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Cautionary tales from the mesoscale eddy transport tensor

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Abstract

The anisotropic mesoscale eddy transport tensor is diagnosed using passive tracers advected online in both an idealized 101-member mesoscale-resolving quasi-geostrophic (QG) double-gyre ensemble, and a realistic 24-member eddying (1/12°) ensemble of the North Atlantic. We assert that the Reynold's decomposition along the ensemble dimension, rather than the spatial or temporal dimension, allows us to capture the intrinsic spatiotemporal variability of the mean flow and eddies. The tensor exhibits good performance in reconstructing the eddy fluxes of passive tracers, here defined as fluctuations about the ensemble thickness-weighted averaged (TWA) mean. However, the inability of the tensor to reconstruct eddy fluxes of QG potential vorticity, which encapsulates the eddy-mean flow interaction, and other active tracers raises the question: To what extent can the diagnosed tensor be applied to inform the parametrization of mesoscale dynamics?

Keywords: Ensemble simulation, mesoscale eddy, eddy diffusivity, thickness-weighted average

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1 1. Introduction

In the field of computational oceanography, there is never enough compu-2 tational power to resolve all the spatiotemporal scales of interest, spanning 3 from on the order of O(1 m) to O(1000 km) and seconds to centuries respec-4 tively. Nevertheless, with the continuous increase in computational power, 5 global fully-coupled ocean simulations with spatial resolution of $O(10 \,\mathrm{km})$ 6 have emerged (e.g. Small et al., 2014; Uchida et al., 2017; Chang et al., 2020). 7 This new generation of ocean simulations have improved the representation of oceanic processes, e.g. the oceanic jets in the separated Gulf Stream and 9 Atlantic Circumpolar Current, and the global oceanic heat transport esti-10 mates match better with observations (Griffies et al., 2015; Chassignet et al., 11 2020). Nevertheless, forced ocean simulations with higher model resolution 12 have shown that even at $O(10 \,\mathrm{km})$ mesoscale eddies and their feedback onto 13 the jets are not sufficiently resolved (Chassignet and Xu, 2021; Uchida et al., 14 2019, 2022c; Hewitt et al., 2022). 15

In order to overcome the insufficient representation of the eddies and their 16 variability, there has been a growing field of research on how to parametrize 17 the effects of eddies in simulations at the grey zone resolution, when the 18 eddy variability is partially resolved. The missing dynamical effects, due 19 to limited resolution, include processes such as energy-backscattering and 20 dissipation of energy and enstrophy (e.g. Bachman et al., 2017; Jansen et al., 21 2019; Bachman, 2019; Guillaumin and Zanna, 2021; Uchida et al., 2022a, and 22 references therein). In this study, we examine the possibility of capturing 23 the effects of these missing dynamical processes within the framework of 24 eddy transport coefficients, where we represent the sub-grid fluxes of tracers 25 via the gradient flux of the resolved tracer fields. In doing so, we utilized 26 two sets of ensemble simulations: an idealized 101-member quasi-geostrophic 27 (QG) double-gyre ensemble at mesoscale-resolving resolution and a realistic 28 eddying $(1/12^{\circ})$ 24-member North Atlantic (NA) ensemble. 29

In the parametrization literature, it is common to frame the eddies as the 30 sub-grid variability and mean flow as the resolved flow under limited model 31 resolution, where the eddy and mean are defined using a Reynold's decom-32 position (Bachman et al., 2015). The assumption, and hope, is that the re-33 duced variability in the mean flow, diagnosed by filtering a high-resolution or 34 observed flow field, would mimic the partially resolved variability at coarser 35 model resolution. In a seminal paper, Young (2012) demonstrated that when 36 the equations of oceanic motions are Reynold's decomposed via a thickness-37

weighted averaging, the net effect of the eddies onto the mean flow can be 38 represented in terms of eddy Ertel's potential vorticity (PV) fluxes on the 39 thickness-weighted averaged (TWA) mean momentum equations. With this 40 interpretation, the goal of the parametrization problem is to represent the 41 eddy QG or Ertel's PV fluxes in terms of the mean fields (Young, 2012; Mar-42 shall et al., 2012; Vallis, 2017). In this study we address the question: Can 43 the eddy fluxes be expressed in terms of a tensor transport model, where 44 the eddy flux is related to the local gradient through a transport tensor? 45 Also, is the transport tensor for active tracers (e.g. PV) similar to a trans-46 port tensor for passive tracers? Our approach is to diagnose the transport 47 coefficients using passive tracers outputs and then to examine whether this 48 can be applied to reconstruct eddy fluxes of active tracers. The potential 49 interchangeability between passive (in the sense that they do not affect the 50 dynamics) and active tracers such as PV has its history in that the governing 51 equations for the two take a similar form of an advective-diffusive equation 52 (with the caveat that PV is directly linked to the momentum and buoyancy 53 while passive tracers are not; Killworth, 1997; Wilson and Williams, 2006; 54 Eden and Greatbatch, 2008). 55

For practical reasons, a time or spatial mean has often been employed to 56 Reynold's decompose the flow into its eddy and mean in diagnostic studies. 57 However, this comes with its own issues regarding interpretation. For a 58 temporally varying system, such as the real ocean, defining the mean flow 59 via a time mean conflates intrinsic variability of the ocean resulting from the 60 non-linearities in governing equations with the variability in the atmospheric 61 forcing (Aiki and Richards, 2008; Fedele et al., 2021; Uchida et al., 2022b). 62 There are also issues surrounding how to choose the filtering scale, and what 63 model resolution, if any, the scale corresponds to (Bachman et al., 2015). An 64 alternative approach is to define the mean flow via an ensemble mean, where 65 the intrinsic variability is expressed as eddies and the oceanic response to 66 atmospheric forcing as the mean (Sérazin et al., 2018; Leroux et al., 2018; 67 Uchida et al., 2022b). Taking the ensemble outputs, we, therefore, define the 68 eddy-mean flow decomposition along the ensemble dimension and attempt 69 to reconstruct the eddy flux of tracers defined as fluctuations about the 70 ensemble TWA mean. Unlike the spatiotemporal filtering approaches, there 71 is less ambiguity about how the eddy and mean are defined (Jamet et al., 72 2022), but the connection to parametrization in coarse-resolution models 73 still remains tenuous. Nonetheless, in this study we examine the eddy-mean 74 flow problem under this framework, which is relatively novel in the ocean 75

⁷⁶ turbulence literature. We also note that because the ensemble dimension is
⁷⁷ orthogonal to the spatiotemporal dimensions, our Reynold's decomposition
⁷⁸ is exact. Our approach can be rephrased as us having the lofty long-term
⁷⁹ goal to parametrize the oceanic intrinsic variability otherwise resolved under
⁸⁰ sufficient model resolution.

The paper is organized as follows: We describe the ensemble model configurations and framework of the anisotropic eddy transport tensor in Section 2. The results are given in Section 3 with a discussion on the structural similarity in eddy transport coefficients that emerge between the two ensembles. We conclude and provide some cautionary notes in Section 4.

86 2. Methods

We describe the quasi-geostrophic (QG) and realistic North Atlantic (NA) ensembles (sections 2.1 and 2.2), and then provide a brief description of the eddy transport tensor (section 2.3).

90 2.1. Quasi-geostrophic ensemble

The model outputs used here are those of Uchida et al. (2021b). For 91 completeness, we provide a brief overview of the configuration here. We use 92 the QG configuration of the Multiple Scale Ocean Model (MSOM; Deremble 93 and Martinez, 2020, hereon referred to as MSQG), based on the Basilisk 94 language (Popinet, 2015), to simulate a three-layer double-gyre flow with 95 a rigid lid and flat bottom. The characteristic length scale of the Rossby 96 radius is prescribed as 50 km and horizontal resolution is ~ 4 km, so we have 97 roughly 12 grid points per radius; our simulation can be considered mesoscale 98 resolving (Hallberg, 2013). 90

The model was forced with a stationary wind stress curl without any 100 buoyancy forcing at the surface. A seasonally varying background stratifica-101 tion was prescribed at the first interface but kept stationary at the second 102 interface, which is consistent with the seasonal variability of stratification 103 being confined in the upper few hundred meters in the real ocean (Chelton 104 et al., 1998). The 101 ensemble members are initialized with stream func-105 tions slightly perturbed at a single grid point randomly selected in the first 106 layer per member and the surface wind stress and temporally varying back-107 ground stratification are kept identical amongst the members. We refer the 108 interested reader to Uchida et al. (2021b) for further details on the model 109 configuration and ensemble generation. 110

In addition, we added four passive tracers to each ensemble member with the governing equation:

$$C_{it} + J(\psi, C_i) = -\mathscr{T}^{-1}(C_i - \dot{C}_i), \qquad (1)$$

where C_i , i = 0, 1, 2, 3 are the four passive tracers and ψ the stream function. They are relaxed towards a profile orthogonal to each other

$$\dot{C}_0 = \frac{x - L/2}{L/2}, \ \dot{C}_1 = \frac{y - L/2}{L/2}, \ \dot{C}_2 = \sin\frac{2\pi x}{L}, \ \dot{C}_3 = \sin\frac{2\pi y}{L},$$
 (2)

with a relaxation time scale of $\mathscr{T} \sim 360$ days for all three vertical layers. 117 $L (= 4000 \,\mathrm{km})$ is the zonal and meridional domain extent, x = [0, L], y =118 [0, L], resulting in the tracers taking values between [-1, 1]. The time scale 119 chosen is similar to previous studies (e.g. Bachman et al., 2020), and meant 120 to be longer than that the typical eddy turn over time scale. In other words, 121 the tracers are passively stirred by the flow realized by the intrinsic variability 122 of each ensemble member but are relaxed towards identical profiles amongst 123 members. The relaxation avoids the tracers from homogenizing (i.e. $\nabla_{\rm h} C_i \neq$ 124 **0** where $\nabla_{\rm h}$ is the horizontal gradient operator). The tracer profiles were 125 initialized with their respective relaxation profiles at the beginning of the 126 ensemble generation and advected prognostically online. 127

The QG eddy flux is $\mathbf{J}^{C_i} = J^{C_i \mathbf{i}} \mathbf{i} + J^{C_i 2} \mathbf{j} \stackrel{\text{def}}{=} \overline{u'C'_i} \mathbf{i} + \overline{v'C'_i} \mathbf{j}$ where $\overline{(\cdot)}$ is the ensemble mean operator and $(\cdot)' \stackrel{\text{def}}{=} (\cdot) - \overline{(\cdot)}$. \mathbf{i}, \mathbf{j} are the horizontal unit vectors in geopotential coordinates. Snapshots of the eddy kinetic energy (EKE) and tracer variance are shown in the Supplementary Material Fig. S1.

132 2.2. Realistic North Atlantic ensemble

We use the model outputs from the realistic simulations described in 133 Jamet et al. (2019, 2020), and Uchida et al. (2022b), which are 48 air-sea 134 partially coupled ensemble members of the NA ocean at mesoscale-permitting 135 resolution $(1/12^{\circ})$ using the hydrostatic configuration of the Massachusetts 136 Institute of Technology general circulation model (MITgcm; Marshall et al., 137 1997). The modelled domain was configured to wrap around zonally in order 138 to reduce memory allocation in running the simulation. Similar to the QG 139 ensemble, in the latter subset of 24 members, four passive tracers per member 140 were added online using the Relaxation Boundary Conditions (RBCS) package 141 with the relaxation profiles of 142

143

113

$$\dot{C}_0 = \frac{y - L^y/2}{L^y/2}; \ \dot{C}_1 = \sin\frac{2\pi x}{L^x}; \ \dot{C}_2 = \frac{z - H/2}{H/2}; \ \dot{C}_3 = \sin\frac{2\pi y}{L^y},$$
 (3)

and the relaxation time scale of $\mathscr{T} = 365$ days. L^x, L^y are the zonal and meridional domain extent respectively and H is the deepest depth in the domain bathymetry. The tracer profiles were again initialized with their respective relaxation profiles at the beginning of the ensemble generation and advected prognostically online.

The connection between primitive equations viewed in the thickness-149 weighted averaged (TWA) framework and quasi geostrophy is that in the 150 latter, the layer thickness $\sigma \stackrel{\text{def}}{=} \zeta_{\tilde{b}}$ only fluctuates on the order of Rossby 151 number (ζ is the depth of the neutral surface and the subscript (\cdot) denotes 152 derivatives in density coordinates). Hence, it can be argued that QG vari-153 ables are implicitly TWA and that for a fair comparison, the primitive equa-154 tions should also be TWA (cf. Marshall et al., 2012). The three-dimensional 155 oceanic motions become quasi two dimensional upon thickness-weighted av-156 eraging (Aoki, 2014; Loose et al., 2022), further elucidating the similarity 157 to quasi geostrophy. We proceed in defining our eddy tracer fluxes within 158 the TWA framework, which gives $\mathbf{J}^{C_i} = J^{C_i 1} \overline{\mathbf{e}}_1 + J^{C_i 2} \overline{\mathbf{e}}_2 \stackrel{\text{def}}{=} \widehat{u'' C_i''} \overline{\mathbf{e}}_1 + \widehat{v'' C_i''} \overline{\mathbf{e}}_2$ 159 where $\widehat{(\cdot)} \stackrel{\text{def}}{=} \overline{\sigma}^{-1} \overline{\sigma(\cdot)}$ and $(\cdot)'' \stackrel{\text{def}}{=} (\cdot) - \widehat{(\cdot)}$ (Young, 2012). $\overline{\mathbf{e}}_1$ and $\overline{\mathbf{e}}_2$ are 160 the horizontal unit vectors along the neutral surface, which reduce to i and 161 **j** respectively when the neutral surfaces are flat $(\nabla_h \zeta = 0$ where ∇_h is the 162 horizontal gradient operator in density coordinates). We note that due to the 163 3rd order direct-space-time (DST) flux-limiter advective scheme used, there 164 are two possible ways to define the eddy flux, i.e. $\widehat{\mathbf{u}''C_i''} \approx \overline{\sigma}^{-1}(\overline{\sigma \mathbf{F}^{C_i}}) - \hat{\mathbf{u}}\widehat{C_i}$ 165 where \mathbf{F}^{C_i} is the DST advective flux computed by MITgcm. The advective 166 scheme was chosen to be consistent with the schemes used for temperature 167 and salinity. Snapshots of the EKE and tracer variance are given in the 168 Supplementary Material Fig. S2. 169

In transforming the three-dimensional model outputs in geopotential co-170 ordinates to TWA variables, we: i) compute the approximately neutral den-171 sity surfaces for each member by removing the effect of compressibility, ii) 172 remap the momentum, isopycnal depth and tracers onto the neutral sur-173 faces, iii) thickness weight the variables and take the ensemble mean, iv) 174 apply Reynold's decomposition about the ensemble TWA mean to obtain 175 the eddy terms $(\cdot)''$, and v) thickness-weighted average the eddy covariance 176 to get the eddy flux. Further details regarding the coordinate remapping 177 from geopotential to approximately neutral surfaces using the xgcm Python 178 package (Abernathey et al., 2021), and the averaging are given in Uchida 179 et al. (2022b). 180

181 2.3. Eddy transport tensor

As the eddy flux of tracers is generally poorly resolved in global forced and coupled ocean simulations, there has been an effort to parametrize this flux in the quasi-adiabatic interior via a local-gradient based model along neutral surfaces (Redi, 1982; Griffies, 2004; Wilson and Williams, 2006; Holmes et al., 2022)

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$$\mathbf{J}^{C_i} = -\kappa \boldsymbol{\nabla}_{\mathrm{h}} \overline{C_i} \,, \tag{4}$$

where κ is the scalar eddy diffusivity, hereon referred to as the transport coefficient. The terminology of 'diffusivity' has its origin in the works by Redi (1982); Gent and McWilliams (1990) and Gent et al. (1995), but eddies not only diffuse but advect tracers (Smith and Gent, 2004; Griffies, 2004; Haigh et al., 2021b), so we have opted for a more general term.

While it is tempting to directly infer a scalar eddy transport coeffi-193 cient from equation (4), assuming an isotropic transport coefficient for an 194 anisotropic flow in realistic simulations is a poor approximation (Smith and 195 Gent, 2004; Ferrari and Nikurashin, 2010; Rypina et al., 2012; Fox-Kemper 196 et al., 2013; Kamenkovich et al., 2015, 2020). A more general or appropri-197 ate model might be to relate the eddy fluxes to the mean gradients via a 198 transport tensor with four parameters (Plumb and Mahlman, 1987), which 199 has some justification in linear wave theories and mixing-length based mod-200 els (Bachman and Fox-Kemper, 2013). In both these models, the inherent 201 assumption is that the scalar transport coefficient or transport tensor is only 202 a function of the flow, and is tracer independent. 203

We, therefore, take the approach of estimating the eddy transport tensor (**K**) from a least-squares best fit to (Plumb and Mahlman, 1987; Abernathey et al., 2013; Bachman and Fox-Kemper, 2013)

$$\underbrace{\begin{pmatrix} J^{C_01} & J^{C_02} \\ J^{C_11} & J^{C_12} \\ J^{C_21} & J^{C_22} \\ J^{C_31} & J^{C_32} \end{pmatrix}}_{\mathbf{J}} = \mathbf{G} \cdot \underbrace{\begin{pmatrix} \kappa^{uu} & \kappa^{vu} \\ \kappa^{uv} & \kappa^{vv} \end{pmatrix}}_{\mathbf{K}}, \tag{5}$$

²⁰⁸ where for the QG ensemble

$$\mathbf{G} = - \begin{pmatrix} \overline{\underline{C}_{0x}} & \overline{\underline{C}_{0y}} \\ \overline{\underline{C}_{1x}} & \overline{\underline{C}_{1y}} \\ \overline{\underline{C}_{2x}} & \overline{\underline{C}_{2y}} \\ \overline{\underline{C}_{3x}} & \overline{\underline{C}_{3y}} \end{pmatrix}, \qquad (6)$$

²¹⁰ and for the realistic NA ensemble

$$\mathbf{G} = - \begin{pmatrix} \widehat{C}_{0\tilde{x}} & \widehat{C}_{0\tilde{y}} \\ \widehat{C}_{1\tilde{x}} & \widehat{C}_{1\tilde{y}} \\ \widehat{C}_{2\tilde{x}} & \widehat{C}_{2\tilde{y}} \\ \widehat{C}_{3\tilde{x}} & \widehat{C}_{3\tilde{y}} \end{pmatrix},$$
(7)

respectively. The least-squares fit can be estimated as $\mathbf{K} = \mathbf{G}^+ \mathbf{J}$ where \mathbf{G}^+ is 212 the Moore-Penrose pseudo inverse of \mathbf{G} for each data point (Bachman et al., 213 2015). The rotational components in \mathbf{J}^{C_i} are not removed prior to inversion. 214 It is possible to invert equation (5) with just two tracers whose gradients are 215 not aligned with each other, and this will return a unique solution specific to 216 the pair of tracers chosen for the inversion (e.g. Haigh and Berloff, 2021; Sun 217 et al., 2021). Here, we instead focus on estimating a single tensor that works 218 for all possible tracer orientations, even if it does not perfectly reconstruct 219 the eddy flux for any single tracer. We have, thus, kept the system over-220 determined by using four tracers. The assumption is that by keeping it over 221 determined, \mathbf{K} would extract the universal component in the relation between 222 eddy fluxes and gradient flux of the mean tracer fields. From a practical point 223 of view, all tracers should be associated with the same transport coefficients 224 in order to reduce the number of model parameters. 225

The eddy flux and mean tracer gradient fields for the QG ensemble were 226 coarse grained by 4×4 grid-point boxcar filter prior to inverting (5) in order 227 to reduce the computational cost. For the NA ensemble, we first spatially 228 smoothed the eddy flux and mean tracer fields by applying a Gaussian kernel 229 with the standard deviation of 50 km using the gcm-filters Python package 230 (Grooms et al., 2021) as we do not expect the linear model (5) to capture 231 grid-scale features. The eddy flux and mean tracer gradient fields were then 232 further coarse grained by 10×10 grid-point boxcar filter in order to reduce 233 the computational cost of inversion. (We demonstrate that other than the 234 significant reduction in computation, the coarse graining has no qualitative 235 impact on our results; Fig. S3. We also note that a boxcar coarse graining 236 commutes with the spatial derivatives and does not result in extra Clark 237 terms. cf. Bachman et al., 2015) Each row in **J** and **G** was then normalized 238 by horizontal median of the magnitude of each mean tracer gradient flux 239 (i.e. $\frac{(\mathbf{J}^{C_i}, \mathbf{G}^{C_i})}{\text{median}[|\mathbf{G}^{C_i}|]}$ where \mathbf{J}^{C_i} and \mathbf{G}^{C_i} are the smoothed and coarse-grained eddy 240 flux and mean gradient flux of an arbitrary tracer C_i prior to the inversion 241 so that each tracer had roughly equal weighting in inverting equation (5). 242

243 3. Results

We present results using the first time step of the fifth year, a time when the ensemble spread has converged for both ensembles (Uchida et al., 2021b; Jamet et al., 2019). The QG outputs are instantaneous snapshots while the North Atlantic (NA) outputs are five-day averaged.

248 3.1. Quasi-geostrophic ensemble

The four components in the eddy transport tensor are provided in the top 249 two rows of Fig. 1 with values reaching up to $O(10^4 \,\mathrm{m^2 \, s^{-1}})$ in the first and 250 second layer. The bottom layer is quiescent with transport coefficients on the 251 order of $O(10^2 \,\mathrm{m^2 \, s^{-1}})$. The diagonal components of the tensor tend to take 252 positive values over the entire domain while the antidiagonal components 253 tend to change signs across the jet centered around $y = 2000 \,\mathrm{km}$. This 254 suggests that the eddies are broadly working to dissipate small-scale variance, 255 as one might expect. Focusing on the first layer, κ^{uv} tends to be coherently 256 negative south of the jet and positive north of the jet. In the lower two layers, 257 κ^{uv} and κ^{vu} tend to mirror each other where there is a sign change across 258 the jet but also within each idealized subtropical and subpolar gyre. These 259 cross diagonal terms of the tensor are largely associated with eddy-induced 260 advection, and often act to oppose the mean flow (Marshall, 2011). 261

Taking the diagnosed tensor, we examine the reconstruction of the eddy flux of C_2 , i.e. $\mathbf{J}_{\text{reconstructed}}^{C_2} \stackrel{\text{def}}{=} - \nabla_{\mathrm{h}} \overline{C_2} \cdot \mathbf{K}$. The middle two rows of Fig. 1 show that the performance of reconstruction is good across all three layers. The spatial correlations between the actual eddy flux and its reconstruction are higher than 0.9 for all four tracers (Table 1). The spatial correlation was computed as

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γ

$$C_{ij} \stackrel{\text{def}}{=} \frac{\sum \left[\left(J^{C_{ij}} - \langle J^{C_{ij}} \rangle \right) \left(J^{C_{ij}}_{\text{reconstructed}} - \langle J^{C_{ij}}_{\text{reconstructed}} \rangle \right) \right]}{\sqrt{\sum \left(J^{C_{ij}} - \langle J^{C_{ij}} \rangle \right)^2} \sqrt{\sum \left(J^{C_{ij}}_{\text{reconstructed}} - \langle J^{C_{ij}}_{\text{reconstructed}} \rangle \right)^2} , \qquad (8)$$

where $\langle \cdot \rangle$ is the horizontal spatial mean, j = 1, 2 correspond to the zonal and meridional orientation, and the summation is taken over the entire domain of interest.

We also exhibit the spatial median of normed relative errors $|\varepsilon^{C_{ij}}|$ computed as

$$\varepsilon^{C_{ij}} \stackrel{\text{def}}{=} \frac{J^{C_{ij}} - J^{C_{ij}}_{\text{reconstructed}}}{J^{C_{ij}}}, \qquad (9)$$

Table 1: Spatial correlation for the four passive tracers and QGPV between the eddy flux and its reconstruction for the zonal and meridional orientation and all three layers. The PV coefficients are not shown for the middle and bottom layer as it is evident from Fig. 1 that the flux and reconstruction are completely decorrelated.

Tracer	Top	Middle	Bottom
$r^{C_0 1}$	0.952	0.989	0.999
$r^{C_0 2}$	0.957	0.990	0.996
$r^{C_{11}}$	0.980	0.966	0.981
$r^{C_{1}2}$	0.999	0.999	0.997
$r^{C_2 1}$	0.939	0.978	0.993
$r^{C_2 2}$	0.949	0.966	0.973
$r^{C_{3}1}$	0.992	0.969	0.980
$r^{C_{3}2}$	0.999	0.999	0.997
r^{q1}	0.844	_	_
r^{q2}	0.906	—	_

in Table 2. This allows us to quantify the normalized error in addition to the 275 sign; $\varepsilon^{C_i j}$ would return positive values if the reconstruction had the correct 276 sign as the actual flux even if it had an offset. When the reconstruction has 277 the wrong sign, the errors would become negative. The spatial median of 278 the normed errors are all positive with values smaller than unity indicating 279 that the reconstruction overall predicts the correct sign of the eddy flux. The 280 spatial fields given in the Supplementary Material Fig. S4 also support the 281 good performance. 282

As the inversion was done as a least squares fit to (5), the good recon-283 struction of \mathbf{J}^{C_i} may not come as a surprise and is consistent with previous 284 studies (e.g. Abernathey et al., 2013; Bachman et al., 2015, 2020). However, 285 it is important to note that such a good fit, although not perfect (Figs. S3) 286 and S4), suggests that the transport tensor model with four free parameters 287 is a good model to represent how the eddies flux different tracers along neu-288 tral surfaces. This model is able to separate the contribution of the flow from 289 any dependence on the orientation of tracer gradients well, and this model 290 of reduced complexity can be a target for parametrizations that are able to 291 represent the eddy fluxes of any arbitrary passive tracer. 292

One may now ask the question: Can the tensor diagnosed from passive tracers be applied to active tracers, here chosen as QG potential vorticity (PV), which is the sole active tracer in quasi geostrophy? Looking at the

Table 2: Spatial median of the normed relative error for the four passive tracers and QGPV between the eddy flux and its reconstruction for the zonal and meridional orientation and all three layers. The PV errors are not shown for the middle and bottom layer for the same reasons as correlation.

Tracer	Top	Middle	Bottom
$ \varepsilon^{C_0 1} $	0.0440	0.0190	0.0122
$ \varepsilon^{C_0 2} $	0.0622	0.0517	0.0169
$ \varepsilon^{C_1 1} $	0.141	0.0746	0.0252
$ \varepsilon^{C_1 2} $	0.0596	0.0153	0.00721
$ \varepsilon^{C_2 1} $	0.0770	0.0326	0.0189
$ \varepsilon^{C_2 2} $	0.112	0.0838	0.0280
$ \varepsilon^{C_31} $	0.135	0.0994	0.0373
$ \varepsilon^{C_3 2} $	0.0596	0.0210	0.0112
$ \varepsilon^{q1} $	1.161	—	—
$ \varepsilon^{q2} $	0.945	_	_

²⁹⁶ bottom two rows of Fig. 1, we see that while the reconstruction $-\nabla_{\rm h}\bar{q}\cdot\mathbf{K}$ ²⁹⁷ captures some features in the top layer (cf. Table 1) and in the regions away ²⁹⁸ from the jet in the middle layer, the reconstruction performs poorly for the ²⁹⁹ bottom layers and in the jet in the middle layer, with the spatial correlations ³⁰⁰ being smaller than 0.1. The normed relative errors are also quite large being ³⁰¹ on the order of O(1) (Table 4; Fig. S5).

302 3.2. Realistic North Atlantic ensemble

Following the QG analyses, we now present the four components of the 303 tensor **K** from the NA ensemble. The magnitude of the tensor components 304 are similar to the QG ensemble, reaching up to $O(10^4 \,\mathrm{m^2 \, s^{-1}})$ (top left four 305 panels in Fig. 2). Also similar to the QG ensemble, the diagonal compo-306 nents tend to take positive values while the antidiagonal components tend 307 to change signs across the separated Gulf Stream (GS). The separated GS 308 can be identified in the top right panel in Fig. 2 where the ensemble-mean 309 depth associated with the neutral surface shoals around 35°N. We also show 310 the vertical transects along 300°E. The patterns in sign persist over depth 311 with the order of magnitude decreasing towards $O(10^2 \,\mathrm{m^2 \, s^{-1}})$ in the abyssal 312 ocean (bottom four panels in Fig. 2). 313

We remind the reader that we define the eddy flux as $\mathbf{J}^{C_i} \stackrel{\text{def}}{=} \widehat{\mathbf{u}''C_i''}$, and following the convention of the TWA framework, the reconstructed eddy flux

Table 3: Spatial correlation for the four passive tracers and temperature and salinity between the eddy flux and its reconstruction for the zonal and meridional orientation along the neutral surface shown in Fig. 2. The correlation coefficients are shown for when they are diagnosed over the entire horizontal domain and only between 10°N-30°N both excluding the hatched regions in Figs. 3 and 4.

Tracer	Entire domain	$10^{\circ}\text{N}\text{-}30^{\circ}\text{N}$
$r^{C_0 1}$	0.918	0.956
$r^{C_0 2}$	0.917	0.971
$r^{C_{1}1}$	0.935	0.959
$r^{C_{1}2}$	0.917	0.936
$r^{C_2 1}$	0.975	0.948
$r^{C_{2}2}$	0.983	0.969
$r^{C_{3}1}$	0.924	0.967
$r^{C_{3}2}$	0.931	0.977
$r^{\Theta 1}$	0.344	0.303
$r^{\Theta 2}$	0.494	0.353
r^{S1}	0.181	0.390
r^{S2}	0.308	0.128

of C_1 becomes $\mathbf{J}_{\text{reconstructed}}^{C_1} \stackrel{\text{def}}{=} -\widetilde{\boldsymbol{\nabla}}_{h}\widehat{C}_1 \cdot \mathbf{K}$. In examining the reconstruction, we limit it to regions where the neutral surface is deeper than 150 m and 316 317 to grids upon the 10×10 coarse graining included no land cells in order to 318 minimize the effect of diabatic mixing (here parametrized by the K-Profile 319 Parametrization; Large et al., 1994). As we see from Fig. 3, the reconstruc-320 tion of eddy passive tracer fluxes is good generally across the entire three 321 dimensional domain with the spatial correlation again higher than 0.9 (Ta-322 ble 3). The largest disagreements between \mathbf{J}^{C_i} and $\mathbf{J}^{C_i}_{\text{reconstructed}}$ can be seen 323 in the separated GS region where eddy activity and vertical fluctuations of 324 the neutral surface are vigorous (Uchida et al., 2022b). The horizontal spa-325 tial correlation improves for the quiescent gyre interior slightly for all four 326 passive tracers. 327

Similar to the QG ensemble, we also show the normalized relative error from the NA ensemble in Table 4. The magnitude of errors are smaller than unity over most of the domain (Fig. S6 in Supplementary Material). As expected from the improvement seen in the spatial correlations, the normed relative errors for passive tracers generally decrease when they are taken over the subdomain of 10°N-30°N.

Table 4: Spatial median of the normed relative errors for the four passive tracers and temperature and salinity between the eddy flux and its reconstruction for the zonal and meridional orientation along the neutral surface shown in Fig. 2. The errors are shown for when they are diagnosed over the entire horizontal domain and only between 10°N-30°N both excluding the hatched regions in Figs. 3 and 4.

Tracer	Entire domain	$10^{\circ}\text{N}\text{-}30^{\circ}\text{N}$
$ \varepsilon^{C_0 1} $	0.0257	0.0141
$ \varepsilon^{C_0 2} $	0.0208	0.00593
$ \varepsilon^{C_1 1} $	0.0118	0.0257
$ \varepsilon^{C_1 2} $	0.0108	0.00847
$ \varepsilon^{C_2 1} $	0.0372	0.0324
$\varepsilon^{C_2 2}$	0.0726	0.0582
$ \varepsilon^{C_3 1} $	0.0334	0.00343
$ \varepsilon^{C_3 2} $	0.0261	0.00153
$ \varepsilon^{\Theta 1} $	0.343	0.286
$ \varepsilon^{\Theta 2} $	0.428	0.331
$ \varepsilon^{S1} $	0.234	0.183
$ \varepsilon^{S2} $	0.314	0.222

We may now also examine if we can use the tensor to reconstruct the 334 eddy temperature and salinity fluxes, variables which were not included in 335 the inversion of (5) and are active tracers. Overall the level of reconstruc-336 tion is poorer than that of passive tracers particularly in the separated GS 337 region; the discrepancy north of 30°N extends vertically down to $\sim 1000 \,\mathrm{m}$ 338 (bottom two rows in Fig. 4). It is interesting, however, that there seems to 339 be some utility of the tensor in the quiescent gyre interior (top three rows 340 of Fig. 4; Table 3); $\mathbf{J}_{\text{reconstructed}}^{\Theta}$ and $\mathbf{J}_{\text{reconstructed}}^{S}$ capture the sign structure south of 30°N in \mathbf{J}^{Θ} and \mathbf{J}^{S} respectively. The normed errors are also on the 341 342 order of O(0.1) indicating some level of reconstructing the eddy flux partic-343 ularly in the quiescent eastern part of the gyre (cf. Fig. S7 in Supplementary 344 Material). Given the QGPV results from the previous section, we did not 345 attempt the reconstruction for Ertel's PV. 346

³⁴⁷ 4. Conclusion and discussion

In this study, we have diagnosed the anisotropic mesoscale eddy transport tensor **K** using passive tracer outputs from two sets of ensemble simulations: an idealized 101-member quasi-geostrophic (QG) double-gyre ensemble and

a realistic 24-member ensemble of the North Atlantic (NA). In decomposing 351 the eddies and mean flow, we have chosen to take the averaging operator over 352 the ensemble dimension rather than the often employed spatial or temporal 353 dimension (e.g. Balwada et al., 2020; Bachman et al., 2020; Kamenkovich 354 et al., 2020; Haigh and Berloff, 2021) with the aim of capturing the intrin-355 sic variability of eddy transport. We have also investigated the tensor in 356 the thickness-weighted averaged (TWA) context, which to our knowledge, 357 is the first study to do so. While we have only utilized one time slice of 358 output, we do not expect the performance of inverting for \mathbf{K} to qualitatively 359 vary over time in the quasi-adiabatic interior of the ocean; in Fig. S8 in the 360 Supplementary Material, we exhibit the time series of the spatial median of 361 the major and minor eigenvalues of the symmetric part of the QG tensor 362 $(\mathbf{S} = (\mathbf{K} + \mathbf{K}^{\mathsf{T}})/2$ where \mathbf{K}^{T} is the transpose). The physical significance of the 363 eigenvalues is that the eddies tend to diffuse the tracers in the direction of 364 the eigenvectors with an associated transport coefficient of each respective 365 eigenvalue (Abernathey et al., 2013; Haigh et al., 2021a). We find a robust 366 seasonal cycle repeating itself (larger values during late summer and smaller 367 values during late winter) with a lag to the seasonality in the prescribed 368 background stratification. When examining the climatological summer aver-369 age of transport coefficients diagnosed at each time step and averaged over 370 five years, they exhibit less spatial structure but with the same tendencies 371 as Fig. 1, i.e. the diagonal components are largely positive and antidiagonal 372 components change sign across the separated jet (Fig. S9). 373

The diagnosed tensor shows good performance in reconstructing the eddy 374 fluxes of passive tracers from the gradient flux of mean passive tracer fields, 375 which were weakly restored with a one-year relaxation timescale. The agree-376 ment between the spatial patterns in the transport coefficients emerging 377 from the QG and NA ensemble in respect to the position of the jet is also 378 comforting; they have similar orders of magnitude and the diagonal compo-379 nents $(\kappa_{uu}, \kappa_{vv})$ tend to be positive while $(\kappa_{uv}, \kappa_{vu})$ tend to have opposite 380 signs across the jet and change signs within each gyre. This partially jus-381 tifies our assumption that there is a universal eddy transport tensor, which 382 is able to represent the eddy flux across passive tracers (at least for pas-383 sive tracers with similar source/sink terms; cf. Fig. S10). As noted in Sec-384 tion 2.2, there are two possible ways to define the eddy tracer fluxes as soon 385 as the advective scheme becomes more complicated than a 2nd-order cen-386 tered scheme. We also diagnosed the tensor with the eddy fluxes defined as 387

³⁸⁸ $\mathbf{J}^{C_i} \stackrel{\text{def}}{=} \overline{\sigma}^{-1}(\overline{\sigma \mathbf{F}^{C_i}}) - \hat{\mathbf{u}}\widehat{C}_i$ but the performance of reconstruction deteriorated ³⁸⁹ compared to when $\mathbf{J}^{C_i} \stackrel{\text{def}}{=} \widehat{\mathbf{u}''C_i''}$ (not shown). We speculate that the linear ³⁹⁰ gradient flux model (5) is unable to capture the non-linearities in the flux-³⁹¹ limiter advective scheme used in our simulations for all passive and active ³⁹² tracers.

For studies using ensemble simulations, whether the ensemble size is large 393 enough to achieve statistical convergence is always in question. We exhibit 394 the QG transport coefficients in the top layer diagnosed from a subset of 395 12. 25 and 50 members in Fig. S11. While noisier, the transport coeffi-396 cients diagnosed from 25 members already demonstrate similar values and 397 spatial patterns to the top left panels in Fig. 1. The histograms also align 398 more closely to the distribution from 101 members and the tails of histogram 399 shorten as the size of subset increases (bottom four panels in Fig. S11). 400

Given the diagnosed transport tensor from passive tracers, we have fur-401 ther examined whether it can be carried over to inform the parametrization 402 of active tracer fluxes. However, when applying the tensor to reconstruct 403 the eddy fluxes of active tracers, here QG potential vorticity (PV), our re-404 sults suggest that passive and active tracers have significantly different eddy 405 transport coefficients. In other words, passive and active tracers have differ-406 ent relations between the eddy fluxes and mean fields and this likely stems 407 from the fact that for QGPV, there is no restoring force, similar to what we 408 prescribed for the passive tracers, particularly below the first layer; the gradi-409 ent of mean QGPV had very little spatial structure in the separated jet region 410 as opposed to the passive tracers (Figs. S12 and S13). Without any restoring 411 for passive tracers, their concentrations would completely homogenize over 412 time $(\nabla_h C_i = \mathbf{0})$ rendering the gradient flux model (5) useless. Our empha-413 sis on the eddy PV flux is because it encapsulates the energy backscattering 414 onto the mean flow (Young, 2012; Marshall et al., 2012; Uchida et al., 2021a). 415 Unlike previous studies (e.g. Mak et al., 2016; Haigh et al., 2021a), we have 416 not split the eddy flux of passive tracers into its divergent and rotational 417 component in diagnosing \mathbf{K} as our interest has been in whether this tensor 418 can be used to approximate the total eddy PV flux itself ($\mathbf{F}^{\#}$ in Young, 2012), 419 and not its divergence, that forces the mean momentum. This being said, 420 our least-square approach does fairly well at reconstructing also the eddy flux 421 divergence of passive tracers in the quiescent gyre interior where the relative 422 errors are small (Figs. S13 and S14). Machine learning methods or further 423 generalizations to the framework may provide a pathway forward in finding 424

the relation for active tracers (e.g. Zanna and Bolton, 2020; Guillaumin and
Zanna, 2021; Frezat et al., 2021; Lu et al., 2022).

Nonetheless, the development of a prognostic and physically consistent **K** 427 will likely benefit biogeochemical modelling since biogeochemical tracers are 428 passive (cf. Jones and Abernathey, 2019; Uchida et al., 2020). We end on 429 the note that for the realistic NA ensemble, the tensor shows some skill in 430 reconstructing the eddy temperature and salinity fluxes in the gyre interior. 431 While temperature and salinity are not purely passive as they affect the 432 dynamics via the hydrostatic pressure, the partial reconstruction may suggest 433 that they have less of a direct role on the dynamics compared to PV. 434

435 Data availability statement

The Jupyter notebooks used for the analyses of the QG and NA ensembles are available via Github (https://github.com/roxyboy/qg_eddy_ diffusivity and https://github.com/roxyboy/TWA-eddy-diffusivity respectively; DOIs will be added upon acceptance of the manuscript).

440 Declaration of competing interest

⁴⁴¹ The authors declare no conflict of interest.

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Figure 1: The eddy transport tensor **K** diagnosed by inverting (5), eddy flux of C_2 and PV and their reconstruction from the QG ensemble for all three layers. The four components of the tensor are exhibited in the top two rows, the eddy flux \mathbf{J}^{C_2} and its reconstruction $-\nabla_{\mathbf{h}}\overline{C_2} \cdot \mathbf{K}$ in the middle two rows, and the tensor applied to PV (q) in the bottom two rows. The eddy PV fluxes in the bottom two layers are two orders of magnitude smaller than the top layer.



Figure 2: The eddy transport tensor **K** diagnosed by inverting (5) from the realistic North Atlantic ensemble on January 3, 1967. The top left four panels show the four components along the neutral surface associated with the ensemble-mean depth $\overline{\zeta}$ shown in the right top panel. The bottom four panels exhibit the vertical transect of the four components along 300°E.





Figure 3: The eddy flux of tracers C_1 and C_2 and their reconstruction from the realistic North Atlantic ensemble on January 3, 1967. The top three rows present the eddy flux \mathbf{J}^{C_i} , reconstruction $-\widetilde{\mathbf{\nabla}}_{h}\widehat{C_i} \cdot \mathbf{K}$, and the difference between the two respectively. The hatches indicate regions where the neutral surface is shallower than 150 m. The bottom two rows exhibit the vertical transect of the flux and reconstruction along 300°E.



Figure 4: The eddy flux of potential temperature and practical salinity, and their reconstruction from the realistic North Atlantic ensemble on January 3, 1967. The top three • rows present the eddy flux $\mathbf{J}^{\Theta}, \mathbf{J}^{S}$, reconstruction $-\widetilde{\boldsymbol{\nabla}}_{h}(\widehat{\Theta}, \widehat{S}) \cdot \mathbf{K}$, and the difference between the two respectively. The hatches indicate regions where the neutral surface is shallower than 150 m. The bottom two rows exhibit the vertical transect of the flux and reconstruction along 300°E.