# Vertical Lagrangian-remapping, generalized vertical coordinates, and spurious diapycnal mixing in ocean models

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Aetherworld

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#### Key points in this talk

- \* SPURIOUS DIAPYCNAL MIXING: This problem corrupts many state-of-the-science ocean simulations, particularly those for climate where errors accumulate to degrade stratification and contribute to spurious tracer evolution.
- \* DYNAMICAL CORE FORMULATION: The vertical Lagrangian-remap method and generalized vertical coordinate formulation of ocean equations can be understood through basic notions of fluid mechanics.
- \* CONJECTURE: Vertical Lagrangian-remapping with an appropriate hybrid vertical coordinate provides a suitable (perhaps optimal) framework to simulate the ocean climate system without incurring physically disruptive spurious mixing.
  - $\longrightarrow$  We are not there yet, but we will show promising results.
- \* ELEMENTS OF THIS TALK ARE TAKEN FROM:
  - A primer on ocean generalized vertical coordinate dynamical cores based on the vertical Lagrangian-remap method, 2020: Griffies, Adcroft, and Hallberg, in revision at JAMES
  - Adcroft et al, 2019: The GFDL Global Ocean and Sea Ice Model OM4.0: Model Description and Simulation Features, *JAMES*.

#### Outline

1 The spurious numerical diapycnal mixing problem

2 Vertical Lagrangian-remapping w/ generalized vertical coordinates

Closing comments

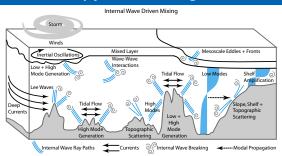


#### Outline

1 The spurious numerical diapycnal mixing problem



#### Physically based diapycnal mixing MacKinnon et al (2017)



- \* There are many physical sources for ocean diapycnal mixing.
- \* Diapycnal mixing impacts on vertical stratification, dynamics, tracer ventilation (heat, carbon), sea level, with effects more important as time increases (e.g., climate).
- \* Coordinated efforts such as the US Climate Process Team on internal gravity wave mixing (2010-2015) and ongoing German TRR 181 on energetic transfers have enhanced integrity of physically based mixing parameterizations used by climate and prediction models.
- \* Unfortunately, numerical transport (i.e., advection schemes) can introduce spurious diapycnal mixing that is larger than physics.



#### Framing the spurious mixing problem

The numerical representation of advection  $= \nabla \cdot (\rho \, C \, v)$  generally introduces spurious mixing and unmixing due to truncation errors

$$\nabla \cdot (\rho \, C \, \mathbf{v})_{\text{model}} = \nabla \cdot (\rho \, C \, \mathbf{v})_{\text{exact}} + \nabla \cdot (\rho \, C \, \mathbf{v})_{\text{error}} \tag{1}$$

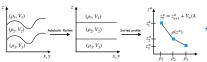
\* Errors in numerical advection can be interpreted as an extra SGS term

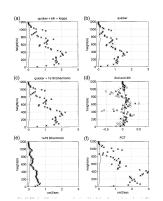
$$\frac{\partial(\rho\,C)}{\partial t} + \nabla\cdot(\rho\,C\,v)_{\text{exact}} = -\nabla\cdot\left[\boldsymbol{J} + (\rho\,C\,v)_{\text{error}}\right]. \tag{2}$$

- \* Error term is not physical nor is it under our direct control. If large it can corrupt physical integrity of the simulation.
- Error term can become larger when refine grid spacing to partially resolve mesoscale eddies, which pump tracer variance to the grid scale.
- \* Spurious mixing from the error term is reduced (but not eliminated) when use higher order accurate advection.
- \* Key concern for climate is spurious diapycnal mixing.
- ⋆ Spurious diapycnal mixing is reduced when use quasi-isopycnal vertical coordinate; errors stopped at layer interface.

#### First diagnostic of spurious diapycnal mixing

Griffies, Pacanowski, Hallberg (2000)





- \* A method based on density sorting to produce a stable background profile,  $\rho_{\rm back}$ , following Winters and D'Asaro (1995).
- \* In an adiabatic simulation, evolution of the background state only arises from spurious numerical sources, which we interpret as an effective diffusivity,  $\kappa_{\it eff}$

$$\frac{\partial \rho_{\text{back}}}{\partial t} = \frac{\partial}{\partial z^*} \left[ \kappa_{\text{eff}} \, \frac{\partial \rho_{\text{back}}}{\partial z^*} \right] \tag{3}$$

- \* Diagnosed levels of  $\kappa_{\it eff}$  from numerical advection can be 10-100x larger than ocean measurements.
- Problems can be enhanced in mesoscale eddying simulations where tracer variance is pumped to the gridscale.
- Spurious mixing scales with lateral grid Reynolds number (see also Ilicak, Adcroft, Griffies, Hallberg, (2012)):

$$Re_{grid} = U \Delta t / \Delta < \mathcal{O}(10).$$
 (4)

Larger Re<sub>grid</sub> allows for noisy vertical velocity from noisy horizontal convergences: recipe for spurious mixing.

But Re<sub>grid</sub> > 10 is very common, thus incurring spurious mixing.



### Many existing measures of spurious (diapycnal) mixing

- \* Sorting along with passive tracer releases
  - Hill, Ferreira, Campin, Marshall, Abernathey, Barrier, 2012: Controlling spurious diapycnal mixing in eddy-resolving height-coordinate ocean models-insights from virtual deliberate tracer release experiments
  - Getzlaff, Nurser, Oschlies, 2012: Diagnostics of diapycnal diffusion in z-level ocean models. Part II: 3-Dimensional OGCM
- \* BACKGROUND/REFERENCE POTENTIAL ENERGY: Global number (though Ilicak, 2016 suggests local)
  - Ilicak, Adcroft, Griffies, Hallberg, 2012: Spurious dianeutral mixing and the role of momentum closure
  - Petersen, Jacobsen, Ringler, Hecht, Maltrud, 2015: Evaluation of the arbitrary Lagrangian-Eulerian vertical coordinate method in the MPAS-Ocean model
  - Zhao and Liu, 2016: Spurious dianeutral mixing in a global ocean model using spherical centroidal vorgon it essellations
    - Ilicak, 2016: Quantifying spatial distribution of spurious mixing in ocean models
  - Gibson, Hogg, Kiss, Shakespeare, Adcroft, 2017: Attribution of horizontal and vertical contributions to spurious mixing in an Arbitrary Lagrangian-Eulerian ocean model
  - VARIANCE METHODS: provides a map for all mixing (no distinction between diapycnal versus isopycnal).
    - Morales-Maqueda and Holloway, 2006: Second-order moment advection scheme applied to Arctic Ocean simulation
    - Burchard, Rennau, 2008: Comparative quantification of physically and numerically induced mixing in ocean models
    - Klingbeil, Mohammadi-Aragh, Grawe, Burchard, (2014): Quantification of spurious dissipation and mixing-discrete variance decay in a Finite-Volume framework
- \* WATERMASS ANALYSIS
  - Lee, Coward, Nurser 2002: Spurious Diapycnal Mixing of the Deep Waters in an Eddy-Permitting Global Ocean Model
  - Urakawa, Hasumi, 2014: Effect of numerical diffusion on the water mass transformation in eddy-resolving models
  - Megann, 2018: Estimating the numerical diapycnal mixing in an eddy-permitting ocean model numerical diapycnal mixing in an eddy-permitting ocean mixing in an eddy-p
  - Holmes, Zika, England, 2019: Diathermal heat transport in a global ocean model

#### Some general points emerging from the studies

- Diagnosing the spurious mixing is useful for understanding its character but insufficient to remove the problem.
- \* Higher order numerics helps [e.g., Hill et al (2012)], though realistic simulatons need flux limiters that add mixing.
- \* Maintenance of modest grid Reynolds number [  $Re_{grid} < \mathcal{O}(10)$ ] is key to suppress velocity noise that translates into spurious mixing [e.g., Ilicak, Adcroft, Griffies, Hallberg (2012)].
- Problem arises from advection in both vertical and horizontal (since isopycnals slope) [e.g., Gibson et al (2017)].
- Claims that the problem is solved by certain advection schemes [e.g., Hill et al (2012)] have ignored flux limiters, which add mixing and yet are needed to ensure positive definite tracer concentrations [e.g., Morales-Maqueda and Holloway (2006)].
- ★ Ilicak et al (2012) and Megann (2018) and Adcroft et al (2019) suggest that 1/4 degree Z—coordinate climate models are poorly situated:
  - Admitting mesoscale eddies w/ 1/4-degree generally requires  $\mathrm{Re}_{\mathrm{grid}} > \mathcal{O}(10)$ .
  - Suggestions (anecdotal) that 1/10-degree Z-model climate simulations have far smaller spurious mixing; perhaps the grid resolves enough of the variance cascade that its dissipation does not require excessive mixing

#### Outline

2 Vertical Lagrangian-remapping w/ generalized vertical coordinates

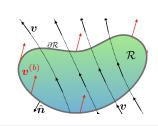


#### Focusing on the vertical solution method

- \* Isopycnal models have direct control over diapycnal transport.
- \* But isopycnal models are have problems for climate modeling (weakly stratified high latitudes) and coastal (weak stratification on shelves).
- \* Hybrid vertical coordinates is a strategy to reduce spurious mixing while allowing for global coverage.
- Vertical Arbitrary-Lagrangian-Eulerian (ALE) method, including the special case of vertical Lagangian-remapping, is a strategy to realize hybrid vertical coordinates.
- \* Proposed terminology:
  - Quasi-Eulerian: restricted set of generalized vertical coordinates, where coordinate is directly related to free surface (Boussinesq) or bottom pressure (non-Boussinesq).
  - Vertical Arbitrary-Lagrangian-Eulerian (ALE) without remapping: as in NEMO-z̃ and MPAS-O.
  - Vertical ALE with remapping, aka Vertical Lagrangian Remapping: as in HYCOM and MOM6.
- \* Here we present some of the fundamentals, aiming to develop intuition based on fluid mechanics rather than numerical algorithm details.

### Finite volume (weak formulation): Leibniz-Reynolds

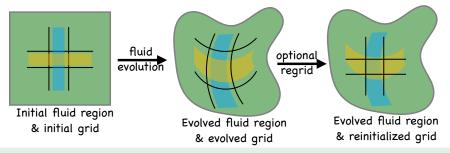
$$\begin{split} \frac{\mathrm{d}}{\mathrm{d}t} \left[ \int_{\mathcal{R}} \rho \, C \, \mathrm{d}V \right] &= -\oint_{\partial \mathcal{R}} \left[ \rho \, C \, (\mathbf{v} - \mathbf{v}^{(b)}) + \mathbf{J} \right] \cdot \hat{\mathbf{n}} \, \mathrm{d}\mathcal{S} \\ \frac{\mathrm{d}}{\mathrm{d}t} \left[ \int_{\mathcal{R}} \rho \, \mathbf{v} \, \mathrm{d}V \right] &= -\int_{\mathcal{R}} \left[ 2 \, \mathbf{\Omega} \wedge \rho \, \mathbf{v} + \rho \, \nabla \Phi \right] \mathrm{d}V \\ &+ \oint_{\partial \mathcal{R}} \left[ -p \, \mathbb{I} - \rho \, \mathbf{v} \otimes (\mathbf{v} - \mathbf{v}^{(b)}) + \mathbb{T} \right] \cdot \hat{\mathbf{n}} \, \mathrm{d}\mathcal{S} \end{split}$$



- $\star$  Discrete equations follow by specializing  ${\cal R}$  to a model grid cell.
- $\star$  Models typically formulate scalar prognostic budgets for extensive quantities: heat, salt, and thus diagnose intensive quantities as in  $C = (C \, \rho \, \Delta V)/(\rho \, \Delta V)$ .
- $\star$  However, we often formulate a discrete velocity equation (intensive),  $\partial_t v$ , rather than a discrete momentum equation (extensive),  $\partial_t (v \, \rho \, \Delta V)$ . Vector-invariant velocity equation (e.g., Sadourny energy-enstrophy) has advantages over advective-form momentum equation.
- Advection refers to the transport of fluid relative to the grid. Fully Lagrangian has zero advection. Fully Eulerian has all motion leading to advection.

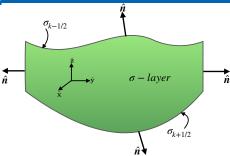
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#### The Arbitrary Lagrangian-Eulerian method (ALE)



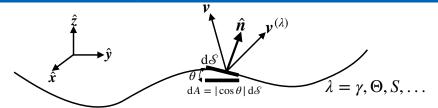
- $\star$  ALE broadly refers to any method that considers moving cell boundaries.
  - STEP ONE: If grid moves with the flow it is a Lagrangian step.
     Non-Lagrangian grid motion is also considered by certain ALE approaches.
  - STEP TWO: The regrid/remap step ideally does not alter the ocean state. Rather, it moves the grid ("regrid") and estimates the ocean state on the new grid ("remap").
- ⋆ Remap step operationally equals to advection (transport relative to grid).
- \* Ocean models restrict their moving meshes to be just in the vertical and formulate equations using generalized vertical coordinates.

# Distinguishing solution methods according to $v^{(b)}$



- \* LATERAL BOUNDARIES:  $\mathbf{v}^{(b)} \cdot \hat{\mathbf{n}}_{\text{sides}} = 0$  (no lateral cell movement).
- $\star$  RIGID-LID Z-MODELS:  $v^{(b)} \cdot \hat{n} = 0$  for all boundaries.
- \* FREE SURFACE MODELS:  $\mathbf{v}^{(b)} \cdot \hat{\mathbf{n}}_{k=1/2} \neq 0$ .
- \* ANALYTICALLY SPECIFIED COORDINATES: barotropic motion specifies  $\mathbf{v}^{(b)} \cdot \hat{\mathbf{n}}_{k\pm 1/2} \neq 0$  for  $\sigma_{\text{terrain}} = (z-\eta)/(H+\eta), z^* = H \sigma_{\text{terrain}}$ , others.
- \* ISOPYCNAL LAYERS:  $\mathbf{v}^{(b)} \cdot \hat{\mathbf{n}}_{k\pm 1/2} \neq 0$  determined by following layer interfaces.
- \* MORE GENERAL ALE:  $v^{(b)} \cdot \hat{n}_{k\pm 1/2} \neq 0$  is arbitrary.

#### Generalized vertical coord & dia-surface transport



Dia-surface velocity component,  $u^{dia}$ , is defined by seawater transport through moving  $\lambda$  surface

 $\mathbf{v} = \text{(barycentric)}$  velocity of fluid element and  $(\partial_t + \mathbf{v}^{(\lambda)} \cdot \nabla) \lambda = 0$ .

$$\mathcal{T} \equiv u^{\text{dia}} \, \mathrm{d}\mathcal{S} \equiv \hat{\pmb{n}} \cdot (\pmb{v} - \pmb{v}^{(\lambda)}) \, \mathrm{d}\mathcal{S} \Longrightarrow \mathrm{can} \mathrm{\ have\ non-zero\ transport\ even\ if\ } \hat{\pmb{n}} \cdot \pmb{v} = 0.$$

$$\hat{a} = \nabla \nabla \nabla \nabla \nabla^{-1}$$
 normal direction pointing to larger  $\nabla$ 

$$\hat{\mathbf{n}} = \nabla \lambda |\nabla \lambda|^{-1} = \text{normal direction pointing to larger } \lambda.$$

Following from these definitions we have

$$\frac{\mathrm{D}\lambda}{\mathrm{D}t} = (\partial_t + \mathbf{v} \cdot \nabla) \, \lambda = [\partial_t + \mathbf{v}^{(\lambda)} \cdot \nabla + (\mathbf{v} - \mathbf{v}^{(\lambda)}) \cdot \nabla] \, \lambda = 0 + u^{\mathsf{dia}} \, |\nabla \lambda|$$

$$\Longrightarrow |\nabla \lambda| \, u^{\mathrm{dia}} = \frac{\mathrm{D}\lambda}{\mathrm{De}} = \dot{\lambda} \Longrightarrow \mathrm{material} \, \mathrm{changes} \, \mathrm{in} \, \lambda \Longleftrightarrow \mathrm{dia-surface} \, \mathrm{transport}.$$

For stably stratified  $\lambda$ -surfaces as in generalized vertical coordinates with  $\lambda = \sigma$ , we define



$$\mathcal{T} \equiv u^{\text{dia}} dS \equiv w^{(\dot{\sigma})} dA = \frac{\partial z}{\partial \sigma} \dot{\sigma} \Longrightarrow \frac{D}{Dt} = \left[ \frac{\partial}{\partial t} \right] + u \cdot \nabla_{\sigma} + w^{(\dot{\sigma})} \frac{\partial}{\partial z}$$

(5)

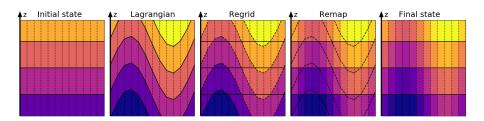
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#### Vertical Lagrangian-Remapping method

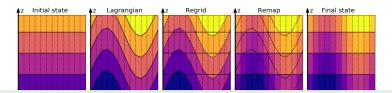


- ⋆ A flavor of ALE where grid cell sides are rigid but top and bottom move.
- \* HYCOM and MOM6 implement the regrid/remap step, constituting the *vertical Lagrangian remap method*.
- \* HYCOM and MOM6 implement the method so that grid layers can vanish and inflate (useful for estuaries and moving ice-shelf grounding lines).
- MPAS-O and NEMO algorithms do not implement the vertical regrid/remap step. They are ALE but not Lagrangian.





#### Comments on vertical Lagrangian-remapping



- WHERE IS DIA-SURFACE ADVECTION? It is part of the evolution of the grid cell thicknesses. Cell interfaces move and carry the state.
  - $\star$  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

$$\nabla \cdot (\rho \, C \, v) = \underbrace{\nabla_{\sigma} \cdot (\rho \, C \, u)}_{\text{horizontal layer advection}} + \text{ remapping.} \tag{11}$$

- There is no CFL associated with vertical remapping; useful for fine vertical grid spacing. But remember stability does not imply accuracy.
- The vertical remapping algorithm can be used for diagnostic purposes to remap and bin grid cell tendencies according to arbitrary surfaces.

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### Distinguishing three solution algorithms

- \* We consider three solution algorithms used by ocean models:
  - quasi-Eulerian (e.g., MITgcm, MOM5, NEMO)
  - vertical ALE without remapping (e.g., NEMO-z̃, MPAS-O)
  - vertical Lagrangian-remapping (e.g., HYCOM, MOM6)
- \* To exemplify the rudiments of the algorithms, consider the following bare-bones suite of model equations consisting just of thickness and thickness-weighted tracer equations.

$$\frac{\partial h}{\partial t} = -\nabla_{\sigma} \cdot (h \mathbf{u}) - \Delta_{\sigma} w^{(\dot{\sigma})}$$
 thickness (12a)

$$\frac{\partial h}{\partial t} = -\nabla_{\sigma} \cdot (h \, \mathbf{u}) - \Delta_{\sigma} w^{(\dot{\sigma})}$$
 thickness (12a) 
$$\frac{\partial (h \, C)}{\partial t} = -\nabla_{\sigma} \cdot [h \, \mathbf{u} \, C] - \Delta_{\sigma} [C \, w^{(\dot{\sigma})}]$$
 thickness weighted tracer. (12b)





## Quasi-Eulerian algorithm

 Vertical coordinate analytically determined by barotropic motion that then determines thickness tendency as in

$$z^* = \frac{z - \eta}{H + \eta} \Longrightarrow dz = (1 + \eta/H) dz^* \Longrightarrow \partial_t(dz) = \frac{dz^*}{H} \partial_t \eta. \tag{13}$$

- \* Example codes: MITgcm, MOM5, NEMO-basic, ROMS
- There is no realization of this algorithm with vanishing layers that maintains machine precision conservation.

#### ALGORITHM STEPS

$$[\Delta_{\sigma} w^{(\dot{\sigma})}]^{(n)} = -[\Delta_{\sigma} w^{\text{grid}}]^{(n)} - \nabla_{\sigma} \cdot [h \mathbf{u}]^{(n)}$$

$$\bullet h^{(n+1)} = h^{\dagger} - \Delta t \, \Delta_{\sigma} \left[ w^{(\dot{\sigma})} \right]^{(n)}$$

grid motion ∝ free surface diagnose dia-surface transport horz advection thickness update horz advection tracer update vert advection thickness update vert advection tracer update.

### Algorithm for vertical ALE without remapping

- ★ General thickness tendency with general vertical coordinates.
- \* Vertical coordinate need not be analytically defined.
- $\star$  Example codes: MPAS-O and NEMO- $\tilde{z}$
- \* There is no realization of this algorithm with vanishing layers that maintains machine precision conservation.

#### ALGORITHM STEPS (ONLY STEP 1 DIFFERS FROM QUASI-EULERIAN)

$$b^{(n+1)} = h^{\dagger} - \Delta t \, \Delta_{\sigma} \left[ w^{(\dot{\sigma})} \right]^{(n)}$$

general layer motion diagnose dia-surface transport

horz advection thickness update

horz advection tracer update vert advection thickness update

vert advection tracer update.



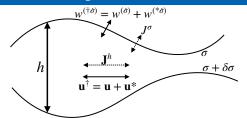
### Algorithm for Vertical Lagrangian-remapping

- ⋆ Pioneered by Bleck (2002).
- ★ General thickness tendency with general vertical coordinates.
- ★ Vertical coordinate need not be analytically defined.
- ★ Lagrangian step includes horizontal dynamics/physics + vertical physics
- ★ Example codes: HYCOM and MOM6
- MOM6 allows for vanishing layers with machine precision conservation.

#### ALGORITHM STEPS

- (a)  $[h C]^{\dagger} = [h C]^{(n)} \Delta t [\nabla_{\sigma} \cdot (h C u)]^{(n)}$  horz advection tracer update
- $\Delta_{\sigma} w^{(\dot{\sigma})} = -(h^{\text{target}} h^{\dagger})/\Delta t$  diagnose dia-surface transport

## Scalar equations for algorithms without remapping

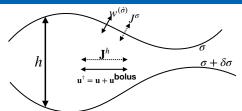


- \* Resolved vertical velocity,  $w^{(\dot{\sigma})}$ , and parameterized vertical velocity (e.g., eddy-induced velocity),  $w^{(*\dot{\sigma})}$ , are diagnosed via continuity equations.
- \* Both  $w^{(\dot{\sigma})}$  &  $w^{(*\dot{\sigma})}$  penetrate layer interfaces as per traditional advection.

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

$$\frac{\partial(h\,\rho\,C)}{\partial t} = 0 \quad \text{(14)}$$

## Scalar equations with vertical Lagrangian remapping

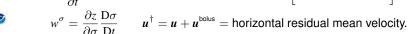


- $\star$  Vertical advection from  $w^{(\dot{\sigma})}$  is handled during the remap step.
- \* Vertical parameterized advection from  $w^{(*\dot{\sigma})}$  is handled during the Lagrangian step via the horizontal convergence  $-\nabla_{\sigma} \cdot [h \mathbf{u}^{\dagger}]$ .
- ★ Use of u<sup>bolus</sup> ensures that horizontal advective transport retains constant layer integrated mass just as in an adiabatic isopycnal layer.

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

$$\frac{\partial(h\rho)}{\partial t} + \nabla_{\sigma} \cdot (h\rho \mathbf{u}^{\dagger}) + \delta_{\sigma}(\rho w^{(\dot{\sigma})}) = 0$$

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



(19)

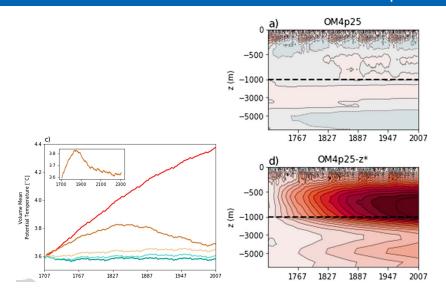
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#### Outline

3 Closing comments



### Choice of vertical coordinate matters for heat uptake!



- $\star$  MOM6/SIS2 at  $0.25^{\circ} \times 75$ -layers forced by interannual CORE.
- $\star$   $z^*$  dominated by spurious mixing relative to hybrid isopycnal- $z^*$ .

### Summary points

- We understand a great deal about ocean mixing and how to parameterize it. However, spurious numerical diapycnal mixing remains a nontrivial problem with many simulations that can corrupt their physical fidelity.
- $\star$  There are a handfull of methods for diagnosing spurious mixing. They all point to the need for improved numerical accuracy and maintenance of modest [Re<sub>orid</sub>  $< \mathcal{O}(10)$ ] grid Reynolds number.
- Vertical Lagrangian-remapping offers a framework for incorporating hybrid/generalized vertical coordinates.
- The design of hybrid coordinates should be targeted at minimizing spurious diapycnal mixing while allowing for an accurate representation of the ocean's multiple regimes of flow.
- More work is needed to improve the choice for vertical coordinate, with no optimal coordinate having been found that satisfies all needs (sometimes subjective needs) for climate and coastal applications.





# Many thanks for your time and attention





