) operators. These operators require only a few moments of the nonlocal eddy diffusivity which can be computed more easily using inverse MFM [1] and the resulting model can be written as a partial differential equation rather than a nonlocal integral.

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1 Introduction

Scalar transport phenomena are critical to a broad range of everyday applications from engineering to biology and geophysics. One commonly used approach for modeling mean scalar transport by a turbulent flow is to Reynolds average the governing equations. This approach leads to an unclosed scalar flux term that must be specified. If the time and length scales over which the mean flow varies are much greater than that of the underlying turbulent fluctuations, then one may apply the Boussinesq approximation \[2\], and write the scalar flux as the product of an eddy diffusivity and the gradient of the mean scalar. Under this approximation, the scalar flux at a given point depends only on the gradient of the mean at that one point, i.e. the Boussinesq approximation is a purely local approximation.

However, in many realistic flows the time and length scales of the fluctuations are not small relative to the scales of the mean flow. In which case, the Boussinesq approximation is not valid. A modification introduced by Berkowicz and Prahm \[3\] allows for the scalar flux to depend on gradients of the mean at all points in space rather than a single point. The eddy diffusivity becomes a nonlocal eddy diffusivity, capturing the spatial dependence of the scalar flux. Moreover, a nonlocal eddy diffusivity may also be modified to capture the temporal dependence of the scalar flux on the history of the gradient of the mean scalar. These ideas and definitions will be made concrete in the problem formulation in Section 1.1.

A nonlocal eddy diffusivity can give a fully accurate description of the scalar flux. Moreover, it can reveal information fundamental to the understanding and prediction of a flow, such as the sensitivity of the scalar flux to gradients in certain regions. The catch is, in practice, a nonlocal eddy diffusivity may be very computationally expensive to obtain. One method to obtain the nonlocal eddy diffusivity is the macroscopic forcing method (MFM), a numerical technique introduced by Mani and Park \[1\], in which one applies an appropriate forcing to the governing equation and measures the averaged response. Through this input-output relationship, one can eventually determine the exact nonlocal eddy diffusivity corresponding to the unclosed term. However, because the full nonlocal eddy diffusivity captures how the scalar flux depends on gradients at all locations, this brute force technique must probe each location, requiring as many simulations as points in the averaged space. Even once obtained, a nonlocal eddy diffusivity may still be impractical to implement in a model due to accounting for the effect of gradients everywhere in space (and time). A spatially nonlocal eddy diffusivity would raise the computational cost from $O(N)$ to $O(N^2)$; a temporally nonlocal eddy diffusivity would require keeping the history of the gradient of the mean scalar stored in memory.

To alleviate the computational cost while keeping the accuracy of the nonlocal eddy diffusivity, we introduce a systematic technique for modeling nonlocal eddy diffusivities using what we call matched moment inverse (MMI) operators. These operators do not require obtaining the full nonlocal eddy diffusivity—as the name suggests, they require only a few moments of the nonlocal eddy diffusivity, which can be cost-effectively obtained using inverse MFM \[1\]. As an alternative to MFM, inverse MFM can obtain the moments of the exact nonlocal eddy diffusivity using just one simulation per moment. Moreover, the resulting MMI model
is in the form of a partial differential equation that can be solved more readily than the nonlocal integral resulting from a regular nonlocal eddy diffusivity formulation. We note that while nonlocal eddy diffusivities for scalar transport have been explored by other works such Hamba [4], the main difference here is that we introduce a systematic procedure for modeling the nonlocal eddy diffusivity which drastically decreases the computational cost.

MFM is introduced in Section 1.2. Section 1.2.2 introduces an alternative (but still costly) linear algebra-based formulation of MFM that works well for small problems and is used for obtaining the exact nonlocal eddy diffusivities in the illustrative examples in this article. Section 1.2.3 introduces inverse MFM, a formulation for easily obtaining the exact moments of the nonlocal eddy diffusivity without going through the full eddy diffusivity. Then using a simple homogeneous problem, we demonstrate obtaining the exact nonlocal eddy diffusivity in Section 2. As noted, this procedure is expensive, but we show it in order to demonstrate what a nonlocal eddy diffusivity looks like and the importance of including nonlocal effects in a model. We then introduce several techniques for approximating a nonlocal eddy diffusivity, culminating in the use of MMI in Section 3. Lastly, we demonstrate the use of MMI for inhomogeneous flows in Section 4 and address some of the challenges with MMI for inhomogeneous wall-bounded flows.

1.1 Problem formulation

Consider a passive scalar, \( c(x, t) \), being transported by a flow with velocity, \( u(x, t) \). The governing equation is

\[
\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_j} (u_j c) = D_M \frac{\partial^2 c}{\partial x_j \partial x_j}
\]  

(1)

where \( D_M \) is the molecular diffusivity. In many applications, instead of the full solution, \( c \), one may be only interested in the average of the solution, \( \bar{c} \). One can derive an equation for \( \bar{c} \) by applying the Reynolds decomposition:

\[
c = \bar{c} + c'
\]

(2a)

\[
u_j = \bar{u}_j + u'_j
\]

(2b)

where \( \bar{() \!} \) denotes a mean quantity and \( ()' \) denotes fluctuations from the mean quantity. Substituting (2a) and (2b) into Equation (1) and then averaging the resulting equation leads to the mean scalar transport equation,

\[
\frac{\partial \bar{c}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_j \bar{c}) = D_M \frac{\partial^2 \bar{c}}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} (u'_j c').
\]

(3)

The scalar flux term, \( \bar{u}_j c' \), cannot be written directly in terms of mean quantities, i.e. this term is unclosed. A commonly-used closure model, introduced by Boussinesq [2], approximates \( -\bar{u}_j c' \) as a diffusive flux:

\[
-\bar{u}_j c'(x) = D \frac{\partial \bar{c}}{\partial x_j} |_{x}
\]

(4)

where \( D \) is known as the eddy diffusivity. The Boussinesq approximation assumes that the mean, \( \bar{c} \), varies over a time scale and a length scale much larger than that of the fluctuations, \( c' \). In other words, the
fluctuations mix very quickly and very locally. In this limit, one can draw an analogy to kinetic theory, where molecules move very quickly and locally due to Brownian motion, but the average motion can be approximated via a diffusive flux. Reliant on a separation of scales, the Boussinesq approximation is a purely local approximation: \(-u_j'c'\) at a given location, \(x\), is only allowed to depend on the gradient of \(\bar{c}\) at the same location, \(x\).

However, such an idealized separation of scales often does not exist in turbulent flows. When the Boussinesq assumption breaks down, a more general form of the eddy diffusivity is introduced by Berkowicz and Prahm [3]:

\[
-\overline{u_j'c'}(x) = \int_y D_{ji}(x,y) \frac{\partial \bar{c}}{\partial x_i} \, dy.
\]

\(-\overline{u_j'c'}\) at a given location, \(x\), may now be influenced by the gradient, \(\partial \bar{c}/\partial x_i\), at another location, \(y\). In this form, there is no requirement of length scale separation, and fluctuations are not assumed to mix locally. \(D_{ji}(x,y)\) is now a nonlocal eddy diffusivity and captures how the scalar flux depends on gradients at other locations. A nonlocal eddy diffusivity can also take into consideration temporal effects [4], [5]:

\[
-\overline{u_j'c'}(x,t) = \int_{y,\tau} D_{ji}(x,y,t,\tau) \frac{\partial \bar{c}}{\partial x_i} |_{y,\tau} \, dy\,d\tau.
\]

\(-\overline{u_j'c'}\) at a given time, \(t\), may now also depend on the time history, \(\tau\), of the gradient of \(\bar{c}\).

If the flow is homogeneous, the nonlocal eddy diffusivity expression in (6) has a simplified form:

\[
-\overline{u_j'c'}(x,t) = \int_{y,\tau} D_{ji}(x-y,t-\tau) \frac{\partial \bar{c}}{\partial x_i} |_{y,\tau} \, dy\,d\tau
\]

where the nonlocal eddy diffusivity does not depend on the specific point, \((x,t)\), but rather only the distance, \((x-y,t-\tau)\). We begin by considering nonlocal eddy diffusivities for homogeneous flows in Section 2 before considering inhomogeneous flows in Section 4.

1.2 Introduction to the Macroscopic Forcing Method (MFM)

We briefly introduce the various formulations of MFM used here; for a more detailed description see [1].

1.2.1 MFM

The scalar transport equation in (1) can be written as

\[
\mathcal{L}c(x_1, \ldots, x_n, t) = 0
\]

where

\[
\mathcal{L} = \frac{\partial}{\partial t} + u_j \frac{\partial}{\partial x_j} - \bar{D}_M \frac{\partial}{\partial x_j} \left( D_M \frac{\partial}{\partial x_j} \right)
\]

is the microscopic operator. The desired mean scalar transport equation is then

\[
\mathcal{\bar{L}}\bar{c}(x_1, \ldots, x_n, t) = 0
\]
where $\hat{L}$ is the \textit{macroscopic operator}. This mean scalar transport equation is entirely in terms of $\bar{c}$, rather than with the unclosed scalar flux. Note both $L$ and $\hat{L}$ must be linear operators. For discussion of application of MFM to the Navier-Stokes equations see [1].

MFM determines the unknown operator $\hat{L}$ by applying a forcing function, $s$, to the right-hand-side of the microscopic equation in (8), with the property $s = \bar{s}$. One can then solve for $c$, compute $\bar{c}$, and use the input-output relationship between $s$ and $\bar{c}$ to solve for $\hat{L}$. In discretized form,

$$[\hat{L}][\bar{c}] = [\bar{s}] \quad (11)$$

where the brackets indicate matrices. Rearranging, the input-output relationship can be written as

$$[\bar{c}] = [\hat{L}]^{-1}[\bar{s}]. \quad (12)$$

The forcing can be specified in various ways. As an example, let $[\bar{s}_1] = [1 \ 0 \ldots \ 0]^T$, and let $[\bar{c}(\bar{s}_1)]$ be the averaged response which can be computed by applying the corresponding forcing, $s_1$, to the microscopic equation in (8) and averaging the corresponding $c(s_1)$. Then the first column of $[\hat{L}]^{-1}$ must be $[\bar{c}(\bar{s}_1)]$. One can repeat the procedure with $[\bar{s}_2] = [0 \ 1 \ldots \ 0]^T$ to find the second column of $[\hat{L}]^{-1}$, etc. and eventually fill out all the columns of $[\hat{L}]^{-1}$. $[\hat{L}]^{-1}$ can then be inverted to find the macroscopic operator $[\hat{L}]$. In this procedure, the forcing acts as a delta-function probe—activating certain locations allows one to determine exactly how $\bar{c}$ depends on what is happening in that location.

Once the macroscopic operator $[\hat{L}]$ is obtained, one can subtract out the closed part of the operator to find the unclosed part of the operator, denoted by $[\hat{L}']$. For example, if averages are taken over all directions except $x_1$ and the unclosed term is simply $\hat{L}'c = \partial/\partial x_1(u_1'c')$, one can then write the unclosed operator as

$$[\hat{L}'] = -[\partial/\partial x_1][D][\partial/\partial x_1]. \quad (13)$$

By removing the appropriate $[\partial/\partial x_1]$ matrices, one can recover the eddy diffusivity, $[D]$, in discretized form. If $[D]$ is a purely diagonal matrix, then the eddy diffusivity is purely local. If instead, there are nonzero off-diagonal entries in $[D]$, which then multiply a spread of corresponding entries in $[\partial \bar{c}/\partial x_1]$, then the eddy diffusivity is nonlocal.

Matrix multiplication can also be expressed as a convolution, and in continuous form, the unclosed term can be written as

$$-u_1' \bar{c}'(x_1) = \int_{y_1} D(x_1, y_1) \frac{\partial \bar{c}}{\partial x_1} \bigg|_{y_1} dy_1, \quad (14)$$

which generalizes to the eddy diffusivity formulation of Berkowicz and Prahm [3] in Equation (5).

Note this approach obtains the entire unclosed operator, $\hat{L}'$. For complex problems with multiple unclosed terms accounted for in $\hat{L}'$, one can instead use the inverse MFM formulation in Section [1,2,3] to probe each unclosed term individually.
1.2.2 Linear algebra-based MFM

Linear algebra-based MFM is an alternative formulation of MFM that works well for the small model problems in this paper, but is not practical for larger problems as it requires computing the inverse of the full microscopic operator, \([\mathcal{L}]\). As with MFM, consider the forcing, \(s\), applied to the microscopic equation in discrete form

\[
[\mathcal{L}][c] = [s].
\]  \hspace{1cm} (15)

Let averaging be defined by

\[
[c] = [P][c]
\]  \hspace{1cm} (16)

where \([P]\) is a projection matrix. We require that \(s = \tilde{s}\), but discretely \([s]\) and \([\tilde{s}]\) may not be vectors of the same size. And so let

\[
[s] = [E][\tilde{s}]
\]  \hspace{1cm} (17)

where \([E]\) is the extension matrix. Then, combining (15), (16), and (17) leads to

\[
[c] = [P][\mathcal{L}]^{-1}[E][\tilde{s}]
\]  \hspace{1cm} (18)

Comparing (18) and (12) implies

\[
[\tilde{\mathcal{L}}]^{-1} = [P][\mathcal{L}]^{-1}[E]
\]  \hspace{1cm} (19)

which can be then be inverted to obtain the same macroscopic operator as before. Note that this approach does not require explicitly specifying the forcing, and thus does not require a new simulation for each new forcing. However, matrix inversion of the full microscopic operator, \([\mathcal{L}]\), may be prohibitively expensive for large problems.

1.2.3 Inverse MFM

In the MFM formulation in Section 1.2.1 one specifies a forcing and computes the corresponding averaged response. In inverse MFM, one specifies the desired averaged response and applies the forcing required to maintain that averaged response.

Consider the forced equation

\[
\frac{\partial c}{\partial t} = f(c, \nabla c, t, \ldots) + s
\]  \hspace{1cm} (20)

and the corresponding averaged equation

\[
\frac{\partial \bar{c}}{\partial t} = \bar{f} + s
\]  \hspace{1cm} (21)

with the condition on the forcing \(s = \tilde{s}\). By pre-specifying \(\bar{c}\) and rearranging (21), one can obtain an expression for \(\tilde{s}\) that can be substituted into (20). This substitution constrains the average to be the pre-specified \(\bar{c}\), but the individual values of \(c\) are free to evolve. In practice, at each time step, one can solve for \(c\) without the forcing, and then shift \(c\) appropriately (still observing the property \(s = \tilde{s}\)) such that the average matches the pre-specified \(\bar{c}\). For a more detailed discussion, see [1].
Inverse MFM allows for cost-effective computation of moments of the nonlocal eddy diffusivity. For example, again assume that averages are taken over all directions except $x_1$ and the unclosed term is

$$- \overline{u_1' c'(x_1)} = \int_{y_1} D(x_1, y_1) \frac{\partial \overline{c'}}{\partial x_1} |_{y_1} dy_1. \tag{22}$$

Consider substitution of $\overline{c} = x_1$ into (22). One recovers the zeroth moment of the nonlocal eddy diffusivity:

$$D^0(x_1) = \int_{y_1} D(x_1, y_1) dy_1 = -\overline{u_1' c'}|_{\overline{c}=x_1}. \tag{23}$$

In other words, if one forces the microscopic equation such that $\overline{c} = x_1$ and post-processes $-\overline{u_1' c'}(x_1)$, then one recovers the zeroth moment of the eddy diffusivity. This requires just one simulation.

Similarly, one can also compute the first moment of the nonlocal eddy diffusivity using

$$D^1(x_1) = \int_{y_1} (y_1 - x_1) D(x_1, y_1) dy_1 = -\left(\overline{u_1' c'}|_{\overline{c}=x_1^2/2} - x_1 \overline{u_1' c'}|_{\overline{c}=x_1}\right). \tag{24}$$

This requires just one additional simulation with the forcing applied such that $\overline{c} = x_1^2/2$. One can compute the second moment of the nonlocal eddy diffusivity using

$$D^2(x_1) = \int_{y_1} \frac{1}{2} (y_1 - x_1)^2 D(x_1, y_1) dy_1 = -\left(\overline{u_1' c'}|_{\overline{c}=x_1^3/6} - x_1 \overline{u_1' c'}|_{\overline{c}=x_1^2/2} + (x_1^2/2) \overline{u_1' c'}|_{\overline{c}=x_1}\right), \tag{25}$$

and so forth.

2 Nonlocal eddy diffusivities in homogeneous flows

2.1 Model problem: dispersion by a parallel flow

As a simple example, consider the dispersion of a passive scalar by a homogeneous, laminar, parallel flow. This problem was first introduced by G. I. Taylor [6] and revisited by [1] to demonstrate how MFM can be used to obtain the exact nonlocal eddy diffusivity. Moreover, this problem can violate the scale separation assumptions of the Boussinesq approximation, requiring the consideration of nonlocal effects. Specifically, consider a two-dimensional problem with the governing equation:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_1}(u_1 c) + \frac{\partial}{\partial x_2}(u_2 c) = D_M \left( \frac{\partial^2 c}{\partial x_1^2} + \frac{\partial^2 c}{\partial x_2^2} \right) \tag{26}$$

where $c(x_1, x_2, t)$ is a passive scalar, $D_M$ is the molecular diffusivity, and $u_j$ is the parallel flow velocity:

$$u_1 = U \cos \left( \frac{2 \pi}{L_2} x_2 \right), \quad u_2 = 0. \tag{27}$$

The domain is $-\infty < x_1 < +\infty$ and $0 \leq x_2 < L_2$ with $L_2 = 2\pi$ and periodic boundary conditions in $x_2$. Nondimensionalizing $x_2$ by $L_2/(2\pi)$, $x_1$ by $UL_2^2/(4\pi^2 D_M)$, and $t$ by $L_2^2/(4\pi^2 D_M)$ leads to the following nondimensionalized equation:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_1}(\cos(x_2) c) = \epsilon^2 \frac{\partial^2 c}{\partial x_1^2} + \frac{\partial^2 c}{\partial x_2^2} \tag{28}$$
where $\epsilon = 2\pi D_M/(L_2 U)$ is the only nondimensional parameter. As in [1], for simplification consider $\epsilon = 0$, corresponding to the limit of large Peclet number, i.e. assume the advective flux is much greater than the diffusive flux in the $x_1$-direction. The governing equation for the homogeneous example problem is

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_1}(\cos(x_2)c) = \frac{\partial^2 c}{\partial x_2^2}. \quad (29)$$

For this problem, averaging is taken over the $x_2$-direction, i.e.

$$\bar{c}(x_1, t) = \frac{1}{L_2} \int_0^{L_2} c(x_1, x_2, t) dx_2. \quad (30)$$

Correspondingly, the mean scalar transport equation for this problem is

$$\frac{\partial \bar{c}}{\partial t} + \frac{\partial}{\partial x_1}(\cos(x_2)c') = 0 \quad (31)$$

where $u'_1 c' = \cos(x_2)c'$ is the unclosed scalar flux. The mean advection, $\partial / \partial x_1 (\bar{u}_1 \bar{c})$, does not appear in (31) since $\bar{u}_1 = \cos(x_2) = 0$. The mean diffusion, $\partial^2 \bar{c} / \partial x_2^2$, also drops from (31) due to averaging over $x_2$ and periodic boundary conditions.

Figure 1a shows the prescribed velocity profile. Figure 1b-d show the initial condition, $c(t = 0) = \exp(-x_1^2/0.025)$, and time snapshots of the dispersed scalar field, $c(x_1, x_2, t)$, and averaged field, $\bar{c}(x_1, t)$, solved using direct numerical simulation (DNS). The goal is to predict the complex behavior of $\bar{c}(x_1, t)$. 

Figure 1: (a) The velocity profile for the homogeneous, parallel flow ($u_1 = \cos(x_2)$, $u_2 = 0$). (b) An initial condition corresponding to the release of a narrow band of passive scalar in the center of the domain ($c(t = 0) = \exp(-x_1^2/0.025)$). (c) The dispersed scalar field, $c(x_1, x_2, t)$, and $x_2$-averaged field, $\bar{c}(x_1, t)$, at time, $t_1 = 0.5$. (d) $c(x_1, x_2, t)$ and $\bar{c}(x_1, t)$ at a later time, $t_2 = 4$. 

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Figure 2: (a) The velocity profile ($u_1 = \cos(x_2), u_2 = 0$). (b) The applied source term, $f(x_1, x_2, t)$, given by $f(x_1, x_2, t) = \exp(ikx_1)\bar{f}(t)$ and shown in physical space for $k = 5$ and $t = 3$. (c) $\bar{f}(t)$ as specified in Equation (30). (d) A snapshot of the resulting scalar field, $c$, solved using DNS and shown in physical space at $t = 3$. (e) The goal is to predict the time-dependent behavior of the averaged scalar field, $\bar{c}(t)$.

However, in order to do so, we first need to build some of the necessary machinery. We will revisit the full spatiotemporal problem in Section 3.4.

2.2 A temporally nonlocal eddy diffusivity

Rather than the dispersion of a narrow band of passive scalar, consider a zero initial condition and an applied source term instead (not to be confused with the MFM forcing). This source term is constrained to only one wavenumber in $x_1$ but allowed to vary in time as shown in Figure 2b-c. One can think of the source term as the injection/removal of a contaminant at a single wavenumber which is then mixed by the flow. The goal is to predict the complex time-dependent behavior of the averaged scalar field, $\bar{c}(t)$, shown in Figure 2e. Although the problem is unphysical, choosing a single wavenumber allows decoupling of spatial and temporal nonlocality, so one may focus solely on temporal nonlocality for now.

The Fourier transform in $x_1$ of the governing equation is

$$\frac{\partial \hat{c}}{\partial t} + ik \cos(x_2)\hat{c} = \frac{\partial^2 \hat{c}}{\partial x_2^2} + \bar{f}(t)$$

where $\bar{f}(t)$ is the source term. Averaging is defined for this problem in the $x_2$-direction by Equation (30).

The Fourier-transformed, mean scalar transport equation is

$$\frac{\partial \bar{c}}{\partial t} + ik \cos(x_2)\bar{c} = \bar{f}(t)$$

where $u'_1\bar{c}' = \cos(x_2)\bar{c}'$ is the unclosed scalar flux. Because the problem is Fourier-transformed in $x_1$ and averaged over $x_2$, now for a given wavenumber, $k$, the nonlocal eddy diffusivity depends only on time. In
other words, for a given $k$, one can write Equation (33) as

$$\frac{d\tilde{c}}{dt} - ik \int_{-\infty}^{t} \hat{D}_k(\tau - t) i k \tilde{c}(\tau) d\tau = \bar{f}(t).$$  (34)

One can now obtain the eddy diffusivity kernel, $\hat{D}_k(\tau - t)$, for a given $k$ using the linear algebra-based MFM formulation in Section 1.2.2. Linear algebra based-MFM gives the eddy diffusivity as a matrix, and because the flow is homogeneous, all the rows are identical, and the eddy diffusivity kernel is just one row of the matrix. Figure 3 shows the kernel for $k = 5$. This kernel is obtained using a second-order central difference discretization on a uniform staggered mesh in space and implicit Euler time-stepping.

Note [1] also use MFM to obtain a nonlocal eddy diffusivity for this example problem; however, their eddy diffusivity is in Fourier space in both space and time. Here, we show the nonlocal eddy diffusivity in physical space in time to make a key point about the shape of the kernel. If the eddy diffusivity were purely local, then the kernel would be a delta function centered at $\tau - t = 0$, so that by the sifting property of the delta function, the unclosed scalar flux would only be a function of $\tilde{c}(t)$ (or more specifically, the gradient of $\tilde{c}(t)$). However, the actual kernel shown for $k = 5$ in Figure 3 is not a delta function—it has a backward decay, implying that the unclosed term at a given time, $t$, depends not only on $\tilde{c}(t)$, but also on the history of $\tilde{c}$. In other words, for this wavenumber, one cannot assume that fluctuations are mixed very quickly relative to the temporal variation of the mean quantity: In order to accurately capture the scalar flux one now needs to know where it came from.

However, the kernel also decays to zero: One needs to consider the history of $\tilde{c}$ but only about one unit or so backwards in time for the wavenumber, $k = 5$. As $k$ increases the kernel width decreases—a larger wavenumber corresponds to smaller features, and thus more local behavior.
3 Approaches for modeling a nonlocal eddy diffusivity

In Section 2.2, we showed the eddy diffusivity for the homogeneous example problem is temporally nonlocal. While this eddy diffusivity is exact (in the sense that if one solves Equation (34) with the eddy diffusivity kernel, \( \hat{D}_k(\tau - t) \), one would recover the same mean scalar field as solving the governing equation and then averaging), one may want to approximate the nonlocal eddy diffusivity to reduce the computational cost of obtaining the eddy diffusivity and implementing a nonlocal integral.

Reducing the computational cost is partially addressed by inverse MFM, which has the capability of getting moments of the eddy diffusivity kernel using just one simulation per moment. The next sections address how to approximate a nonlocal eddy diffusivity using only these moments. The challenge lies in using this very limited information about the true eddy diffusivity kernel to reconstruct the approximate behavior of the full eddy diffusivity kernel. We now show several approaches for modeling with increasing sophistication and illustrate when these approaches are valid and why they often fail. The culminating result, using matched moment inverse (MMI) operators, is a systematic technique for capturing nonlocality accurately and cost-effectively.

3.1 The Boussinesq approximation: a purely local approach

We begin by revisiting the commonly used Boussinesq approximation [2], which uses an assumption of scale separation to draw upon an analogy to kinetic theory and approximates the eddy diffusivity as a purely local quantity. For the Fourier-transformed, homogeneous, dispersion problem in Section 2.2, the mean scalar transport equation in (34) is approximated as

\[
\frac{d\tilde{c}}{dt} + k^2 \hat{D}_0^k \tilde{c} = \bar{f}(t)
\]

where \( \hat{D}_0^k \) is the purely local eddy diffusivity. Since the velocity field is steady, \( \hat{D}_0^k \) is the same value at all times, i.e. the eddy diffusivity is a constant for a given wavenumber.

One can obtain the local eddy diffusivity, \( \hat{D}_0^k \), one of several ways: 1) Consider the exact nonlocal integral in (34): \( k^2 \int_{-\infty}^{t} \hat{D}_k(\tau - t)\tilde{c}(\tau) d\tau \). A local approximation implies that \( \tilde{c}(\tau) \approx \tilde{c}(t) \) and can be taken out of the integral. Therefore, \( \hat{D}_0^k = \int_{-\infty}^{t} \hat{D}_k(\tau - t) d\tau \). In other words, the eddy diffusivity found using the Boussinesq approximation is the area of the full eddy diffusivity kernel in Section 2.2 (more precisely, the local eddy diffusivity is a delta function kernel with the same area as the full kernel). We can use MFM to compute the full kernel, and then compute the area to obtain the equivalent Boussinesq eddy diffusivity. 2) Because \( \hat{D}_0^k \) is equal to the area of the kernel, i.e. the zeroth moment of the kernel, we can also use inverse MFM to get the zeroth moment directly without getting the full kernel. 3) We can analytically obtain \( \hat{D}_0^k \) for this problem using Taylor’s approach for dispersion by a parallel flow [6]. This approach uses the transport equation for the fluctuations, \( \tilde{c}' \), and applies the same length/time scale separation assumption as the Boussinesq approximation to find the leading-order term balance. The resulting model is the same as that of the Boussinesq approximation. Taylor’s approach for this problem is shown in detail in [1].
Figure 4: The local eddy diffusivity vs. wavenumber. The Boussinesq approximation is only valid for small wavenumber where $\hat{D}_k^0$ is constant. For large wavenumber, $\hat{D}_k^0$ scales as $k^{-1}$.

Figure 4 shows the local eddy diffusivity, $\hat{D}_k^0$, vs. the wavenumber, $k$. $\hat{D}_k^0$ is only constant for small wavenumbers and scales as $k^{-1}$ for large wavenumbers, i.e. the Boussinesq approximation is only valid for small wavenumber and breaks down for large wavenumber. This result is expected as the Boussinesq approximation is valid when the gradient of the mean varies slowly and smoothly which happens only for small wavenumber.

To test the model, the source function is specified as:

$$\tilde{f}(t) = \begin{cases} 
0 & \text{if } t < 1 \\
-1/4(t - 1)(t - 5) & \text{if } t \geq 1
\end{cases}$$  \hspace{1cm} (36)

as shown in Figure 2. The response, $\hat{c}(t)$, is then computed using Equation (35). For comparison, the same source is applied to the Fourier-transformed governing equation in (32), $\hat{c}(x_2, t)$ is computed and then averaged over $x_2$ for the DNS solution. The initial condition is $\hat{c}(t = 0) = 0$, and correspondingly, $\hat{\tilde{c}}(t = 0) = 0$.

Figure 5 shows the Boussinesq model and the DNS solution for an intermediate wavenumber, $k = 5$. In this regime, the Boussinesq approximation is not valid, and the model lags the DNS response. This source function and wavenumber were specifically chosen as an illustrative, challenging test case to improve on in the next sections. Note if a smaller wavenumber for which the Boussinesq approximation is valid had been chosen, the model would have done significantly better. Similarly, if a more slowly varying source function were chosen, such that the response also varied more slowly, the model would have also done better. The goal is to understand how to improve upon the Boussinesq model in a simplified setting before generalizing to more complicated problems.
3.2 Taylor series expansion: corrections to the Boussinesq approximation

In the previous section, we showed that the Boussinesq approximation is only valid in the limit of small wavenumber for this problem and does poorly for intermediate wavenumbers. One then might add corrections to the Boussinesq approximation by considering the following Taylor series expansion about $\tau = t$:

$$
\int_{-\infty}^{t} \hat{D}_k(\tau - t)\tilde{c}(\tau)d\tau = \int_{-\infty}^{t} \hat{D}_k(\tau - t)[\tilde{c}(t) + (\tau - t)\frac{d\tilde{c}}{dt}t + \frac{1}{2}(\tau - t)^2\frac{d^2\tilde{c}}{dt^2}t + \ldots]d\tau. \quad (37)
$$

In this Taylor series expansion, the nonlocal integral on the left-hand-side that depends on $\tilde{c}$ at all previous times, $\tau$, is expanded locally, such that the integral on the right-hand-side now only depends on $\tilde{c}$ and the derivatives of $\tilde{c}$ at the current time, $t$. Since, $\tilde{c}$ no longer depends on $\tau$, $\tilde{c}$ (and its derivatives) can now be taken out of the integral to obtain:

$$
\int_{-\infty}^{t} \hat{D}_k(\tau - t)\tilde{c}(\tau)d\tau = \hat{D}_k^0\tilde{c}(t) + \hat{D}_k^1\frac{d\tilde{c}}{dt}t + \hat{D}_k^2\frac{d^2\tilde{c}}{dt^2}t + \ldots \quad (38)
$$

where

$$
\hat{D}_k^0 = \int_{-\infty}^{t} \hat{D}_k(\tau - t)d\tau
$$
$$
\hat{D}_k^1 = \int_{-\infty}^{t} (\tau - t)\hat{D}_k(\tau - t)d\tau
$$
$$
\hat{D}_k^2 = \int_{-\infty}^{t} \frac{1}{2}(\tau - t)^2\hat{D}_k(\tau - t)d\tau
$$
$$
\vdots
$$

$\hat{D}_k^0$ is the zeroth moment and corresponds to the area of the kernel, $\hat{D}_k^1$ is the first moment and captures the asymmetry of the kernel, etc. Each moment carries successively more information about the shape of the
Figure 7: For $k = 5$: The Boussinesq model is given in Equation (35). “With $\hat{D}_k^1$ correction” corresponds to including $\hat{D}_k^1 d\tilde{c}/dt$ in the model. “With $\hat{D}_k^1$ and $\hat{D}_k^2$ correction” corresponds to solving Equation (39). Successive corrections actually make the Boussinesq model worse.

kernel, $\hat{D}_k(\tau - t)$. If one truncates the Taylor series expansion at the zeroth moment, letting $\int_{-\infty}^{t} \hat{D}_k(\tau - t)\tilde{c}(\tau)d\tau \approx \hat{D}_k^0 \tilde{c}(t)$, one recovers the Boussinesq approximation where $\hat{D}_k^0$ is the eddy diffusivity. Using the Taylor series expansion, one can add corrections to the Boussinesq approximation by including more terms from the expansion. If one includes up to the second moment, the model equation becomes:

$$
\frac{d\tilde{c}}{dt} + k^2 \left( \hat{D}_k^0 \tilde{c} + \hat{D}_k^1 \frac{d\tilde{c}}{dt} + \hat{D}_k^2 \frac{d^2\tilde{c}}{dt^2} \right) = \bar{f}(t).
$$

One can now test this model by applying the same source term, $\bar{f}(t)$, as in Equation (36). Since this is now a second-order ordinary differential equation, one needs two initial conditions: Assuming that before the start of the problem, $\tilde{c}(x_2, t)$ is zero for long enough such that $\tilde{c}(t)$ and all of its derivatives are zero, and at $t = 0$, the source term, $\bar{f}(t)$, is suddenly turned on, implies the initial condition should be $\tilde{c}(t = 0) = 0$ and $\frac{d\tilde{c}}{dt}(t = 0) = 0$.

This model is again expected to do very well in the limit of small wavenumber where one recovers the Boussinesq approximation. In this limit, the large scale features vary slowly in time; thus, the higher-order derivatives of $\tilde{c}$ are close to zero, and drop out of the Taylor series expansion in (38). Figure 7 shows what happens if one adds corrections for the intermediate wavenumber, $k = 5$. Surprisingly, the model actually gets worse—successive corrections cause the solution to blow up.

The Taylor series expansion in Equation (38) is a non-converging Taylor series. Convergence requires keeping infinite terms in the series for error cancellation. The non-converging Taylor series is also shown for a spatially nonlocal eddy diffusivity in [1], and has a previous analogue [7] to the Kramers-Moyal expansion that describes stochastic processes associated with Brownian dynamics.

To understand why the truncated Taylor series approach does not work, consider the shape of the modeled
kernel as corrections are added. The zeroth moment corresponds to a purely local kernel, i.e. a delta function
kernel. Higher-order terms correspond to the superposition of higher-order derivatives of the delta function.
Whereas, as shown in Figure 3 for \( k = 5 \), the actual kernel looks nothing like a delta function. The truncated Taylor series expansion can only add highly local corrections, rather than capture the nonlocal shape of the full kernel.

3.3 Matched Moment Inverses (MMI): capturing the shape of the nonlocal eddy diffusivity

In Section 3.2, we showed that correcting a purely local eddy diffusivity by including finite additional terms from the Taylor series expansion in (38) does not improve the model. The additional terms in the Taylor series expansion add corrections with the shape of higher-order derivatives of the delta function, i.e. additional terms add highly local corrections. Matched Moment Inverse (MMI) operators work by more closely approximating the nonlocal shape of the full kernel.

Consider the eddy diffusivity kernel for \( k = 5 \) in Figure 3 which resembles an exponential function. For now let us approximate it such:

\[
\int_{-\infty}^{t} \hat{D}_{k}^{t}(\tau-t)\hat{c}(\tau)d\tau \approx \int_{-\infty}^{t} \beta e^{\alpha(\tau-t)}\hat{c}(\tau)d\tau. \tag{40}
\]

This exponential has two parameters, \( \alpha \) and \( \beta \), that can be found by matching the zeroth and first moments of the eddy diffusivity kernel:

\[
\hat{D}_{k}^{0} = \int_{-\infty}^{t} \hat{D}_{k}(\tau-t)d\tau = \int_{-\infty}^{t} \beta e^{\alpha(\tau-t)}d\tau, \tag{41a}
\]

\[
\hat{D}_{k}^{1} = \int_{-\infty}^{t} (\tau-t)\hat{D}_{k}(\tau-t)d\tau = \int_{-\infty}^{t} (\tau-t)\beta e^{\alpha(\tau-t)}d\tau. \tag{41b}
\]

Analytically, this requires \( \alpha = -\hat{D}_{k}^{0}/\hat{D}_{k}^{1} \) and \( \beta = -\hat{D}_{k}^{0}\hat{D}_{k}^{0}/\hat{D}_{k}^{1} \). The approximate exponential kernel for \( k = 5 \) is shown in Figure 8 and closely matches the shape of the actual kernel. Note that obtaining \( \alpha \) and \( \beta \) does not require the full kernel, only the exact temporal moments of the kernel, \( \hat{D}_{k}^{0} \) and \( \hat{D}_{k}^{1} \).

![Figure 8: For \( k = 5 \): The eddy diffusivity kernel and the approximate exponential kernel matching the zeroth and first moments of the full kernel.](image)
After this step, the model equation is

$$\frac{d\tilde{c}}{dt} + k^2 \int_{-\infty}^{t} \beta e^{(\tau-t)} \tilde{c} \, d\tau = \tilde{f}(t).$$  \hspace{1cm} (42)$$

At this point, we have a formulation using only moments, and thus have avoided the cost of getting the full eddy diffusivity. But we still have not addressed the second computational cost concern: Implementation of the nonlocal integral is also expensive, since in this case, it requires keeping a time history of $\tilde{c}$ in memory. Let

$$\gamma = \int_{-\infty}^{t} \beta e^{(\tau-t)} ik\tilde{c} \, d\tau.$$  \hspace{1cm} (43)$$

Taking the time derivative of both sides and simplifying leads to

$$\frac{d\gamma}{dt} + \alpha \gamma = \beta ik\tilde{c}.$$  \hspace{1cm} (44)$$

The nonlocal integral in Equation (43) is an approximate model for $-\overline{u'_1\bar{c}'\prime}$ for one wavenumber and can be expressed by the ordinary differential equation in Equation (44). The full model is the following coupled system:

$$\frac{d\tilde{c}}{dt} + ik\overline{u'_1\bar{c}'\prime} = \tilde{f}(t)$$  \hspace{1cm} (45a)$$

$$\left[\frac{d}{dt} - \frac{D_k^0}{D_k^1}\right] (\overline{u'_1\bar{c}'\prime}) = -\overline{D_k^0 D_k^0} ik\tilde{c}. $$  \hspace{1cm} (45b)$$

Again, this model can be assessed using the same source function specified in Equation (36). The initial condition is $\tilde{c}(0) = 0$ and $\overline{u'_1\bar{c}'\prime}(0) = 0$, assuming there is enough time before the source term is applied such that the fluctuations smooth out to zero.

Because the model in Equations (45a) and (45b) exactly captures the true low order moments of the eddy diffusivity, the model is again expected to do well in the small wavenumber limit as the higher-order terms of the Taylor series expansion become negligible. Figure 9 shows that for the more challenging, intermediate wavenumber of $k = 5$, this model performs much better than the Boussinesq model.

The model in Equations (45a) and (45b) performs well because it closely approximates the shape of the nonlocal eddy diffusivity. We specifically introduced the derivation above to emphasize the importance of capturing the shape of kernel. We now present an alternative and more generalizable derivation of Equation (45b) that uses matched moment inverse (MMI) operators. Consider the model form:

$$\left[ a_1 \frac{d}{dt} + 1 \right] (-\overline{u'_1\bar{c}'\prime}) = a_0 ik\tilde{c},$$  \hspace{1cm} (46)$$

where $a_0$ and $a_1$ are unknown coefficients. Rearranging leads to

$$-\overline{u'_1\bar{c}'\prime} = \left[ 1 + a_1 \frac{d}{dt} \right]^{-1} a_0 ik\tilde{c}. $$  \hspace{1cm} (47)$$

Consider the Taylor series expansion of (47):

$$-\overline{u'_1\bar{c}'\prime} = \left[ 1 - a_1 \frac{d}{dt} + \ldots \right] a_0 ik\tilde{c},$$  \hspace{1cm} (48)$$
For $k = 5$: The model presented in Equations (45a) and (45b) (MMI model) which approximates the
kernel as an exponential closely matches the DNS solution. The Boussinesq model is shown for comparison.

and the Taylor series expansion of the nonlocal eddy diffusivity kernel:

\[-\bar{u}_1' \bar{c}' = \int_{-\infty}^{t} D_k(\tau - t)\bar{k}\bar{c}(\tau)d\tau = \left[ D^0_k + \frac{D^1_k}{D^0_k} \frac{d}{dt} \ldots \right] ik\bar{c} \]  

(49)

We obtain $a_0$ and $a_1$ by matching the zeroth and first temporal moments of the inverse operator in square
brackets in (48) with those of the exact nonlocal eddy diffusivity kernel in (49). Hence, the operator in (47)
is known as a *matched moment inverse operator*. This leads to $a_0 = \frac{D^0_k}{D^0_k}$, $a_1 = -\frac{D^1_k}{D^0_k}$, and

\[- \frac{D^1_k}{D^0_k} \frac{d}{dt} + 1 \left( -\bar{u}_1' \bar{c}' \right) = \frac{D^0_k}{D^0_k} ik\bar{c} \]  

(50)

which results in the original model in Equation (45b) after some rearrangement. Note that the truncated
Taylor series expansion in Section 3.2 fails because one needs to keep an infinite Taylor series for error
cancellation. By using MMI, we keep an infinite Taylor series and simply match the low-order moments with
those of the actual nonlocal eddy diffusivity.

### 3.4 MMI for modeling a spatiotemporally nonlocal eddy diffusivity

For the homogeneous example problem, we isolated a temporally nonlocal eddy diffusivity by Fourier trans-
morphing in the $x_1$-direction and averaging in the $x_2$-direction. Then, we introduced MMI for approximating
a temporally nonlocal eddy diffusivity and showed good agreement with the DNS. We are now ready to
revisit the full spatiotemporal problem shown in Figure 1 which considers the dispersion of a narrow band
of passive scalar.

Figure 10a shows the full spatiotemporally nonlocal eddy diffusivity. For details on obtaining the spatiotemporal
eddy diffusivity using inverse MFM, see Appendix A. The eddy diffusivity has a wide spread in
the $x_1$-direction and thus is highly nonlocal in space as well as in time.
Figure 10: (a) The exact spatiotemporally nonlocal eddy diffusivity, $D(x_1 - y_1, t - \tau)$, for the homogeneous problem. (b) The modeled eddy diffusivity using MMI.

In physical space, the MMI model equations are:

$$\frac{\partial \bar{c}}{\partial t} + \frac{\partial}{\partial x_1} u'_1 c' = 0 \quad (51a)$$

$$\left[ a_3 \frac{\partial}{\partial t} + \left( 1 + a_1 \frac{\partial}{\partial x_1} + a_2 \frac{\partial^2}{\partial x_1^2} \right) \right] (\bar{u}_1' c') = a_0 \frac{\partial \bar{c}}{\partial x_1} \quad (51b)$$

where $a_0, \ldots, a_3$ are unknown coefficients to be obtained by matching the low-order spatiotemporal moments with those of the nonlocal eddy diffusivity. For a homogeneous problem, these coefficients are constant. To obtain $a_0, \ldots, a_3$, rearrange Equation (51b),

$$- \bar{u}_1' c' = \left[ 1 + a_1 \frac{\partial}{\partial x_1} + a_2 \frac{\partial^2}{\partial x_1^2} + a_3 \frac{\partial}{\partial t} \right]^{-1} a_0 \frac{\partial \bar{c}}{\partial x_1} \quad (52)$$

and Taylor series expand the MMI,

$$- \bar{u}_1' c' = \left[ 1 - a_1 \frac{\partial}{\partial x_1} + a_2 \frac{\partial^2}{\partial x_1^2} + a_3 \frac{\partial}{\partial t} \left( a_1 \frac{\partial}{\partial x_1} \right) + \cdots - a_3 \frac{\partial}{\partial t} + \cdots \right] a_0 \frac{\partial \bar{c}}{\partial x_1} \quad (53)$$

Consider the nonlocal eddy diffusivity expression for the unclosed scalar flux:

$$- \bar{u}_1' c' = \int_{-\infty}^{t} \int_{-\infty}^{\infty} D(x_1 - y_1, t - \tau) \frac{\partial \bar{c}}{\partial x_1} \bigg|_{y_1, \tau} dy_1 d\tau \quad (54)$$

Taylor series expanding about $y_1 = x_1$ and $\tau = t$ leads to

$$- \bar{u}_1' c' = \left[ D^{0,0} + D^{1,0} \frac{\partial}{\partial x_1} + D^{2,0} \frac{\partial^2}{\partial x_1^2} + \cdots + D^{0,1} \frac{\partial}{\partial t} + \cdots \right] \frac{\partial \bar{c}}{\partial x_1} \quad (55)$$

where the superscript $n_s$ denotes the $n$th spatial moment and $m_t$ denotes the $m$th temporal moment, such
that

\[
D^{0,0_t} = \int_{-\infty}^{t} \int_{-\infty}^{\infty} D(x_1 - y_1, t - \tau) dy_1 d\tau \\
D^{1,0_t} = \int_{-\infty}^{t} \int_{-\infty}^{\infty} (y_1 - x_1) D(x_1 - y_1, t - \tau) dy_1 d\tau \\
D^{2,0_t} = \int_{-\infty}^{t} \int_{-\infty}^{\infty} \frac{1}{2} (y_1 - x_1)^2 D(x_1 - y_1, t - \tau) dy_1 d\tau \\
\vdots \\
D^{0,1_t} = \int_{-\infty}^{t} \int_{-\infty}^{\infty} (\tau - t) D(x_1 - y_1, t - \tau) dy_1 d\tau \\
\vdots
\]

There are also mixed moments, e.g. \(D^{1,1_t}\), not shown in the expansion.

The unknown coefficients, \(a_0 \ldots a_3\), in (53) can be obtained by matching them with the exact eddy diffusivity moments in Taylor series expansion in (55). This leads to \(a_0 = D^{0,0_t}\), \(a_1 = -D^{1,0_t}/D^{0,0_t}\), \(a_2 = -D^{2,0_t}/D^{0,0_t} + (D^{1,0_t}/D^{0,0_t})^2\), and \(a_3 = -D^{0,1_t}/D^{0,0_t}\).

The resulting MMI model equations for the homogeneous example problem are:

\[
\frac{\partial \bar{c}}{\partial t} + \frac{\partial}{\partial x_1} (u'_1 \bar{c}') = 0, \tag{56a}
\]

\[
\left[ \frac{\partial}{\partial t} + \left( 1 - \frac{1}{16} \frac{\partial^2}{\partial x_1^2} \right) \right] \left( -u'_1 \bar{c}' \right) = \frac{1}{2} \frac{\partial \bar{c}}{\partial x_1}. \tag{56b}
\]

In terms of shape, Equation (56b) approximates the kernel as an exponential in time, capturing up to the first moment of the exact nonlocal eddy diffusivity in time, and a double-sided exponential in space, capturing up to the second moment in space (the first moment is zero since the kernel is symmetric in \(x_1\)).

Figure 10b shows the shape of the approximate kernel, which reasonably resembles the shape of the actual kernel. Note that although like a second-moment closure model, there is an additional equation for the unclosed scalar flux, \(-u'_1 \bar{c}'\), the additional equation in (56b) is not a transport equation. This equation is instead for accurately approximating the shape of the true eddy diffusivity and cost-effectively capturing the effect of the nonlocal integral.

Consider the dispersion of a narrow band of passive scalar in the center of the domain, i.e. the initial condition \(c(t = 0) = \exp(-x_1^2/0.025)\). Figure 11 shows the evolution of the averaged field, \(\bar{c}(x_1, t)\). Compared with the DNS solution, the MMI model closely predicts the spread of the averaged field. Also shown for comparison is the leading-order Taylor model given by

\[
\frac{\partial \bar{c}}{\partial t} = \frac{1}{2} \frac{\partial^2 \bar{c}}{\partial x_1^2} \tag{57}
\]

and the higher-order Taylor model given by

\[
\frac{\partial}{\partial t} \left( \bar{c} + \frac{1}{2} \frac{\partial^2 \bar{c}}{\partial x_1^2} \right) = \frac{1}{2} \frac{\partial^2 \bar{c}}{\partial x_1^2} + \frac{1}{32} \frac{\partial^4 \bar{c}}{\partial x_1^4}. \tag{58}
\]
Figure 11: Model comparison of the averaged field, $\bar{c}(x_1,t)$, using the initial condition $c(t = 0) = \exp(-x_1^2/0.025)$. The MMI model closely captures the spread of the averaged field, whereas the leading-order Taylor and higher-order Taylor models overpredict the spread of the averaged field.

The leading-order Taylor model is the physical space analogue the Boussinesq model in Section 3.1, and the higher-order Taylor model is the physical space analogue of adding additional Taylor series correction terms in Section 3.2. The leading-order Taylor model causes the mean field to spread out too quickly, and the higher-order Taylor model, as noted before with adding additional terms to the truncated Taylor series, does even worse.

Figure 12 shows the model comparison at an early time, $t = 0.5$, and a later time, $t = 4$. The MMI model reasonably captures the early time solution, whereas the leading-order Taylor model and higher-order Taylor model do poorly. The MMI model excellently captures the late time solution, outperforming both the Taylor models. All three models are expected to do well at late times in the limit of large and slowly varying mean field, i.e. where the Boussinesq approximation becomes valid. However, in this case the MMI model does well even outside of this limit. Note also that the higher-order Taylor model actually produces a negative solution, whereas the MMI model does not have this issue.
3.5 Comparison with other nonlocal eddy diffusivity models

We now compare the MMI model in Section 3.4 with another nonlocal model presented in [1] for the same dispersion problem. [1] also find the full nonlocal eddy diffusivity but in Fourier space in both space and time. They then write down a pen and paper approximate eddy diffusivity operator fitted to match the limits of $k, \omega \to 0$ and $k, \omega \to \infty$ where $k$ is the wavenumber corresponding to the Fourier transform in $x_1$-direction and $\omega$ the frequency corresponding to the Fourier transform in time. Transforming back into physical space, the unclosed scalar flux is approximated as

$$- \overline{u_1'c}(x_1, t) = \left[ -\sqrt{\left( I + \frac{\partial}{\partial t}\right)^2 - \frac{\partial^2}{\partial x_1^2}} + \left( I + \frac{\partial}{\partial t}\right) \right] \overline{c}(x_1, t)$$

where $I$ is the identity operator. Note that this MFM-inspired, eddy diffusivity operator does not have the cost-saving advantages of using MMI. In order to obtain this form for the unclosed term, [1] have to first find the full eddy diffusivity which is a computationally expensive procedure. However, we show a comparison of the MMI model with this MFM-inspired model to address a more general modeling question: Is it more appropriate to match the limits of large and small $k$ and $\omega$ or the low-order moments of the nonlocal eddy diffusivity?

Figure 13 shows a comparison between the MMI model and the MFM-inspired model at early and late time. At early time, the MFM-inspired model performs better; whereas at late time, the MMI model performs better. Because the MFM-inspired model matches the limit of large $k$ and $\omega$, i.e. small and fast features, it performs better at early time where the solution is a very narrow feature that quickly disperses. The MMI model matches low-order moments and is thus only expected to do well for large and slowly varying features where the higher-order terms of the Taylor series expansion become negligible. For early time, how well the MMI model does depends on how well the high-order moments of the MMI model happen to match the true high-order moments, and we see that it does reasonably in this case. For late time, even though the
Early time comparison.

Late time comparison.

Figure 13: MMI model and MFM-inspired model comparison at early time, $t = 0.5$, and late time, $t = 4$.

Figure 14: (a) A spatially nonlocal eddy diffusivity. (b) The same eddy diffusivity shown in Fourier space.

The answer to the question of whether a model should match the limits of $k$ and $\omega$ or the low-order moments of the nonlocal eddy diffusivity is that it depends. If there is a singularity or very sharp feature in the solution, then a model matching the limits of $k$ and $\omega$ may be more appropriate. Otherwise, if the solution is reasonably smooth (as is true for many practical applications), then a model matching the low-order moments is more appropriate. Figure 14 shows an example spatially nonlocal eddy diffusivity kernel in both physical space and Fourier space. The shaded area in blue under the eddy diffusivity in physical space, $D^0$, corresponds to $\hat{D}(0)$ in Fourier space. The first spatial moment of eddy diffusivity, $D^1$, corresponds to the first derivative of the kernel in Fourier space, $\hat{D}'(0)$, and so forth. Whereas, the shaded area in red representing high wavenumber in Fourier space corresponds to the peak in physical space at $D(0)$. Matching low-order moments better captures the overall shape of the nonlocal eddy diffusivity, whereas matching the limits of $k$ and $\omega$ captures the high and low wavelength/frequency features of the eddy diffusivity.

There exist other nonlocal models as well. Since there has been a lot of recent interest surrounding fractional-order operators, a comparison with a simple fractional-order Laplacian is shown in Appendix B.
4 Nonlocal eddy diffusivities in inhomogeneous flows

We now generalize the MMI model for inhomogeneous flows. In inhomogeneous flows, the moments of the eddy diffusivity are functions of space, and correspondingly the coefficients of the MMI model will also be functions of space. In this case, the MMI coefficients cannot analytically be matched with the eddy diffusivity moments since an infinite number of higher-order derivatives of the unknown coefficients appear in the Taylor series expansion of the MMI operator. We present a modified procedure for determining the MMI coefficients in order to match the low-order moments of the eddy diffusivity. We begin with an inhomogeneous example with periodic boundary conditions, and then discuss wall-bounded flows and the challenges of determining the MMI coefficients in the near-wall region.

4.1 Inhomogeneous problem with periodic boundary conditions

Consider a two-dimensional domain corresponding to the cross-section of a channel with periodic boundary conditions at the left and right walls at \( x_1 = \pm \pi \), and a no flux condition, \( \partial c / \partial x_2 = 0 \), at the top and bottom walls at \( x_2 = 0, 2\pi \). The flow consists of two vortices given by the velocity field:

\[
\begin{align*}
 u_1 &= \frac{1}{2}[2 + \cos(x_1)] \cos(x_2), \\
 u_2 &= \frac{1}{2} \sin(x_1) \sin(x_2).
\end{align*}
\]  

Streamlines of the velocity field are shown in Figure 15a. The steady, governing equation is

\[
\frac{\partial}{\partial x_1} (u_1 c) + \frac{\partial}{\partial x_2} (u_2 c) = \epsilon^2 \frac{\partial^2 c}{\partial x_1^2} + \frac{\partial^2 c}{\partial x_2^2} + f
\]  

where \( c(x_1, x_2) \) is a passive scalar, and \( f(x_1, x_2) \) is an external source function. \( \epsilon^2 \) results from directional nondimensionalization as in Section 2.1. For this example problem, we consider \( \epsilon^2 = 0.05 \) and \( f \) to be an oscillatory source function given by \( f = \cos(x_1) \).

Figure 15b shows contours of \( c(x_1, x_2) \) from DNS. The problem is discretized using second-order central difference on a uniform staggered mesh with \( N_1 = 200 \) grid points in \( x_1 \) and \( N_2 = 50 \) grid points in \( x_2 \).
to the boundary conditions of the problem, \(c(x_1, x_2)\) can arbitrarily be shifted by a constant. Hence, there is an additional constraint such that at the first point in \(x_1\) the average of \(c(x_1, x_2)\) over \(x_2\) is zero.

As in Section 2.1, averaging is defined in the \(x_2\)-direction as

\[
\bar{c}(x_1) = \frac{1}{L_2} \int_{0}^{L_2} c(x_1, x_2) \, dx_2
\]

where \(L_2 = 2\pi\). The corresponding mean scalar transport equation for this problem is

\[
\frac{d}{dx_1} \bar{u}' \bar{c} = \bar{c} \frac{d^2 \bar{c}}{dx_1^2} + \bar{f}.
\]

### 4.2 MMI for inhomogeneous flows

For an inhomogeneous problem, recall that the unclosed term can be written exactly as

\[
- \bar{u}' \bar{c}(x_1) = \int_{y_1} D(x_1, y_1) \frac{d\bar{c}}{dx_1}|_{y_1} \, dy_1
\]

where \(D(x_1, y_1)\) is a spatially nonlocal eddy diffusivity. Since the problem is inhomogeneous, the eddy diffusivity is now a function of \(x_1\). Correspondingly, each spatial moment of the eddy diffusivity, \(D^0(x_1), D^1(x_1), \) etc., is now also a function of \(x_1\) and can be computed using inverse MFM. The periodic boundary conditions may be incompatible with the required \(\bar{c}(x_1)\) for inverse MFM, e.g. \(\bar{c} = x_1\). Appendix C provides a remedy for periodic problems.

The steady MMI model for the unclosed scalar flux is

\[
\left[1 + a_1(x_1) \frac{d}{dx_1} + a_2(x_1) \frac{d^2}{dx_1^2}\right] (-\bar{u}' \bar{c}) = a_0(x_1) \frac{d\bar{c}}{dx_1}
\]

where the coefficients, \(a_0, a_1,\) and \(a_2\), are now also functions of \(x_1\) and yet to be determined. The MMI coefficients can be found by matching the low-order moments of the eddy diffusivity numerically.

Consider the local Taylor series expansion of the eddy diffusivity:

\[
- \bar{u}' \bar{c}(x_1) = \left[D^0(x_1) + D^1(x_1) \frac{d}{dx_1} + D^2(x_1) \frac{d^2}{dx_1^2} + \cdots\right] \frac{d\bar{c}}{dx_1}.
\]

To obtain the low-order moments of the eddy diffusivity using inverse MFM, the forcing is applied such that \(\bar{c} = x_1, \bar{c} = x_1^2/2,\) etc. Substituting these \(\bar{c}(x_1)\) into Equation (66) and post-processing the corresponding \(-\bar{u}' \bar{c}|_{\bar{c}}\) leads to:

\[
- \bar{u}' \bar{c}|_{\bar{c}=x_1} = D^0(x_1),
\]

\[
- \bar{u}' \bar{c}|_{\bar{c}=x_1^2/2} = x_1 D^0(x_1) + D^1(x_1),
\]

\[
- \bar{u}' \bar{c}|_{\bar{c}=x_1^3/6} = \frac{x_1}{2} D^0(x_1) + x_1 D^1(x_1) + D^2(x_1).
\]

If \(-\bar{u}' \bar{c}|_{\bar{c}}\) are directly available from inverse MFM, then one should use them directly. Otherwise, if only the moments are available, one should form \(-\bar{u}' \bar{c}|_{\bar{c}}\) using the expressions above in Equations (67a)-(67c). \(-\bar{u}' \bar{c}|_{\bar{c}}\) contains exact information about the low-order moments of the true eddy diffusivity that one can
now incorporate into the MMI model in Equation (65). One can form three equations for $a_0(x_1)$, $a_1(x_1)$, and $a_2(x_1)$ by substituting $c = x_1$, $\bar{c} = x_1^2/2$, and $\bar{c} = x_1^3/6$ and the corresponding $-\bar{u}' c'$ from Equations (67a)-(67c) into Equation (65):

\begin{align}
-\bar{u}' c'|_{\bar{c}=x_1} + a_1 \frac{d}{dx_1}(-\bar{u}' c'|_{\bar{c}=x_1}) + a_2 \frac{d^2}{dx_1^2}(-\bar{u}' c'|_{\bar{c}=x_1}) &= a_0, \\
-\bar{u}' c'|_{\bar{c}=x_1^2/2} + a_1 \frac{d}{dx_1}(-\bar{u}' c'|_{\bar{c}=x_1^2/2}) + a_2 \frac{d^2}{dx_1^2}(-\bar{u}' c'|_{\bar{c}=x_1^2/2}) &= a_0 x_1, \\
-\bar{u}' c'|_{\bar{c}=x_1^3/6} + a_1 \frac{d}{dx_1}(-\bar{u}' c'|_{\bar{c}=x_1^3/6}) + a_2 \frac{d^2}{dx_1^2}(-\bar{u}' c'|_{\bar{c}=x_1^3/6}) &= a_0 x_1^2/2.
\end{align}

This linear system of equations for $a_0$, $a_1$, and $a_2$ is solved pointwise to obtain the MMI coefficients at each $x_1$ location. Figure 16a shows the MMI coefficients for the inhomogeneous problem with periodic boundary conditions described in Section 4.1.

To understand the role of each of the MMI coefficients, assume that $a_0$, $a_1$, and $a_2$ are smooth and can be approximated locally as a constant around a given $x_1$ location. To obtain the kernel at that given $x_1$ location, let $dc/dx_1 = \delta(x_1)$ and solve for $-\bar{u}' c'$ as for obtaining the full kernel for the homogeneous problem in Appendix A. Consider $a_0 > 0$ and $a_2 < 0$ as with the coefficients shown in Figure 16a and ignoring $a_1$ momentarily, the Green’s function solution to Equation (65) is a symmetric double-sided exponential whose growth/decay constant is $\pm 1/\sqrt{|a_2|}$, i.e. $a_2$ controls the width of the kernel, while $a_0$ controls the height. $a_1$ adds asymmetry to the shape of the kernel with $a_1 d/dx_1$ acting as an advection-like term.

Figure 16b shows the exact eddy diffusivity obtained using linear algebra-based MFM and the approximate eddy diffusivity from the MMI model at various $x_1$ locations for the inhomogeneous problem with periodic boundary conditions. Details for obtaining the exact eddy diffusivity for periodic problems are given in Appendix C. The MMI model closely captures the double-sided exponential shape of the exact eddy diffusivity including the slight asymmetry at some $x_1$ locations.
Figure 17 shows a comparison between the MMI model and DNS solution for the inhomogeneous problem with periodic boundary conditions. The DNS solution corresponds to averaging the full solution in Figure 15b over the $x_2$-direction. The Boussinesq model given by

$$-\frac{d}{dx_1} \left( D^0(x_1) \frac{dc}{dx_1} \right) = \epsilon^2 \frac{d^2 \bar{c}}{dx_1^2} + \bar{f}$$

is also shown for comparison. The Boussinesq model greatly underpredicts the solution while the MMI model solution is almost indistinguishable from the DNS solution.

However, the MMI model achieves this fully accurate solution at a fraction of the cost of DNS. The MMI model solution requires only solving a one-dimensional system by inverting a $N_1 \times N_1$ matrix. On the other hand, the DNS solution requires solving the full two-dimensional system by inverting a $(N_1 \times N_2) \times (N_1 \times N_2)$ matrix. There is also some cost associated with the obtaining the low-order moments of the eddy diffusivity used in the MMI model. Obtaining the true eddy diffusivity using brute force MFM would have required $N_1$ DNS simulations. Using linear algebra-MFM, as is done for this problem, requires inverting a $(N_1 \times N_2) \times (N_1 \times N_2)$ matrix; this method works for small problems such as the current example problem, but is impractical for most applications. Obtaining the moments directly using inverse MFM (and bypassing obtaining the full eddy diffusivity) requires just three DNS simulations, one for each low-order moment used in the MMI model. While this is more expensive than running a single DNS for this problem, the MMI model is expected to be accurate for a wide variety of forcing scenarios for $f$ due to the closeness of the approximate eddy diffusivity kernel with the true eddy diffusivity kernel.

4.3 Wall-bounded inhomogeneous flows

As an example application of the MMI model to wall-bounded inhomogeneous flows, consider the same two-dimensional channel geometry as in Section 4.1, but now replace the periodic boundary conditions with solid walls and Dirichlet boundary conditions $c(x_1 = \pm \pi) = 0$. To satisfy the no-slip and no-penetration
Figure 18: (a) Streamlines of the velocity field in Equation (70). (b) Contour plot of $c(x_1, x_2)$ from DNS.

Figure 19: (a) MMI coefficients for Equation (65) for the wall-bounded inhomogeneous problem. (b) The exact eddy diffusivity and eddy diffusivity from the MMI model shown for various $x_1$ approaching the wall.

conditions at the solid wall, the velocity field is modified to be:

$$u_1 = [1 + \cos(x_1)] \cos(x_2), u_2 = \sin(x_1) \sin(x_2).$$  \hspace{1cm} (70)

Streamlines of the velocity field are shown in Figure 18a. The governing equation is given by Equation (61) with $\epsilon^2 = 0.05$ as before. The source function, $f$, is specified to be a constant, $f = 1$. Contours of $c(x_1, x_2)$ from DNS with grid resolution $N_1 = 200$ and $N_2 = 50$ are shown in Figure 18b. Averaging is defined over $x_2$ by Equation (62), and the corresponding mean scalar equation is given by Equation (63) as before.

The steady MMI model is given in Equation (65), and the coefficients are found via the procedure described in Section 4.2. Figure 19a shows the MMI coefficients for the wall-bounded inhomogeneous flow. The coefficients are well-behaved in the center of the domain; however, near the wall, there is a sharp spike in the MMI coefficients at $x_1 \approx \pm 2.5$.

To gain an understanding of why this singularity occurs, Figure 19b shows the exact eddy diffusivity ob-
Figure 20: Model comparison for the inhomogeneous problem with periodic boundary conditions. The MMI model is almost indistinguishable from the DNS solution.

tained using linear algebra-based MFM at various \( x_1 \) locations approaching the wall. While the approximate eddy diffusivity from the MMI model closely follows the exact eddy diffusivity, both the eddy diffusivities deviate from a double-sided exponential shape, gradually becoming smoother and smaller in magnitude near the wall as the flow also diminishes.

Reexamining the Green’s functions solutions to the MMI model in Equation (65), and assuming that the coefficients are smooth, the general kernel solutions are exponentials with decay/growth constants \((-a_1 \pm \sqrt{a_1^2 - 4a_2})/2a_2\) that join at the location of the delta function forcing, \( x_1 \). However, due to the presence of the wall and the no-slip/no-penetration boundary conditions, this kernel solution must also go zero at the walls. In the center of the domain, the decay/growth constants are real with one positive and one negative corresponding to a double-sided exponential kernel. At the wall, the decay/growth constants are imaginary corresponding to a smooth rounded kernel. In the transition region between the center of the domain and the wall, the kernel still has a sharp peak but also must rapidly go to zero at the wall: the decay/growth constants are actually both positive corresponding to two exponentially growing solutions that cancel each other out at the wall to satisfy the zero boundary condition. The transition in kernel behavior due to the presence of the wall causes the singularity seen in the MMI coefficients. It is an error with our model form.

However, despite the ill-behaved coefficients, the resulting \( \bar{c}(x_1) \) from the MMI model is still very accurate, greatly outperforming the Boussinesq model given in Equation (69), as shown in Figure 20. Near the wall, viscous effects dominate, and the eddy diffusivity model is unimportant.

This leads to a coefficient regularization technique to remedy the singularity in the MMI coefficients in Figure 19a. Because the model is unimportant near the wall, a small parameter \( \varepsilon \) is added for determining the MMI coefficients:

\[
\left[ 1 + a_1(x_1) \frac{d}{dx_1} + a_2(x_1) \frac{d^2}{dx_1^2} \right] \left( -u'_1 \bar{c}' + \varepsilon \frac{d\bar{c}}{dx_1} \right) = a_0(x_1) \frac{d\bar{c}}{dx_1}.
\]

(71)

As \(-u'_1 \bar{c}'\) goes to zero near the wall, the added \( \varepsilon d\bar{c}/dx_1 \) term ensures that the MMI coefficients will still
be well-behaved. In terms of kernel shape, $\varepsilon \bar{c}/dx_1$ is an added delta function that keeps the kernel from diminishing. To ensure that the final MMI model perfectly matches the zeroth moment, i.e. case when $\bar{c} = x$, $\varepsilon$ is subtracted from $a_0(x)$ in the final model:

$$
1 + a_1(x_1) \frac{d}{dx_1} + a_2(x_1) \frac{d^2}{dx_1^2} \left(-\bar{u}'c'\right) = (a_0(x_1) - \varepsilon) \frac{d\bar{c}}{dx_1}.
$$

(72)

The presence of $\varepsilon$ will effect the higher order moments; for example substituting $\bar{c} = x^2/2$ into Equation (72) results in an extra $\varepsilon(x_1 + a_1)$ compared with Equation (68b). However, as along as $\varepsilon$ is small, this error in the higher moments is also small.

Figure 21a shows the MMI coefficients for the wall-bounded inhomogeneous problem with the coefficient regularization technique. $\varepsilon$ is chosen to be $0.1\epsilon^2$ where $\epsilon^2$ is the nondimensionalized diffusivity in the $x_1$-direction. With the regularization technique the coefficients are now well-behaved; however, this technique is not yet systematic with regards to choice of $\varepsilon$.

Figure 21b shows a comparison between the MMI model with coefficient regularization in Equation (72) and the DNS solution. The MMI model with coefficient regularization performs even slightly better the original MMI model in Equation (65) although this depends strongly on the choice of $\varepsilon$. While the coefficient regularization technique performs well for this wall-bounded inhomogeneous problem, this does not address the original issue with the model form error. The MMI model form in Equation (65) admits a variety of exponential kernel shapes, but there are some shapes it cannot capture, and the model form may need to be modified. Alternative formulations for the MMI are shown in Appendix D but this is still an area of ongoing investigation.
5 Conclusion

A nonlocal eddy diffusivity can greatly improve modeling of mean scalar transport when the Boussinesq approximation is invalid. However, obtaining and implementing the full nonlocal eddy diffusivity can often be too computationally expensive for practical applications, and thus we introduce matched moment inverse (MMI) operators to approximate the nonlocal eddy diffusivity. These operators can accurately predict mean scalar transport by capturing the shape of the nonlocal eddy diffusivity using only a few low-order moments. The resulting model is in the form of a differential equation rather than a computationally- or memory-intensive nonlocal integral. Moreover, we show that MMI are expected to perform well as long the mean scalar field is reasonably smooth; for fields with sharp features, one may want to consider other operators that match the large and small wavenumber limits instead.

In this work, we demonstrate the application of MMI to homogeneous and inhomogeneous example problems. We discuss challenges in inhomogeneous wall-bounded flows where the scalar flux goes to zero near the wall, and show a coefficient regularization technique although this is not yet systematic. Future work will show MMI for modeling scalar transport in fully turbulent flows and extension of MMI for modeling momentum transport, i.e. RANS modeling and active scalar transport.

6 Acknowledgements

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A Obtaining the spatiotemporal eddy diffusivity for the homogeneous model problem

For the homogeneous model problem in Section 2.1 the unclosed scalar flux can be written as

\[-\overline{u_1'}c'(x_1, t) = \int_{-\infty}^{t} \int_{-\infty}^{\infty} D(x_1 - y_1, t - \tau) \frac{\partial \bar{c}}{\partial x_1} \big|_{y_1, \tau} dy_1 d\tau \] (73)

where \(\overline{()}\) denotes averaging in the \(x_2\)-direction, and \(D(x_1 - y_1, t - \tau)\) is the spatiotemporal eddy diffusivity. Using inverse MFM and prescribing \(\partial \bar{c}/\partial x_1\) as a delta function in both space and time:

\[-\overline{u_1'}c'(x_1, t) = \int_{-\infty}^{t} \int_{-\infty}^{\infty} D(x_1 - y_1, t - \tau) \delta(y_1, \tau) dy_1 d\tau, \] (74)

then by the sifting property of the delta function:

\[-\overline{u_1'}c'(x_1, t) = D(x_1, t). \] (75)

The spatiotemporal eddy diffusivity can be obtained by postprocessing \(-\overline{u_1'}c'(x_1, t)\).
B Comparison with a fractional-order operator

Several recent works [8][9][10] examine using fractional-order operators for nonlocal models. A simple model with a fractional-order Laplacian for the homogeneous problem in Section 2.1 is:

\[
\frac{\partial \tilde{c}}{\partial t} = \frac{1}{2} \left( \frac{\partial^2}{\partial x_1^2} \right)^{\alpha/2} \tilde{c}
\]

where \(0 < \alpha < 2\), and the coefficient in front of the fractional-order Laplacian is chosen such that when \(\alpha = 2\), the model reduces to the leading-order Taylor model (Boussinesq model) in Equation (57). Equation (76) can be solved by Fourier transforming in \(x_1\):

\[
\frac{\partial \hat{\tilde{c}}}{\partial t} = \frac{1}{2} \left( -\left( k^2 \right)^{\alpha/2} \right) \hat{\tilde{c}}
\]

where \(k\) is the corresponding wavenumber in \(x_1\), and time-advancing in Fourier space.

To obtain the nonlocal eddy diffusivity, recall that the right-hand-side of Equation (77) is a model for the derivative of the unclosed scalar flux:

\[
\hat{ik}(-u'_i c') = \frac{1}{2} \left( -\left( k^2 \right)^{\alpha/2} \right) \hat{\tilde{c}}
\]

Rearranging,

\[
- u'_i c' = \frac{1}{2} \left( k^2 \right)^{\alpha/2-1} (ik\hat{\tilde{c}})
\]

where the gradient of \(\tilde{c}\) in Fourier space is \(ik\hat{\tilde{c}}\), and correspondingly the nonlocal eddy diffusivity in Fourier space is:

\[
\hat{D}(k) = \frac{1}{2} \left( k^2 \right)^{\alpha/2-1}.
\]

Figure 22 shows the nonlocal eddy diffusivity in Fourier space for several \(\alpha\) in comparison with the exact nonlocal eddy diffusivity obtained using MFM.

![Figure 22](image)

Figure 22: Nonlocal eddy diffusivity of the simple fractional-order model shown in Fourier space for various choices of \(\alpha\) compared with the exact nonlocal eddy diffusivity obtained from MFM.
Figure 23: Fractional-order model comparison for the homogeneous problem in Section 2.1 at early time, \( t = 0.5 \), and late time, \( t = 4 \).

Figure 23 shows an early time (\( t = 0.5 \)) and late time (\( t = 4 \)) comparison of the MMI model with the fractional-order model for several choices of \( \alpha \). For early time, the simple fractional-order model with a constant \( \alpha \) does not capture the double-peaked feature in the DNS solution of \( \bar{c}(x_1) \) whereas the MMI model does. For late time, the fractional-order model overpredicts the spread of \( \bar{c}(x_1) \). As shown in Figure 22, the nonlocal eddy diffusivity of the fractional-order model shown is larger than the exact nonlocal eddy diffusivity in both the limits of large \( k \) and small \( k \). Thus, the fractional-order model solution diffuses too quickly for both early time where narrow (large wavenumber) features are present and late time where very smooth (small wavenumber) features are present.

This result may be remedied by a more sophisticated fractional-order model with a variable \( \alpha \) but is not considered here.

C  MFM for periodic problems

C.1  Inverse MFM for periodic problems

The \( \bar{c} \) required for inverse MFM, e.g. \( \bar{c} = x_1 \) for the zeroth moment, may be incompatible with the periodic boundary conditions of the problem as for the inhomogeneous model problem in Section 4.1. The remedy is to decompose \( \bar{c}(x_1, x_2) = \bar{c}(x_1) + c'(x_1, x_2) \) where \( \bar{c}(x_1) \) may be nonperiodic but \( c'(x_1, x_2) \) is periodic.

Moreover, following a similar line of reasoning as for the input-output relationship between \(-u_1 \bar{c}'(x_1)\) and \( \bar{c}(x_1), c'(x_1, x_2) \) can be Taylor series expanded as

\[
c'(x_1, x_2) = g^0(x_1, x_2) \frac{\partial \bar{c}}{\partial x_1} + g^1(x_1, x_2) \frac{\partial^2 \bar{c}}{\partial x_1^2} + g^2(x_1, x_2) \frac{\partial^3 \bar{c}}{\partial x_1^3} + \ldots \tag{81}
\]

where \( g^0(x_1, x_2), g^1(x_1, x_2), \) etc. are to be determined. Once determined, to get to the desired moments,
According to Equation (81), multiply Equation by \(-u_1'(x_1, x_2)\) and average over \(x_2\),

\[
-\bar{u}'_1\bar{c}'(x_1) = -\bar{u}_1'g^0(x_1)\frac{\partial \bar{c}}{\partial x_1} - \bar{u}_1'g'(x_1)\frac{\partial^2 \bar{c}}{\partial x_1^2} - \bar{u}_1'g''(x_1)\frac{\partial^3 \bar{c}}{\partial x_1^3} - \ldots,
\]

which leads to \(D^0(x_1) = -\bar{u}_1'g^0(x_1), D^1(x_1) = -\bar{u}_1'g'(x_1), D^2(x_1) = -\bar{u}_1'g''(x_1), \ldots\).

For example, to obtain the zeroth moment for the inhomogeneous model problem in Section 4.1, substitute \(\bar{c} = x_1\) into Equation (81) to get \(\bar{c}'(x_1, x_2) = g^0(x_1, x_2)\), and substitute \(c(x_1, x_2) = x_1 + g^0(x_1, x_2)\) into the governing equation for the inhomogeneous model problem (Equation (81)):

\[
u_1 + u_1 \frac{\partial g^0}{\partial x_1} + u_2 \frac{\partial g^0}{\partial x_2} = \epsilon^2 \frac{\partial^2 g^0}{\partial x_1^2} + \frac{\partial^2 g^0}{\partial x_2^2} + s(x_1)
\]

where \(s(x_1)\) is the MFM forcing required to enforce \(\bar{c}'(x_1) = g^0(x_1) = 0\). One can then solve for \(g^0(x_1, x_2)\), and obtain the zeroth moment by forming \(D^0(x_1) = -\bar{u}_1'g^0(x_1)\). Using Equation (83) for \(g^0(x_1, x_2)\) rather than the full governing equation for \(c(x_1, x_2)\) bypasses the issue of needing to explicitly enforce \(\bar{c}\) with periodic boundary conditions.

Similarly, to obtain the first moment, substitute \(c(x_1, x_2) = x_1^2/2 + g^0(x_1, x_2)x_1 + g^1(x_1, x_2)\) into the governing equation for the inhomogeneous model problem, and subtract \(x_1\) times Equation (83):

\[
u_1 g^0 + u_1 \frac{\partial g^1}{\partial x_1} + u_2 \frac{\partial g^1}{\partial x_2} = \epsilon^2 \frac{\partial^2 g^1}{\partial x_1^2} + \epsilon^2 \frac{\partial^2 g^1}{\partial x_2^2} + \frac{\partial^2 g^1}{\partial x_1^2} + s(x_1)
\]

where \(s(x_1)\) is the forcing required to enforce \(\bar{c}'(x_1) = 0\). One can then solve for \(g^1(x_1, x_2)\), and obtain the first moment by forming \(D^1(x_1) = -\bar{u}_1'g^1(x_1)\). Note Equation (84) relies on having \(g^0(x_1, x_2)\) from Equation (83).

One can obtain the second moment from solving the equation for \(g^2(x_1, x_2)\), and so forth. As with inverse MFM where obtaining the second moment relies on having the zeroth and first moments, the equation for \(g^2(x_1, x_2)\) relies on having \(g^0(x_1, x_2)\) and \(g^1(x_1, x_2)\). However, this decomposition does not raise the cost of obtaining the moments, still requiring one simulation per moment.

### C.2 Linear algebra-based MFM for periodic problems

This section provides details for obtaining the nonlocal eddy diffusivity for the inhomogeneous problem with periodic boundary conditions in Section 4.1. Using linear algebra-based MFM, the matrix, \([\tilde{L}]\), can be obtained via Equation (19) and can be further written as

\[
[\tilde{L}] = -[d/dx_1]|([D] + \epsilon^2[I])|d/dx_1|,
\]

where \([D]\) is the desired nonlocal eddy diffusivity matrix and \([I]\) is the identity matrix. Due to the periodic boundary conditions, \([d/dx_1]\) is uninvertible and thus one cannot simply solve for \([D]\) using Equation (85).

Rather, the decomposition in Section C.1 can be applied, and let

\[
[c'] = [g]|d\bar{c}/dx_1|
\]
which is the non Taylor-series expanded form of Equation (81). Then,

\[ -u_1'c' = -[P][u_1'][c'] = -[P][u_1'][g][d\bar{c}/dx_1] = [D][d\bar{c}/dx_1], \tag{87} \]

where \([P]\) is the projection (i.e. averaging) matrix, and thus the nonlocal eddy diffusivity matrix is

\[ [D] = -[P][u_1'][g]. \tag{88} \]

To obtain \([g]\), substitute \(c = \bar{c} + c'\) into the governing equation for the inhomogeneous model problem (Equation (61)) with the MFM forcing, \(s(x_1)\):

\[ u_1 \frac{\partial c'}{\partial x_1} + u_2 \frac{\partial c'}{\partial x_2} - \epsilon^2 \frac{\partial^2 c'}{\partial x_1^2} = -u_1 \frac{\partial \bar{c}}{\partial x_1} + c' \frac{\partial^2 \bar{c}}{\partial x_1^2} + s(x_1). \tag{89} \]

where the role of \(s(x_1)\) is to enforce the condition \(\bar{c}(x_1) = 0\). In matrix operator form,

\[ [\mathcal{L}][c'] = [\tilde{\mathcal{L}}_1][\partial \bar{c}/\partial x_1] + [s] \tag{90} \]

where \([\tilde{\mathcal{L}}_1] = -[u_1] + \epsilon^2[\partial/\partial x_1]\). Substituting \([s] = [E][\bar{s}]\) into Equation (90), and forming a matrix system to simultaneously solve for \([c']\) and \([\bar{s}]\) such that \([P][c'] = 0\) leads to:

\[ \begin{pmatrix} \mathcal{L} & -E \\ P & 0 \end{pmatrix} \begin{pmatrix} c' \\ \bar{s} \end{pmatrix} = \begin{pmatrix} \tilde{\mathcal{L}}_1 \\ 0 \end{pmatrix} \begin{pmatrix} \partial \bar{c} \\ \partial x_1 \end{pmatrix}. \tag{91} \]

Rearranging,

\[ \begin{pmatrix} c' \\ \bar{s} \end{pmatrix} = \begin{pmatrix} \mathcal{L} & -E \\ P & 0 \end{pmatrix}^{-1} \begin{pmatrix} \tilde{\mathcal{L}}_1 \\ 0 \end{pmatrix} \begin{pmatrix} \partial \bar{c} \\ \partial x_1 \end{pmatrix} = \begin{pmatrix} g \\ \bar{s} \end{pmatrix} \begin{pmatrix} \partial \bar{c} \\ \partial x_1 \end{pmatrix}, \tag{92} \]

allows one to obtain \([g]\).

## D An alternative MMI formulation

For the inhomogeneous problems in Section 4, an alternative to the steady MMI model in Equation (65) is

\[ \begin{pmatrix} 1 + a_1(x_1) \frac{d}{dx_1} + a_2(x_1) \frac{d^2}{dx_1^2} \end{pmatrix} \begin{pmatrix} -u_1'c' \\ \frac{a_0(x_1)}{a_0(x_1)} \end{pmatrix} = \frac{d\bar{c}}{dx_1}. \tag{93} \]

By choosing \(a_0(x_1) = D^0(x_1)\), the MMI formulation in Equation (93) matches the zeroth moment of the exact nonlocal eddy diffusivity (i.e. for \(\bar{c} = x_1\), the model recovers \(-u_1'c'|_{\bar{c}=x_1} = D^0\)). The remaining coefficients, \(a_1(x_1)\) and \(a_2(x_1)\), can be determined by matching the other low-order moments via specifying \(\bar{c} = x_1^2/2\) and \(\bar{c} = x_1^3/6\) as done in Section 4.2. This alternative formulation has one fewer coefficient to solve for than the original MMI formulation, but may have singularity issues if the zeroth moment goes to zero, for example near a wall.

Figure 24(a) shows the coefficients of the alternative MMI formulation for the wall-bounded inhomogeneous model problem in Section 4.3, and Figure 24(b) shows the resulting solution, \(\bar{c}(x_1)\), of the alternative MMI
formulation closely matching the DNS solution. Although the solution of the alternative MMI formulation is very similar to that of the original MMI formulation in Figure 20, the coefficients show some differences particularly in $a_1(x_1)$ and the location of singularities. At the wall, both $u_1'c'(x_1)$ and $D^0(x_1)$ go to zero, leading to a zero divided by zero and numerical issues in determining the coefficients at the wall. However, at the wall, viscous effects also dominate and the eddy diffusivity model is unimportant leading to a well-behaved solution.

To remedy the issues at the wall, a coefficient regularization technique similar to the one shown Section 4.3 is used. A small parameter $\varepsilon$ is introduced for determining the MMI coefficients:

$$
1 + a_1(x_1) \frac{d}{dx_1} + a_2(x_1) \frac{d^2}{dx_1^2} \left( \frac{-u_1'c' + \varepsilon \frac{dc}{dx_1}}{D^0 + \varepsilon} \right) = \frac{dc}{dx_1}.
$$

Equation (94) is used purely for determining the model coefficients; for ease of implementation, the final model is still Equation (93) with $a_0(x_1) = D^0(x_1)$. As with the previous coefficient regularization technique in Section 4.3, this introduces a small amount of error in matching the first- and second-order moments, but the tradeoff is better-behaved coefficients. Figure 25a shows the coefficients for the alternative MMI formulation using coefficient regularization with $\varepsilon = 0.01c^2$, and Figure 25b shows a comparison of the model solution with DNS. While the alternative MMI model with coefficient regularization performs slightly better than the without coefficient regularization, the choice of $\varepsilon$ is not yet systematic.
Figure 25: (a) Coefficients for the alternative MMI formulation with coefficient regularization and $\varepsilon = 0.01\varepsilon^2$. (b) Model comparison for the wall-bounded inhomogeneous problem in Section 4.3.

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