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Computing eddy-driven effective diffusivity using Lagrangian particles

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A B S T R A C T

A novel method to derive effective diffusivity from Lagrangian particle trajectory data sets is developed and then analyzed relative to particle-derived meridional diffusivity for eddy-driven mixing in an idealized circumpolar current. Quantitative standard dispersion- and transport-based mixing diagnostics are defined, compared and contrasted to motivate the computation and use of effective diffusivity derived from Lagrangian particles. The effective diffusivity is computed by first performing scalar transport on Lagrangian control areas using stored trajectories computed from online Lagrangian In-situ Global High-performance particle Tracking (LIGHT) using the Model for Prediction Across Scales Ocean (MPAS-O). The Lagrangian scalar transport scheme is compared against an Eulerian scalar transport scheme. Spatially-variable effective diffusivities are computed from resulting time-varying cumulative concentrations that vary as a function of cumulative area. The transport-based Eulerian and Lagrangian effective diffusivity diagnostics are found to be qualitatively consistent with the dispersion-based diffusivity. All diffusivity estimates show a region of increased subsurface diffusivity within the core of an idealized circumpolar current and results are within a factor of two of each other. The Eulerian and Lagrangian effective diffusivities are most similar; smaller and more spatially diffused values are obtained with the dispersion-based diffusivity computed with particle clusters.

1. Introduction

Mesoscale eddies arise from baroclinic instability and strongly contribute to oceanic transport (Volkov et al., 2008)– especially for ventilation in the Southern Ocean (Abernathey and Ferreira, 2015), biogeochemistry (José et al., 2014; Salmon et al., 2015), oceanic heat content (Griffies et al., 2015) and feedbacks to the atmosphere and climate system (Frenger et al., 2013). Parameterizations of eddy-induced mixing are particularly important for climate simulation (Fox-Kemper et al., 2013; Klocker and Abernathey, 2014) and are typically developed and tested using mixing diagnosed from remote sensing observations, Lagrangian drifters, and model analysis (Ferreira et al., 2005; Abernathey and Marshall, 2013; Cole et al., 2015; Bachman et al., 2015, etc.).

Mixing estimates can be broadly grouped into Eulerian (Fox-Kemper et al., 2013) and Lagrangian (LaCasce, 2008) approaches. The data available in these frames of reference has historically resulted in physically different diagnostic techniques. For example, scalar gradients are typically used in the Eulerian frame. Gradients are produced from advective and diffusive contributions, i.e., the scalar field evolves due to the combined action of transport producing stirring and small-scale mixing that eliminates resultant large scalar gradients. In contrast, Lagrangian particle tracking may be performed with a variety of velocity fields and background subgrid scale mixing parameterizations (e.g., Griffa, 1996; van Sebille et al., revised, 2017), although without explicit dependence on concentration gradient. This distinction has to date precluded Lagrangian particle tracking data from being used for diffusivity diagnostics that rely on the evolution of scalar concentrations and gradients, e.g., the Nakamura (1996) effective diffusivity, which is hereafter referred to as simply “effective diffusivity”. However, estimation of effective diffusivity from Lagrangian datasets would be useful because of the increasing capability to derive a Lagrangian perspective of the flow from global circulation models (Wolfram et al., 2015; van Sebille et al., revised, 2017) and observational datasets, e.g., via Argo and RAFOS floats and Global Drifter Program data (Roemmich et al., 2009; Rossby et al., 1986; Roemmich and Gilson, 2009). The computation of a Lagrangian-based effective diffusivity is a natural reuse and repurposing of Lagrangian particle trajectories to provide alternative estimates of mixing that can be directly compared with standard particle-based methods. The effective diffusivity approach, consequently, is complementary to standard Lagrangian diffusivity approaches. Standard Lagrangian

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diffusivity approaches are computed from the time rate of change of particle dispersion; the effective diffusivity is computed from the evolving cumulative concentration that accounts for mixing occurring across a variety of spatial scales by large-scale straining and small scale diffusion in the fluid.

Despite these advantages to computing effective diffusivity from Lagrangian particle trajectories, no complete method to compute effective diffusivity from particles has been presented to date (Shuckburgh and Haynes, 2003). However, an estimated bound for effective diffusivity computed solely from particle separation, without use of concentration fields, has been developed (Klocker et al., 2012). A method to compute effective diffusivity from concentration fields derived from particle data is useful because it provides an alternative approach to quantifying fluid diffusivity using the same particle dataset typically analyzed with standard dispersion-based approaches. To this end, we present a novel *post-facto* method for the evolution of a passive scalar concentration field using Lagrangian data. This data can subsequently be used to estimate concentration dependent mixing diagnostics, enabling use of the effective diffusivity diagnostic.

In order to best motivate development and use of the proposed novel particle-based effective diffusivity diagnostic we first examine the role of scalar mixing diagnostics relative to governing scalar transport processes for broader context by introducing two general conceptual frameworks to better understand mixing diagnostics, which are presented in Section 2. The effective diffusivity calculation is outlined in Section 3 and its application via Lagrangian particles is developed in Section 4. The idealized circumpolar current (Ringler et al., 2017; Wolfram and Ringler, 2017) used to explore the mixing diagnostics is described in Section 5 and the mixing diagnostics used to evaluate the effective diffusivity diagnostic are presented in Section 6. Results are presented in Section 7, discussed in Section 8, and general conclusions are made in Section 9.

2. Frameworks to quantify scalar mixing

Scalar transport is composed of an unsteady term, an advective term for a velocity $\mathbf{u}$, and a term parameterizing mixing for some background diffusivity $\boldsymbol{\kappa}$, i.e.,

$$\underbrace{\overbrace{\frac{\partial c}{\partial t}}^{\text{Dispersion-based}} + \mathbf{u}\cdot\nabla c = \nabla\cdot(\boldsymbol{\kappa}\nabla c)}_{\text{Transport-based}}, \tag{1}$$

where c is the scalar concentration and t is time. The scalar evolves from some initial condition $c(t=0)=c_0$. Mixing diagnostics can be classified as 1) dispersion- and 2) transport-based methods. Dispersion-methods account for unsteadiness and strain. Transport-based methods account for mixing occurring due to unsteadiness; tracer filaments produced by stirring ultimately result in mixing via the combined action of produced tracer gradients and the fluid diffusivity (Welander, 1955; Fischer et al., 1979). Note that the transport-based diagnostic fully accounts for temporally destroyed scalar variance due to the diffusive destruction of the enhanced gradients produced by advection, which is accounted for by κ in (1). In contrast, particle-based diffusivities account for shear but are fully independent of κ. However, particle- and tracer-based diffusivities are typically found to agree because tracers and particles are both passively advected and mixing is predominantly due to advection in a turbulent flow that is chaotic and irreversible (Klocker et al., 2012; Tulloch et al., 2014; LaCasce et al., 2014).

2.1. Dispersion-based methods

Particle-based mixing metrics have been relegated to dispersion-based metrics because of their natural applicability and use within the Lagrangian reference frames. Their scientific use in understanding mixing is vibrant and widespread (e.g., LaCasce, 2008; van Sebille et al., revised, 2017). Diagnostically, dispersion-based methods are readily computed using particle-based methods because in their simplest implementation, particle tracking is accomplished by solving

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t), \tag{2}$$

where $\mathbf{x}$ is the position of a particle with the initial condition $\mathbf{x}(t=0)=\mathbf{x}_0$. These numerical trajectories simulate data collected by real-world floats. An excellent comparison of different particle-based approaches as applied to float-derived isopycnal diffusivities for the Diapycnal and Isopycnal Mixing Experiment in the Southern Ocean (DIMES) is given by LaCasce et al. (2014).

Note that Eq. (2) cannot account for concentration-based mixing because, in isolation, it contains no information related to the scalar concentration c but instead tracks Lagrangian pathlines within the fluid. Diagnosed diffusivities are consequently derived from advective fluid kinematics. Conceptually, particle-based dispersion methods consequently measure the capability of the fluid to mix out *sufficiently* strong and constant concentration gradients (Klocker et al., 2012), independent of the particular mixing of a scalar. This estimate may be reasonably close to the diffusivity encountered for scalar transport under reasonable initial conditions, as evident by near equivalence of different mixing metrics measured for particular flows (Klocker et al., 2012; Abernathey et al., 2013) because the flow is chaotic and turbulent, which effectively permits an advection-dominated description of the mixing (Klocker et al., 2012; Tulloch et al., 2014; LaCasce et al., 2014).

2.2. Transport-based methods

In contrast, transport-based methods use the evolution of a scalar from some initial concentration distribution to make inferences about mixing, potentially including diagnosis of the full diffusivity tensor and quantification of irreversible mixing. At the largest spatial scale, the global diffusivity may be computed from a global concentration variance budget (Marshall et al., 2006). At smaller spatial scales, mixing may be quantified via computation of scalar moments for each tracer (Aris, 1956; Holleman et al., 2013). Additionally, a least squares fit using multiple tracers can be used to directly compute the mixing from a Reynold's stress decomposition via spatial and/or temporal averaging operations $\bar{\cdot}$ and associated decomposed eddy $\cdot'$ components (Bachman et al., 2015), yielding

$$\overline{\mathbf{u}'c'} = -\mathbf{R}\nabla\bar{c}. \tag{3}$$

$\mathbf{R}$ includes both advective and diffusive properties corresponding to its antisymmetric and symmetric components (Garrett, 2006; Fox-Kemper et al., 2013). However, $\mathbf{R}$ neglects the time-varying nature of mixing; some "mixing" processes in (3) may be reversible and may be viewed in a time-averaged sense as diffusivity noise. But, the form of (3) is more amenable to parameterization schemes where this variability is unimportant, e.g., Redi (1982) and Gent and Mcwilliams (1990) parameterizations for the symmetric and antisymmetric components of $\mathbf{R}$, respectively.

Alternatively, methods such as the effective diffusivity and the *local* Osborn and Cox (1972) diffusivity quantify irreversible mixing occurring due to flux of tracer normal to tracer contours. Note that at shorter times than the decorrelation timescale, diffusivity estimates are dependent upon the initial choice of scalar concentration. Osborn and Cox (1972) diffusivity, in contrast to effective diffusivity, computes the irreversible mixing occurring at a point as opposed to across a tracer contour within a tracer-based coordinate system. However, this local mixing measure requires advection of tracer variance to be small relative to variance dissipation