WMT analysis in ocean models: some thoughts and questions

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Traditional lands of the Bedegal people of the Eora Nation

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Ongoing issues

Goals for this talk

- * CONCEPTUAL AND PRACTICAL: Aspects of WMT analysis that impacts our ability to use the method in numerical models (largely from Groeskamp et al 2019).
- ★ MODEL ALGORITHMS AND BUDGETS: How do models evolve tracers?
 - → A bit on quasi-Eulerian (traditional) and quasi-Lagrangian (and ALE) methods.
- * TAKE-HOME POINT: To write rigorous and thorough code for 3d process-based WMT analysis requires expertise in WMT analysis, process physics and BGC. and numerical algorithms.
 - → It is for us to determine if the investment has sufficient payoff.



- The WMT elevator speech
- What we need from the models
- Scalar equations in ocean models
- Ongoing issues

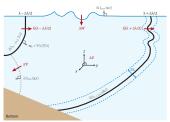






Basic mathematical expressions (Grosskamp et al 2019)

MEASURE SEAWATER TRANSPORT ACROSS ISO-SURFACES OF A SCALAR PROPERTY.



$$G(\lambda) = \iint_{\lambda} \rho \, u^{\text{dia}} \, dA = \iint_{\lambda} \frac{\rho \, \dot{\lambda} \, dA}{|\nabla \lambda|} \tag{1}$$

Fundamental theorem of calculus renders the more useful form

$$G(\lambda) = \frac{\partial}{\partial \lambda} \iiint_{\lambda' \le \lambda} \rho \,\dot{\lambda}' \,\mathrm{d}V. \tag{2}$$

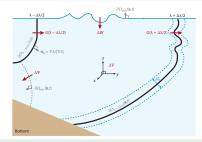
Discretized form for numerical calculations

$$G(\lambda) \approx \frac{1}{\Delta \lambda} \sum_{n=1}^{N} \sum_{i,i,k} \Pi(\lambda_n, \lambda, \Delta \lambda) \left(\rho \,\dot{\lambda}\right)_{i,j,k} V_{i,j,k}. \tag{3}$$

Box-car binning of the material change $\rho \dot{\lambda}$ into N-bins



Notable conceptual characteristics (Grosskamp et al 2019)



- A powerful kinematic framework for studying tracer dynamics.
 - $\star~\lambda$ surfaces can be non-monotonic and disconnected.
 - $\star~\lambda$ is typically density (which one?), temperature, or salinity.
 - * Geographical non-locality \Longrightarrow distinct from strict isopycnal analysis.
 - \star Generalizable to ΘS space (Döös, Zika, Groeskamp, collaborators).
 - * Generalizable to arbitrary 3-scalar space (Nurser, Zika, Griffies ongoing).
- Geographical non-locality means WMT phase space is not suitable for spatially local contact forces such as pressure and stress.
 - ★ ⇒ Still need Eulerian or Lagrangian kinematics for momentum dynamics.
 - $\star \implies$ Perfect-fluid dynamical processes ($\dot{\lambda} = 0$) are invisible to WMT.





2 What we need from the models



Models need to carefully diagnose $\rho \,\dot{\lambda} = -\nabla \cdot \boldsymbol{J}$.

• KINEMATIC METHOD: Direct calculation but offers no process information

$$\underbrace{\rho \,\dot{\lambda}}_{\text{material change}} = \underbrace{\frac{\partial(\rho \,\lambda)}{\partial t}}_{\text{local tendency}} + \underbrace{\nabla \cdot (\rho \,\lambda \,\nu^{\dagger})}_{\text{residual mean advection}} \qquad \text{with} \qquad \nu^{\dagger} = \nu + \nu^{\text{sgs}}. \tag{4}$$

PROCESS METHOD: Indirect calculation offering full process information

$$\rho \, \dot{\lambda} = -\nabla \cdot \textbf{\textit{J}} = \sum (\text{interior processes + boundaries}). \tag{5}$$

- SOME NUMERICAL ISSUES THAT MAKE CAREFUL BUDGETS TOUGH:
 - * Models generally have changing cell thicknesses, thus requiring care to keep track of cell volume along with tracer evolution (more later).
 - ★ Multi-step time stepping means ocean is incrementally updated; e.g., time-implicit vertical diffusion ⇒ tough to diagnostically close budgets.
 - Numerial algorithms often preclude fine-scale decomposition of budgets;
 e.g., nonlinear numerical advection

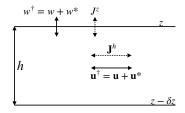
$$v^{\dagger} = v + v^{\text{sgs}}$$
 and yet $\nabla \cdot (\rho C v^{\dagger}) \neq \nabla \cdot (\rho C v) + \nabla \cdot (\rho C v^{\text{sgs}})$. (6)







Z-coordinate scalar eqns w/ eddy-induced v^*



Scalar equations in ocean models

$$\frac{\mathsf{D}^\dagger}{\mathsf{D}t} = \frac{\partial}{\partial t} + \mathsf{v}^\dagger \cdot \nabla, \quad \mathsf{v}^\dagger = \mathsf{v} + \mathsf{v}^* \quad \mathsf{w/ local mass conserve eddy} \Longrightarrow \nabla \cdot (\rho \, \mathsf{v}^*) = 0 \quad (7)$$

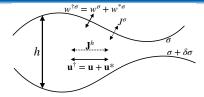
$$\frac{\mathrm{D}^{\dagger}(\rho\,\delta V)}{\mathrm{D}t} = 0 \Longrightarrow \frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\,\mathbf{v}) = 0 \quad \text{usual continuity equation even with } \mathbf{v}^* \neq 0 \quad \text{(8)}$$

$$\rho \frac{\mathsf{D}^{\dagger} C}{\mathsf{D} t} = -\nabla \cdot \mathbf{J} \Longrightarrow \frac{\partial (\rho \, C)}{\partial t} + \nabla \cdot (\rho \, C \, \mathbf{v}^{\dagger}) = -\nabla \cdot \mathbf{J}. \tag{9}$$

Some tracers, especially BGC tracers, also have sources. Ignore here for brevity.



The WMT elevator speech



$$\frac{\partial (h\,\rho)}{\partial t} + \nabla_{\sigma} \cdot (h\,\rho\,\boldsymbol{u}^{\dagger}) + \delta_{\sigma}(\rho\,\boldsymbol{w}^{\dagger\sigma}) = 0 \quad \text{and} \quad \nabla_{\sigma} \cdot (h\,\rho\,\boldsymbol{u}^{*}) + \delta_{\sigma}(\rho\,\boldsymbol{w}^{*\sigma}) = 0 \quad (10)$$

$$\frac{\partial(h\,\rho\,C)}{\partial t} + \nabla_{\sigma}\cdot(h\,\rho\,C\,\boldsymbol{u}^{\dagger}) + \delta_{\sigma}(\rho\,C\,\boldsymbol{w}^{\dagger\,\sigma}) = -\left[\nabla_{\sigma}\cdot(h\boldsymbol{J}^{h}) + \delta_{\sigma}J^{\sigma}\right] \tag{11}$$

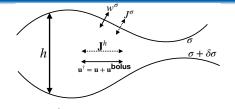
$$z_{\sigma} = \frac{\partial z}{\partial \sigma} \qquad h = z_{\sigma} \, d\sigma \qquad w^{\dagger \sigma} = \frac{\partial z}{\partial \sigma} \frac{D^{\dagger \sigma}}{Dt} = w^{\sigma} + v^* \cdot z_{\sigma} \nabla \sigma = w^{\sigma} + w^{*\sigma}$$
(12)
$$\delta_{\sigma} = d\sigma \, \frac{\partial}{\partial \sigma} \qquad \nabla_{\sigma} = \nabla_z + \mathbf{S} \, \partial_z \qquad \mathbf{S} = \nabla_{\sigma} z = -z_{\sigma} \nabla_z \sigma \qquad J^{\sigma} = z_{\sigma} \nabla \sigma \cdot \mathbf{J}$$
(13)

$$\delta_{\sigma} = d\sigma \frac{\partial}{\partial z}$$
 $\nabla_{\sigma} = \nabla_{z} + S \partial_{z}$ $S = \nabla_{\sigma} z = -z_{\sigma} \nabla_{z} \sigma$ $J^{\sigma} = z_{\sigma} \nabla \sigma \cdot J$ (13)

- Coordinate transformation of the z-coordinate equations (e.g., Griffies 2004).
- w^{σ} & $w^{*\sigma}$ are diagnosed via the continuity equation: a *kinematic* approach.
- Quasi-Eulerian codes: MOM5, MITgcm, NEMO, ROMS.
- Example coordinates are those that do not vanish (unless lose ocean to rock) ⇒ isopycnal coordinates are not available.



Quasi-Lagrangian scalar egns w/ eddy-induced u^{bolus}



$$\frac{\partial(h\,\rho)}{\partial t} + \nabla_{\sigma} \cdot (h\,\rho\,\boldsymbol{u}^{\dagger}) + \delta_{\sigma}(\rho\,\boldsymbol{w}^{\sigma}) = 0 \tag{14}$$

$$\frac{\partial (h \, \rho \, C)}{\partial t} + \nabla_{\sigma} \cdot (h \, \rho \, C \, \boldsymbol{u}^{\dagger}) + \delta_{\sigma} (\rho \, C \, w^{\sigma}) = -\left[\nabla_{\sigma} \cdot (h \, \boldsymbol{J}^{h}) + \delta_{\sigma} J^{\sigma}\right] \tag{15}$$

$$w^{\sigma} = \frac{\partial z}{\partial \sigma} \frac{D\sigma}{Dt} \qquad u^{\dagger} = u + u^{\text{bolus}}$$
 (16)

- w^{σ} is specified based on dia-surface processes such as mixing: a thermodynamic or process approach.
- Makes use of u^{bolus} to ensure advective transport retains constant mass layers, even if not an adiabatic isopycnal layer.
 - * A choice stemming from isopycnal models, here chosen also for any coordinate.
 - * See McDougall and McIntosh (2001), Griffies (2004), Young (2012) for relation between u^{bolus} and v^* .
- Quasi-Lagrangian codes: HYCOM, MOM6, MPAS-O, NEMO (immature?).

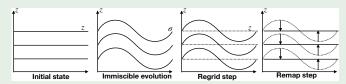


Arbitrary Lagrangian Eulerian (ALE) method for the scalar equations (Based on AJ Addroin)

• IMMISCIBLE LAYER STEP: Using the quasi-Lagrangian formulation, evolve ocean state to time $t+\Delta t$ using $\dot{\sigma}=0$ (constant mass layers) yet with the full suite of SGS parameterizations

$$\frac{\partial(h\,\rho)}{\partial t} + \nabla_{\sigma} \cdot (h\,\rho\,\mathbf{u}^{\dagger}) = 0 \qquad \frac{\partial(h\,\rho\,C)}{\partial t} + \nabla_{\sigma} \cdot (h\,\rho\,C\,\mathbf{u}^{\dagger}) = -\left[\nabla_{\sigma} \cdot (h\,\mathbf{J}^{h}) + \delta_{\sigma}J^{\sigma}\right].$$

- REGRIDDING STEP: New grid with thicknesses h^* fitting in the model domain.
- Remapping step: Take the new state and map it onto h^* . Use a very high order accurate one-dimensional scheme to minimize spurious mixing/unmixing.



- WHERE IS DIA-SURFACE ADVECTION? It is part of the evolution of the grid cell thicknesses. Cell interfaces move and carry the state.
- Z-COORDINATE EXAMPLE: Define h* according to fixed z-levels. Remapping
 moves the state onto the fixed z-grid: operationally same as vertical advection.



Ongoing issues





Spurious mixing and unmixing

The numerical representation of advection $= \nabla \cdot (\rho \, C \, v^\dagger)$ generally introduces spurious mixing and unmixing due to truncation errors (Griffies et al 2000 and others)

$$\nabla \cdot (\rho \, C \, v^{\dagger})_{\text{model}} = \nabla \cdot (\rho \, C \, v^{\dagger})_{\text{exact}} + \nabla \cdot (\rho \, C \, v^{\dagger})_{\text{noise}} \tag{17}$$

* Noise in numerical advection can be interpreted as an extra SGS term

$$\frac{\partial(\rho\,\lambda)}{\partial t} + \nabla\cdot(\rho\,\lambda\,v^{\dagger})_{\text{exact}} = -\nabla\cdot\left[\boldsymbol{J} + (\rho\,\lambda\,v^{\dagger})_{\text{noise}}\right]. \tag{18}$$

- Noise term is not physical. Hence, if it is large it can corrupt the physical integrity of the simulation.
- ⋆ Noise term can become larger when refine grid spacing to partially resolve mesoscale eddies, which pump tracer variance to the grid scale. Need to move into the very fine spacing regime before spurious mixing reduces: 0.25° → 0.1°.
- * After 20 years of trying, there is no exact and general means to locally diagnose $\nabla \cdot (\rho \, C \, v^\dagger)_{\text{noise}}$ in a realistic ocean climate simulation. However, there are ideas that might get us part of the way there (e.g., Ryan Holmes).
- Noise is reduced when use higher order accurate advection and when move to ALE vertical remapping (with high order accurate remapping).



Ambiguity and noise in the binning process

The discrete water mass transformation expression is given by

$$G(\lambda) \approx \frac{1}{\Delta \lambda} \sum_{n=1}^{N} \sum_{i,j,k} \Pi(\lambda_n, \lambda, \Delta \lambda) \left(\rho \,\dot{\lambda}\right)_{i,j,k} V_{i,j,k} \tag{19}$$

Box-car binning of the material change $\rho \dot{\lambda}$ into N-bins

with analogous expressions for layer tracer budgets.

- What bin size should we use?
 - * Bin size can have a nontrivial impact on the results.
- It is useful for debugging the binning code to check that the depth/layer integrated budget adds up to the native model budget.
- Even so, there is no obvious sanity check on WMT within any particular bin.
 - ★ We are aiming for quantitatively robust results, and yet there is no direct means to double-check the numbers. That is a problem.
- Are we ready for a detailed best-practices for WMT analysis, at least to help minimize obvious mistakes?



A final solution for best globally defined buoyancy?

For buoyancy-based WMT analysis, we remain using non-optimal density fields such as $\gamma^{\rm n}$ or potential density.

- Aspirations for any new-and-improved γ field.
 - \star An equation for γ to allow online binning.
 - \star An expression for γ that is general enough to allow for arbitrary model state; not limited to an observational dataset.
 - \star Dispense with the dreaded *b*-factor in the following relation from McDougall and Jackett (2005) and ludicone et al (2008)

$$\frac{\dot{\gamma}}{\gamma} = b \frac{\dot{\rho}^{\text{local}}}{\rho^{\text{local}}} = b \left(-\alpha \,\dot{\Theta} + \beta \,\dot{S} \right) \qquad b = \frac{|\nabla \gamma|}{|\nabla \rho^{\text{local}}|} \approx 1??$$
 (20)

 Jeff Stanley's ongoing work with Trevor to generalize the Klocker and McDougall (2009) ω -surfaces holds some promise.

