Diagnosing the effective diapycnal diffusivity in the Regional Oceanic Modeling System

1 Diagnostic method

We estimate an effective diapycnal diffusivity in the model (at each point in space and time) based on the calculation of non-advective buoyancy fluxes that we project in the diapycnal direction. To do this, we first diagnose the temperature and salinity budgets, including all numerical sources of mixing. We use them to compute a buoyancy budget and in particular to isolate the non-advective buoyancy fluxes. Finally, we project the fluxes in the direction orthogonal to the local isopycnal surfaces (based on local adiabatic density gradients) to obtain an effective diffusivity. The different steps are detailed below:

1.1 Tracer budgets

We first diagnose non-advective tracer fluxes ($\vec{F^T}$,$\vec{F^S}$) for the potential temperature T and salinity S by closing the following budgets:

$$\frac{DT}{Dt} = \underbrace{T_t}_{T_{rate}} + \underbrace{\vec{u} \cdot \vec{\nabla} T}_{T_{adv}} = \underbrace{-\vec{\nabla} \cdot \vec{F^T}}_{T_{rhs}}$$

$$\frac{DS}{Dt} = \underbrace{S_t}_{S_{rate}} + \underbrace{\vec{u} \cdot \vec{\nabla} S}_{S_{adv}} = \underbrace{-\vec{\nabla} \cdot \vec{F^S}}_{S_{rhs}}$$

where the flux divergence on the r.h.s. includes contributions from: surface or bottom forcings, explicit horizontal mixing or implicit horizontal mixing due to the advection scheme (Shchepetkin & McWilliams, 2005), parameterized vertical mixing (from KPP or GLS), and all other possible sources of numerical mixing such as implicit vertical advection (Shchepetkin, 2015), stabilisation of the isoneutral diffusive operator (Lemarié *et al.*, 2012), or aspects related to the model time-stepping (Shchepetkin & McWilliams, 2008).

Horizontal advective schemes for tracers in ROMS include centered (C2, C4 or C6), upstream biased (UP3 or UP5), split and rotated upstream biased (RSUP3 or RSUP5), and weighted essentially non-oscillatory (WENO5) schemes. For numerical schemes with implicit diffusivity (UP3, UP5, RSUP3, RSUP5 and WENO5), the implicit part is estimated by removing the contribution of the next higher-order centered advection scheme (C4 or C6). The horizontal advective part on the l.h.s. of the budget is then taken as $T_{Hadv} = T_{Hadv}^{C4/C6}$, while the remainder is included in the r.h.s. as the contribution to horizontal mixing (T_{Hmix}), such that for UP3/RSUP3: $T_{Hmix} = T_{Hadv}^{UP3/RSUP3} - T_{Hadv}^{C4}$, and for UP5/RSUP5 or WENO5: $T_{Hmix} = T_{Hadv}^{UP5/RSUP5/WENO5} - T_{Hadv}^{C6}$.

Vertical advective schemes for tracers in ROMS include centered (C2), 4th-order compact (SPLINES), 4th-order compact with harmonic averaging (AKIMA), and weighted essentially non-oscillatory (WENO5). When SPLINES, AKIMA, or WENO5 are used, the vertical advection on the l.h.s. is taken as the contribution of the SPLINES scheme, whose dissipative part is assumed to be small compared to other sources (Shchepetkin & McWilliams, 2005; Ménesguen *et al.*, 2018). The rest is included in the r.h.s. as a contribution to vertical mixing. A possible contribution from the adaptive, courant number-dependent implicit scheme for vertical advection is also included in the r.h.s. (Shchepetkin, 2015).

Note that this method of estimating the implicit diffusivities for the advective schemes is only valid as long as essentially dissipative schemes are used. Using a scheme with dispersive errors (e.g. C4 without adding an explicit diffusivity) would lead to an underestimation of the effective diffusivity.

1.2 Buoyancy equation

Non-advective buoyancy fluxes are computed by combining the tracer fluxes:

$$\vec{\mathcal{B}} = -g(-\alpha \vec{F^T} + \beta \vec{F^S})$$

where the thermal expansion coefficient $\alpha = -\frac{1}{\rho_0}\left(\frac{\partial \rho}{\partial T}\right)_S$ and the saline contraction coefficient $\beta = \frac{1}{\rho_0}\left(\frac{\partial \rho}{\partial S}\right)_T$, are computed using a local (3d) linear equation of state of the model (Shchepetkin & McWilliams, 2011).

More precisely, we use the equation of state of Shchepetkin & McWilliams (2011):

$$\rho(T, S, z) = \rho_1(T, S) + q_1(T, S)|z|(1 - q_2|z|)$$

where ρ_1 is the potential density referenced at the surface, and z is the depth. Such that density gradients can be written as :

$$\frac{\partial \rho}{\partial x_i} = \frac{\partial \rho_1}{\partial x_i} + \frac{\partial qp_1}{\partial x_i}\,|z|\,(1 - q_2|z|) + q_1 \frac{\partial\,|z|}{\partial x_i}(1 - 2\,q_2|z|) \tag{1}$$

The first 2 terms in the r.h.s. correspond to the adiabatic part, and the third one to the compressible part, such that the adiabatic gradients are computed as:

$$\left.\frac{\partial \rho}{\partial x_i}\right|_{adiab} = \frac{\partial \rho_1}{\partial x_i} + \frac{\partial q_1}{\partial x_i}\,|z|\,(1 - q_2|z|)$$

Thermal expansion and saline contraction coefficients are written in the same way as:

$$\alpha = -\frac{1}{\rho_0}\left(\frac{\partial \rho}{\partial T}\right)_S = -\frac{1}{\rho_0}\left(\left(\frac{\partial \rho_1}{\partial T}\right)_S + \left(\frac{\partial qp_1}{\partial T}\right)_S |z|\,(1 - qp2 * |z|)\right)$$

$$\beta = \frac{1}{\rho_0}\left(\frac{\partial \rho}{\partial S}\right)_T = \frac{1}{\rho_0}\left(\left(\frac{\partial \rho_1}{\partial S}\right)_T + \left(\frac{\partial qp_1}{\partial S}\right)_T |z|\,(1 - qp2 * |z|)\right)$$

1.3 Effective diffusivity

Finally, to get an effective diapycnal diffusivity, we project the buoyancy fluxes ($\vec{F^B}$) in the direction orthogonal to the isopycnal surfaces $\vec{n} = \frac{\vec{\nabla} b}{|\vec{\nabla} b|}$ (where $\vec{\nabla} b$ are the adiabatic buoyancy gradients based on the adiabatic density gradients of Eq. 1) and divide by the norm of the same gradient:

$$K_{eff} = \vec{\mathcal{B}} \cdot \frac{\vec{\nabla} b}{\left|\vec{\nabla} b\right|^2}$$

Note that if the mixing is dominated by the vertical mixing parameterization ($\vec{F_b} \approx (0, 0, \kappa \frac{\partial b}{\partial z})$, where κ is the mixing coefficient parameterized via KPP or GLS), and if the horizontal buoyancy gradients are small compared to the vertical stratification ($\left|\frac{\partial b}{\partial x}\right|, \left|\frac{\partial b}{\partial y}\right| \ll \left|\frac{\partial b}{\partial z}\right|$) , we should recover: $K_{eff} = \kappa$.

References

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