# WMT analysis in ocean models: some thoughts and questions

*Watermass Transformation Meeting 2019*
4-6 Feb 2019

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# Goals and apologies

- ⋆ 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?

  $\longrightarrow$ 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.

  $\longrightarrow$ It is for us to determine if the investment has sufficient payoff.
- ⋆ APOLOGIES for the heaps of maths.
  "Everything should be made as simple as possible, but not simpler." A. Einstein.

# Outline

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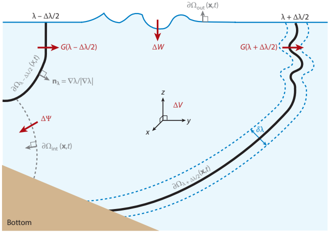
# Basic mathematical expressions (Groeskamp et al 2019)

MEASURE SEAWATER TRANSPORT ACROSS ISO-SURFACES OF A SCALAR PROPERTY.
Assume smooth $\lambda$ surfaces $\Longrightarrow$ average over microstructure as per De Szoeke and Bennett (1993).




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

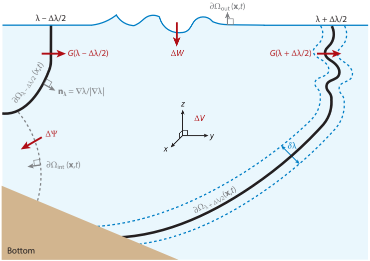
Fundamental theorem of calculus renders the more useful form

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

Discretized form for numerical calculations

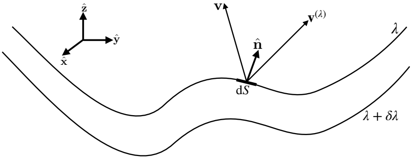
$$G(\lambda) \approx \underbrace{\frac{1}{\Delta\lambda} \sum_{n=1}^{N} \sum_{i,j,k} \Pi(\lambda_n, \lambda, \Delta\lambda)\, (\rho\, \dot{\lambda})_{i,j,k}\, V_{i,j,k}.}_{\text{Box-car binning of the material change } \rho\,\dot{\lambda} \text{ into } N\text{-bins}} \tag{3}$$

# Notable conceptual characteristics (Groeskamp et al 2019)




- Suitable kinematic framework for studying tracer dynamics.
  - $\lambda$ surfaces can be non-monotonic and disconnected.
  - $\lambda$ is typically density (which one?), temperature, or salinity.
  - Geographical non-locality $\Longrightarrow$ distinct from strict isopycnal analysis.
  - Generalizable to $\Theta - S$ 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.
  - $\Longrightarrow$ Still need Eulerian or Lagrangian kinematics for momentum dynamics.
  - $\Longrightarrow$ Perfect-fluid dynamical processes ($\dot{\lambda} = 0$) are invisible to WMT.

# Tutorial on dia-surface transport (Section 6.7 of Griffies 2004)




In Groeskamp et al (2019), we define the dia-surface velocity component, $u^{\text{dia}}$, according to the volume of seawater transported across a moving surface

$$\mathcal{T} \equiv u^{\text{dia}}\, \mathrm{d}S \equiv \hat{\boldsymbol{n}} \cdot (\boldsymbol{v} - \boldsymbol{v}^{(\lambda)})\, \mathrm{d}S \tag{4}$$

$$\hat{\boldsymbol{n}} = \frac{\nabla\lambda}{|\nabla\lambda|} = \text{ surface outward normal direction} \tag{5}$$

$$\boldsymbol{v} = \text{fluid parcel velocity} \qquad \text{and} \qquad \frac{\partial\lambda}{\partial t} + \boldsymbol{v}^{(\lambda)} \cdot \nabla\lambda = 0. \tag{6}$$

Following from these definitions we have

$$\frac{\mathrm{D}\lambda}{\mathrm{D}t} = \frac{\partial\lambda}{\partial t} + \boldsymbol{v} \cdot \nabla\lambda = \frac{\partial\lambda}{\partial t} + \boldsymbol{v}^{(\lambda)} \cdot \nabla\lambda + (\boldsymbol{v} - \boldsymbol{v}^{(\lambda)}) \cdot \nabla\lambda = 0 + u^{\text{dia}}\, |\nabla\lambda| \tag{7}$$

$$\Longrightarrow u^{\text{dia}} = \frac{1}{|\nabla\lambda|} \frac{\mathrm{D}\lambda}{\mathrm{D}t} = \frac{\dot{\lambda}}{|\nabla\lambda|}. \tag{8}$$

# Outline

2 What we need from the models

# Budget analysis

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

- KINEMATIC METHOD: Direct calculation but offers no process information

$$\underbrace{\rho\,\dot{\lambda}}_{\text{material change}} = \underbrace{\frac{\partial(\rho\,\lambda)}{\partial t}}_{\text{local tendency}} + \underbrace{\nabla \cdot (\rho\,\lambda\,\boldsymbol{v}^{\dagger})}_{\text{residual mean advection}} \qquad \text{with} \qquad \boldsymbol{v}^{\dagger} = \boldsymbol{v} + \boldsymbol{v}^{\text{sgs}}. \tag{9}$$

- PROCESS METHOD: Indirect calculation offering full process information

$$\rho\,\dot{\lambda} = -\nabla \cdot \boldsymbol{J} = \sum(\text{interior processes + boundaries}). \tag{10}$$

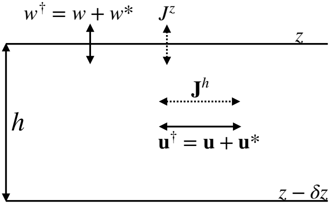
- SOME NUMERICAL ISSUES THAT MAKE CAREFUL BUDGETS TOUGH:
  - ⋆ Models generally have changing cell thicknesses, thus requiring care to keep track of cell volume along with tracer evolution (more later).
  - ⋆ Multi-step time stepping means ocean is incrementally updated; e.g., time-implicit vertical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

$$\boldsymbol{v}^{\dagger} = \boldsymbol{v} + \boldsymbol{v}^{\text{sgs}} \quad \text{and yet} \quad \nabla \cdot (\rho\,C\,\boldsymbol{v}^{\dagger}) \neq \nabla \cdot (\rho\,C\,\boldsymbol{v}) + \nabla \cdot (\rho\,C\,\boldsymbol{v}^{\text{sgs}}). \tag{11}$$

# Outline

3 Scalar equations in ocean models

# Z-coordinate scalar eqns w/ eddy-induced $\boldsymbol{v}^*$



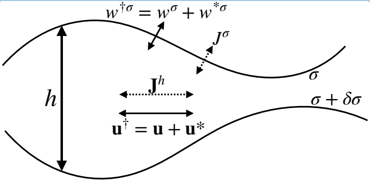

$$\frac{\mathrm{D}^\dagger}{\mathrm{D}t} = \frac{\partial}{\partial t} + \boldsymbol{v}^\dagger \cdot \nabla, \quad \boldsymbol{v}^\dagger = \boldsymbol{v} + \boldsymbol{v}^* \ \text{ w/ local mass conserve eddy} \Longrightarrow \nabla \cdot (\rho\, \boldsymbol{v}^*) = 0 \tag{12}$$

$$\frac{\mathrm{D}^\dagger(\rho\,\delta V)}{\mathrm{D}t} = 0 \Longrightarrow \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\, \boldsymbol{v}) = 0 \ \text{ usual continuity equation even with } \boldsymbol{v}^* \neq 0 \tag{13}$$

$$\rho\, \frac{\mathrm{D}^\dagger C}{\mathrm{D}t} = -\nabla \cdot \boldsymbol{J} \Longrightarrow \frac{\partial(\rho\, C)}{\partial t} + \nabla \cdot (\rho\, C\, \boldsymbol{v}^\dagger) = -\nabla \cdot \boldsymbol{J}. \tag{14}$$

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

# Quasi-Eulerian scalar eqns w/ eddy-induced $\boldsymbol{v}^*$




$$\frac{\partial(h\,\rho)}{\partial t} + \nabla_\sigma \cdot (h\,\rho\,\boldsymbol{u}^{\dagger}) + \delta_\sigma(\rho\,w^{\dagger\sigma}) = 0 \;\text{ and }\; \nabla_\sigma \cdot (h\,\rho\,\boldsymbol{u}^{*}) + \delta_\sigma(\rho\,w^{*\sigma}) = 0 \tag{15}$$

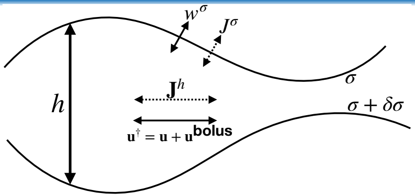
$$\frac{\partial(h\,\rho\,C)}{\partial t} + \nabla_\sigma \cdot (h\,\rho\,C\,\boldsymbol{u}^{\dagger}) + \delta_\sigma(\rho\,C\,w^{\dagger\sigma}) = -\left[\nabla_\sigma \cdot (h\,\boldsymbol{J}^h) + \delta_\sigma J^\sigma\right] \tag{16}$$

$$z_\sigma = \frac{\partial z}{\partial \sigma} \qquad h = z_\sigma\,\mathrm{d}\sigma \qquad w^{\dagger\sigma} = \frac{\partial z}{\partial \sigma}\frac{\mathrm{D}^{\dagger}\sigma}{\mathrm{D}t} = w^{\sigma} + \boldsymbol{v}^* \cdot z_\sigma \nabla\sigma = w^{\sigma} + w^{*\sigma} \tag{17}$$

$$\delta_\sigma = \mathrm{d}\sigma\,\frac{\partial}{\partial\sigma} \qquad \nabla_\sigma = \nabla_z + \boldsymbol{S}\,\partial_z \qquad \boldsymbol{S} = \nabla_\sigma z = -z_\sigma \nabla_z \sigma \qquad J^\sigma = z_\sigma \nabla\sigma \cdot \boldsymbol{J} \tag{18}$$

- Coordinate transformation of the z-coordinate equations (e.g., Griffies 2004).
- $w^\sigma$ & $w^{*\sigma}$ 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) $\Longrightarrow$ isopycnal coordinates are not available.

# Quasi-Lagrangian scalar eqns w/ eddy-induced $\boldsymbol{u}^{\text{bolus}}$



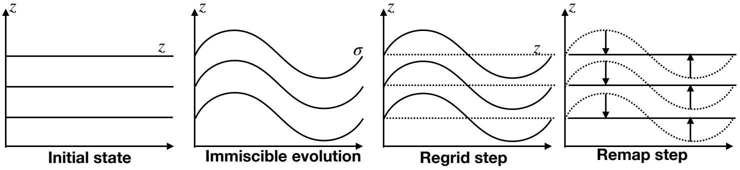

$$\frac{\partial (h\,\rho)}{\partial t} + \nabla_\sigma \cdot (h\,\rho\,\boldsymbol{u}^\dagger) + \delta_\sigma(\rho\,w^\sigma) = 0 \tag{19}$$

$$\frac{\partial (h\,\rho\,C)}{\partial t} + \nabla_\sigma \cdot (h\,\rho\,C\,\boldsymbol{u}^\dagger) + \delta_\sigma(\rho\,C\,w^\sigma) = -\left[\nabla_\sigma \cdot (h\,\boldsymbol{J}^h) + \delta_\sigma J^\sigma\right] \tag{20}$$

$$w^\sigma = \frac{\partial z}{\partial \sigma}\frac{\mathrm{D}\sigma}{\mathrm{D}t} \qquad \boldsymbol{u}^\dagger = \boldsymbol{u} + \boldsymbol{u}^{\text{bolus}} = \text{horizontal residual mean velocity.} \tag{21}$$

- $w^\sigma$ is specified based on dia-surface processes such as mixing: a *thermodynamic* or *process* approach.
- Makes use of $\boldsymbol{u}^{\text{bolus}}$ to ensure advective transport retains layer integrated constant mass, 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 $\boldsymbol{u}^{\text{bolus}}$ and $\boldsymbol{v}^*$.
- Quasi-Lagrangian codes: HYCOM, MOM6, MPAS-O, NEMO (immature?).

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

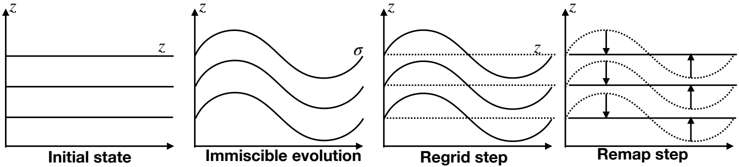



- IMMISCIBLE LAYER STEP: Using the quasi-Lagrangian formulation, evolve ocean state to time $t + \Delta t$ using $\dot{\sigma} = 0$ (so integrated mass is constant in each layer) yet with the full suite of SGS parameterizations

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

- 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.

# Comments about ALE




- 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, a step that is the operationally same as vertical advection.
- To diagnose the full advection operator, we need to diagnose the contribution from remapping so that

$$\nabla \cdot (\rho\, C\, \boldsymbol{v}^{\dagger}) = \underbrace{\nabla_{\sigma} \cdot (\rho\, C\, \boldsymbol{u}^{\dagger})}_{\text{horizontal layer advection}} + \text{remapping}. \tag{22}$$

- There is no CFL associated with vertical remapping; useful for fine vertical grid spacing.
- The vertical remapping algorithm can be used for diagnostic purposes to remap and bin grid cell tendencies according to arbitrary surfaces.

# Outline

# Spurious mixing and unmixing

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

$$\nabla \cdot (\rho \, C \, \boldsymbol{v}^{\dagger})_{\text{model}} = \nabla \cdot (\rho \, C \, \boldsymbol{v}^{\dagger})_{\text{exact}} + \nabla \cdot (\rho \, C \, \boldsymbol{v}^{\dagger})_{\text{noise}} \tag{23}$$

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

$$\frac{\partial(\rho \, \lambda)}{\partial t} + \nabla \cdot (\rho \, \lambda \, \boldsymbol{v}^{\dagger})_{\text{exact}} = -\nabla \cdot \left[ \boldsymbol{J} + (\rho \, \lambda \, \boldsymbol{v}^{\dagger})_{\text{noise}} \right]. \tag{24}$$

- ⋆ Noise term is not physical. Hence, if it is large it can corrupt the physical integrity of the simulation; e.g., spurious watermass trends can be induced.
- ⋆ 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: $0.25^{\circ} \longrightarrow 0.1^{\circ}$.
- ⋆ Noise is reduced when use higher order accurate advection and when move to ALE vertical remapping (with high order accurate remapping).
- ⋆ After 20 years of trying, there is no exact and general means to locally diagnose $\nabla \cdot (\rho \, C \, \boldsymbol{v}^{\dagger})_{\text{noise}}$ in a realistic ocean climate simulation. However, there are ideas that might get us part of the way there (e.g., Ryan Holmes).

# Ambiguity with the binning process

The discrete water mass transformation expression is given by

$$G(\lambda) \approx \underbrace{\frac{1}{\Delta\lambda} \sum_{n=1}^{N} \sum_{i,j,k} \Pi(\lambda_n, \lambda, \Delta\lambda)\, (\rho\, \dot{\lambda})_{i,j,k}\, V_{i,j,k}}_{\text{Box-car binning of the material change } \rho\,\dot{\lambda} \text{ into } N\text{-bins}} \tag{25}$$

with analogous expressions for layer tracer budgets.

- What bin size should we use?
  - In many cases, bin size can have a nontrivial impact on the results.
  - Is that because we are using poor numerics?
  - Perhaps ALE remapping will help?
- 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.
  - Given sentivities to numerical choices (binning algorithm, binning classes), the lack of a double-check is a real problem.
  - The analogous issue does *not* arise with native-grid budget analyses, since we can check “left hand side = right hand side” at each grid cell.
- Should we consider a detailed best-practices guide for WMT analysis?

# What is the best globally defined buoyancy?

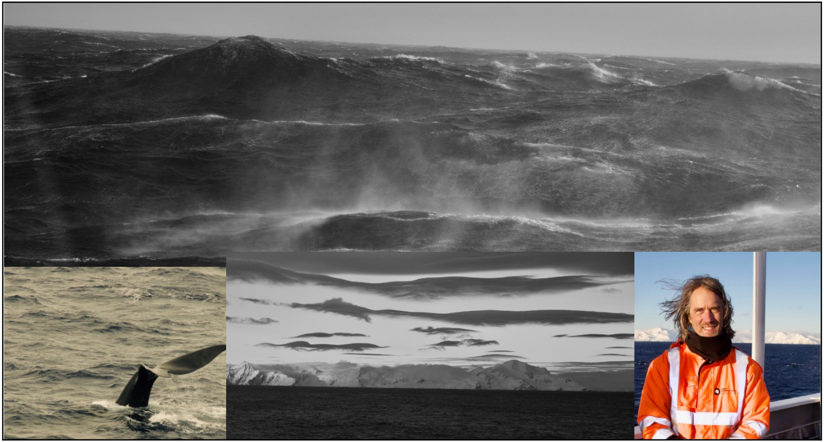
For buoyancy-based WMT analysis, we remain using non-optimal density fields such as $\gamma^{\mathrm{n}}$ or potential density.

- A wish-list for a new-and-improved $\gamma$ field.
  - ⋆ A state-dependent equation for $\gamma$ to allow online binning.
  - ⋆ An expression for $\gamma$ that is general enough to allow for arbitrary model state: paleoclimate and climate change.
  - ⋆ No direct connection to observational data so that there is no geographical dependence.
  - ⋆ Accurate enough so that the material changes in $\gamma$ are very close to those of locally referenced potential density.
  - ⋆ Stated alternatively, we wish to have the $b-$factor from McDougall and Jackett (2005) and Iudicone et al (2008) near unity everywhere

$$\frac{\dot{\gamma}}{\gamma} = b\,\frac{\dot{\rho}^{\mathrm{local}}}{\rho^{\mathrm{local}}} = b\,(-\alpha\,\dot{\Theta} + \beta\,\dot{S}) \qquad b = \frac{|\nabla\gamma|}{|\nabla\rho^{\mathrm{local}}|} \approx 1. \tag{26}$$

- Geoff Stanley's ongoing work with Trevor to generalize the Klocker and McDougall (2009) $\omega$-surfaces holds some promise.

# Many thanks for your time and attention



From the Weddell Sea and Scotia Sea, autumn 2017 on the RRS James Clark Ross