Response to Referee # 1

Fast Macroscopic Forcing Method

Bryngelson, Schäfer*, Liu, Mani*

We are grateful for the referee's constructive suggestions that have led to improving the quality of this paper. We quote the comments of the referee and discuss changes made to the paper in response to these comments in the following.

Referee #1

1. References are needed for "Still, full-resolution simulations of them stretch computational resources."

   We agree. This sentence is far too vague to start a paper. We have revised this and the preceding sentence to be more precise and include appropriate references. In particular, the initial phrasing: "Well-established equations describe even the most complicated flow physics. Still, full-resolution simulations of them stretch computational resources." has been changed to "Significant computational resources are required to solve fluid dynamics problems; for example, Yang and Griffin Physics of Fluids (2021) discuss resolution requirements for a turbulent boundary layer with application to a simulation of a ship hull (Liefvendahl and Fureby Ocean Engineering (2017))."

2. Eq. (11), I appreciate that the authors are using different symbols for the dummy variable that is being integrated, but using y can cause some confusion. Maybe use another symbol?

   We agree and changed this notation as $y \to x'$ in the integrals of equations (10, 12, 15, 17, 23, 26, 30, 33) in the revised manuscript, which follows the notation of previous works and, in our view, is more intuitive and runs less risk of confusion.

3. Section 4.1. Typo. "top and bottom walls with $x_2 = 0\ldots$" should be "top and bottom walls *at* $x_2 = 0\ldots$"

   We agree; this has been changed.

4. I think some statements need to be tuned down. For example, I believe that the authors could only say that when the forward simulation is sufficiently resolved, the number of DNSs needed does not depend on the grid points.

   We agree and have revised our phrasing to accommodate this limitation. Following the referee's comment, the revised phrasing of the relevant text in the abstract as "Our results show that a similar number of simulations are required to reconstruct the operators to the same accuracy under grid refinement. Thus, the accuracy corresponds to the physics of the problem, not the numerics, so long as the grid is sufficiently refined." And to the second to last passage in section 4.1, we revised to: "This indicates that, so long as the forward simulation is fully resolved and mesh-independent, the Fast MFM reconstruction is dependent on the physical locality of the operator, not a numerical or discretized one."

5. Complex geometry and flows at higher Reynolds numbers are naturally extensions which could be discussed.

We agree that these are indeed natural extensions, and at the very least, the reader should be aware of this and the caveats associated with addressing these other flows. In response to this, we have added the following paragraph to the conclusion and discussion: "The Fast MFM formulation is natural for other turbulent flows. For example, higher Reynolds numbers can be analyzed in the same way. In such cases, the relative advantage of Fast MFM over traditional MFM will depend on the degree of locality in the flow. Multiphase flows can also be studied under the same strategy. One such previous example includes MFM analysis of the Rayleigh–Taylor instability (Lavacot et al. arXiv:2307.13911 (2023)). Flows in complex geometries are also tractable, though they require particular attention to the boundary condition formulations."

Response to Referee # 2
Fast Macroscopic Forcing Method
Bryngelson, Schäfer*, Liu, Mani*

We are grateful for the referee's constructive suggestions that have led to improving the quality of this paper. We quote the comments of the referee and discuss changes made to the paper in response to these comments in the following.

Referee #2

1. Can the authors give a practical example of the field s?

   We have added text in the third paragraph of section 2.1. to clarify the use of s. This is the first place in the manuscript that s is used mechanically. Specifically, we have added "For example, discretely specifying $\bar{s} = [1\ 0 \dots 0]^\top$ (a Dirac delta function at $x_{1,1}$), solving the microscopic equations for c, and averaging to obtain $\bar{c}$ leads to the first column of $\overline{\mathcal{L}}^{-1}$ via $\bar{c} = \overline{\mathcal{L}}^{-1}\bar{s}$. Discretely specifying $\bar{s} = [0\ 1\ 0 \dots 0]^\top$ leads to the second column of $\overline{\mathcal{L}}^{-1}$, etc."

2. At page 3 the authors claim that their technique can be applied to a wide number of situations. Can they be more precise and add another example different from the averaging in space?

   We have included a specific, recent reference for multiphase flow in the context of the Rayleigh–Taylor instability assessed by MFM to the penultimate paragraph of the introduction: "indeed, multiphase flow has already been considered in this context for the Rayleigh–Taylor instability (Lavacot et al. arXiv:2307.13911 (2023)) However, we do not show such examples in this work." We have modified the paragraph of page 4 of the revised manuscript to clarify that one could address closure operators of turbulent multiphase flow via this strategy, though these are also spatio-temporal. Specifically, this part of the manuscript now reads: "[...] and is similar to the averaging in the steady laminar channel example problem in section 4.1. In the turbulent channel example problem in section 4.2, we average over temporal and homogeneous spatial directions. However, we point out that the techniques outlined in this work apply to a wider range of possible averaging operations, for example closure operators for turbulent multiphase flow, but leave such discussion for the conclusion." We added discussion of multiphase flows in the conclusion: "Multiphase flows can also be studied under the same strategy. One such previous example includes MFM analysis of the Rayleigh–Taylor instability (Lavacot et al. arXiv:2307.13911 (2023))."

3. The operators P and E are not clearly introduced. Can the authors do an effort in explaining better their form?

   We have added example definitions of $\boldsymbol{P}$ and $\boldsymbol{E}$ via equations following eq. 5, which buttress the descriptive text rather than replace it. Specifically, the equations and text added are "In other words, let $c(x_1, x_2)$ be discretized as a $N_1 N_2 \times 1$ vector, $[c_{1,1}\ c_{2,1} \dots c_{N_1,1} \dots c_{N_1,N_2}]^\top$. Then $\boldsymbol{P}$ is a $N_1 \times N_1 N_2$ matrix that averages over the appropriate $c_{i,j}$, e.g., $\boldsymbol{P} = 1/N_2[\mathcal{I}\ \mathcal{I} \dots \mathcal{I}]$ where $\mathcal{I}$ is a $N_1 \times N_1$ identity matrix, and $\boldsymbol{E} = N_2 \boldsymbol{P}^\top$."

4. How equation 7 is obtained is not clear.

In the revised manuscript, we have added a detailed reference, including page number, to clarify how one obtains eq. 7 from the previous ones. Ultimately, it is a single identity following the Schur complement and enabling eq. 7. Specifically, the reference is [pg. 19, F. Zhang, The Schur Complement and its Applications, Vol. 4 (2006)]. This is all added to the revised text.

5. Section 2.3. the sentence "If (1) is an evolution PDE, this procedure can be interpreted as a control problem, where at each time step, the microscopic portion of the forcing s is chosen to maintain a target average." needs further explanation. Equations will strongly help.

   We have added text and equations to clarify the referee's specific comment above and the IMFM procedure more fully. Specifically, we have added these equations and text to buttress this subsection: "For example, at a given time step, n, the next c^{n+1} needs to satisfy $\bar{c}^{n+1} = \bar{c}$. One can time advance the governing equations without including the forcing and solve for an intermediate c^*, which may not have the requisite $\bar{c}$. The forcing is added in a correction step, $c^{n+1} = c^* + \bar{c} - \overline{c^*}$, such that $\bar{c}^{n+1}$ now satisfies $\bar{c}^{n+1} = \bar{c}$ and the implied s satisfies $s = \bar{s}$. For example, if a first order explicit timestepping scheme is used, the implied s is $s = (\bar{c} - \overline{c^*})/\Delta t$, where Δt is the time step size. "

6. Since the authors discuss turbulence modeling in Section 2.4, I believe that some introduction to those models will be useful. Reynolds decomposition needs to be explained.

   We have added a more thorough and appropriate discussion of turbulence modeling to the introduction and the discussion of the eddy diffusivity operator in section 2.4. We have also added a new section (section 2.5) to specifically discuss the eddy viscosity operator and expanded discussion of the anisotropic Boussinesq eddy viscosity shown in section 4.2.

   Specifically, in the introduction we added: "However, RANS models (Spalart and Allmaras (1992), Menter (1994), Wilcox (1998)), often rely on ad hoc modeling assumptions (Boussinesq (1877)) that are invalid for complex flows (Jespersen et al. (2016), Probst et al (2010), Park et al. (2022))."

   The changes in section 2.4 and newly-added section 2.5 are lengthy, and rather than pasting here, we refer the referee to the revised manuscript with highlighted changes. Regarding the specific comment about the Reynolds decomposition in section 2.4, we have expanded the text and also added a citation: "In general $c \neq \bar{c}$, and the difference between the averaged field $\bar{c}$ and instantaneous field c (and analogously for the velocity field $\boldsymbol{u}$) can be expressed as

$$\boldsymbol{u} = \bar{\boldsymbol{u}} + \boldsymbol{u}' \quad \text{and} \quad c = \bar{c} + c', \tag{1}$$

   where $(\cdot)'$ denotes fluctuations about the mean, and is commonly-known as a Reynolds decomposition (Reynolds (1895))".

In the turbulent channel example in section 4.2, we have clarified the anisotropic Boussinesq eddy viscosity that is shown for comparison: "For comparison, the anisotropic Boussinesq eddy viscosity corresponding to the leading term of the Taylor series expansion of eq. 30 around $x_2' = x_2$ is

$$-\overline{u_i' v_j'}(x_2) = \mathcal{D}_{ij21}^{\text{Boussinesq}}(x_2)\frac{\partial \bar{v}_1}{\partial x_2}, \tag{2}$$

where

$$\mathcal{D}_{ij21}^{\text{Boussinesq}}(x_2) = \int_{x_2'} \mathcal{D}_{ij21}(x_2, x_2')\mathrm{d}x_2'. \tag{3}$$

"

7. What is the equation which defines the eddy diffusivity matrix? What about its generalization?

   We have added this definition below eq. 13. Specifically, we added the equation: "$-\overline{u_1' c'} = \mathcal{D}\partial\bar{c}/\partial x_1$" and text where "$\overline{u_1' c'}$ is a $N_1 \times 1$ vector, $\mathcal{D}$ is a $N_1 \times N_1$ matrix, and $\partial\bar{c}/\partial x_1$ a $N_1 \times 1$ vector." We have also added the definition of the eddy viscosity matrix in eq. 31: "Discretely, for a given direction, e.g., $i = 2$ and $j = 1$:

$$-\overline{u_2' v_1'} = \mathcal{D}_{2121}\frac{\partial \bar{v}_1}{\partial x_2}, \tag{4}$$

   where $-\overline{u_2' v_1'}$ is a $N_2 \times 1$ vector, $\mathcal{D}_{2121}$ is a $N_2 \times N_2$ eddy viscosity operator, and $\partial\bar{v}_1/\partial x_2$ is a $N_2 \times 1$ vector, where $N_2 = 144$."

8. At the end of pg. 6 the authors claim "The objective of the present work is to recover D, and thus L, from as few matrix-vector products as possible, as accurately as possible." However, from the beginning of the manuscript it seemed that their goal was much broader: they wanted to propose a new methodology for L and not for the specific case considered in section 2.4. Please specify.

   We perform Fast MFM (and brute force) MFM, for the problems of this paper, on $\mathcal{D}$ and not $\overline{\mathcal{L}}$ because it has a more local matrix structure, giving better results. This is because, in the case of our Reynolds stress closures, $\overline{\mathcal{L}}$ has an additional diffusion that is already known and thus does not need to be *recovered*. This is shown in the manuscript as:

$$\overline{\mathcal{L}} = -\left(\frac{\partial}{\partial x_1}\right)(\mathcal{D} + a\mathcal{I})\left(\frac{\partial}{\partial x_1}\right).$$

   So, we can recover $\mathcal{D}$ and then compute $\overline{\mathcal{L}}$ from $\mathcal{D}$ as needed. In cases with no such $\mathcal{D}$; for example, outside of the turbulence context, one can perform the same algorithm on the more general $\overline{\mathcal{L}}$ matrix. We do not perform such a case here, but again agree that the above points should be clarified so that Fast MFM can be understood outside of the RANS context.

We made the existing abstract text more explicit, noting that we recover eddy diffusivity and viscosity rather than the more general $\overline{\mathcal{L}}$. Specifically, this part of the abstract now reads: "We demonstrate the algorithm's performance for the eddy diffusivity and eddy viscosity operators, which correspond to the unclosed parts of the ensemble-averaged transport equations, excluding the analytically known, closed parts of such equations. However, the algorithm can also be applied to the full operators as needed."

We revised the manuscript to show the meaningful distinction between $\overline{\mathcal{L}}$ and $\mathcal{D}$ for our algorithm and its examples. We note the existence and utility of such a $\mathcal{D}$ in the cases we analyze and how they can likewise be used for more general cases via $\overline{\mathcal{L}}$. Specifically, we have added to section 2.3 the leading text "We perform Fast (and brute force) MFM on $\mathcal{D}$, corresponding to an eddy diffusivity, and not $\overline{\mathcal{L}}$ because it has a more local matrix structure. In the case of our turbulence closures, $\overline{\mathcal{L}}$ has an additional diffusion that is already known and thus does not need to be *recovered*. So, we can recover $\mathcal{D}$ and then compute $\overline{\mathcal{L}}$ from $\mathcal{D}$ as needed. In cases with no such $\mathcal{D}$, for example, outside of the turbulence context, one can perform the same algorithm on the more general $\overline{\mathcal{L}}$ matrix."