



# Applying Implicit Energetics Ideas to Simulate Full-Water-Column Ocean Mixing

Robert Hallberg

NOAA / GFDL

with contributions from Brandon Reichl





# Diapycnal Mixing, Turbulent Kinetic Energy and the Osborn Relationship

A simplified, dominant balance for the turbulent kinetic energy budget allows (hard to observe) turbulent vertical buoyancy fluxes to be related to the (more easily inferred) dissipation of turbulent kinetic energy. (Osborn, *JPO* 1980)

A typical turbulent kinetic energy (TKE or  $E$ ) balance equation:

$$\frac{DE}{Dt} = \nabla \cdot \mathbf{F}_Q - \overline{\mathbf{u}'w'} \frac{\partial \bar{\mathbf{u}}}{\partial z} + \overline{w'b'} - \nu_{mol} \overline{\nabla \mathbf{u}' \cdot \nabla \mathbf{u}'}$$

$$\approx \frac{\partial}{\partial z} \left( \nu_E \frac{\partial E}{\partial z} \right) + \nu_u \left\| \frac{\partial \bar{\mathbf{u}}}{\partial z} \right\|^2 + Src_{IGW} - \kappa N^2 - \varepsilon$$

$$E \equiv \frac{1}{2} \overline{(u'^2 + v'^2 + w'^2)}$$

$$N^2 \equiv -\frac{g}{\rho} \frac{\partial \rho}{\partial z}$$

$\kappa \equiv$  Turbulent diffusivity of heat & salt

$\varepsilon \equiv$  Dissipation of TKE

$P \equiv$  Production of TKE

In the interior ocean, the local balance often works pretty well:

$$0 \approx Src_{Shear} + Src_{IGW} - \kappa N^2 - \varepsilon$$

$$P = \kappa N^2 + \varepsilon$$

The flux Richardson number ( $R_f \equiv \kappa N^2 / P$ ) is typically less than a critical value of  $\sim 0.15$ .

$$\kappa N^2 / R_f = \kappa N^2 + \varepsilon$$

$$\kappa = \frac{\Gamma \varepsilon}{N^2}$$

$$\Gamma \equiv \frac{R_f}{1 - R_f} \leq \sim 0.2$$

The buoyancy frequency and dissipation can both be determined observationally.

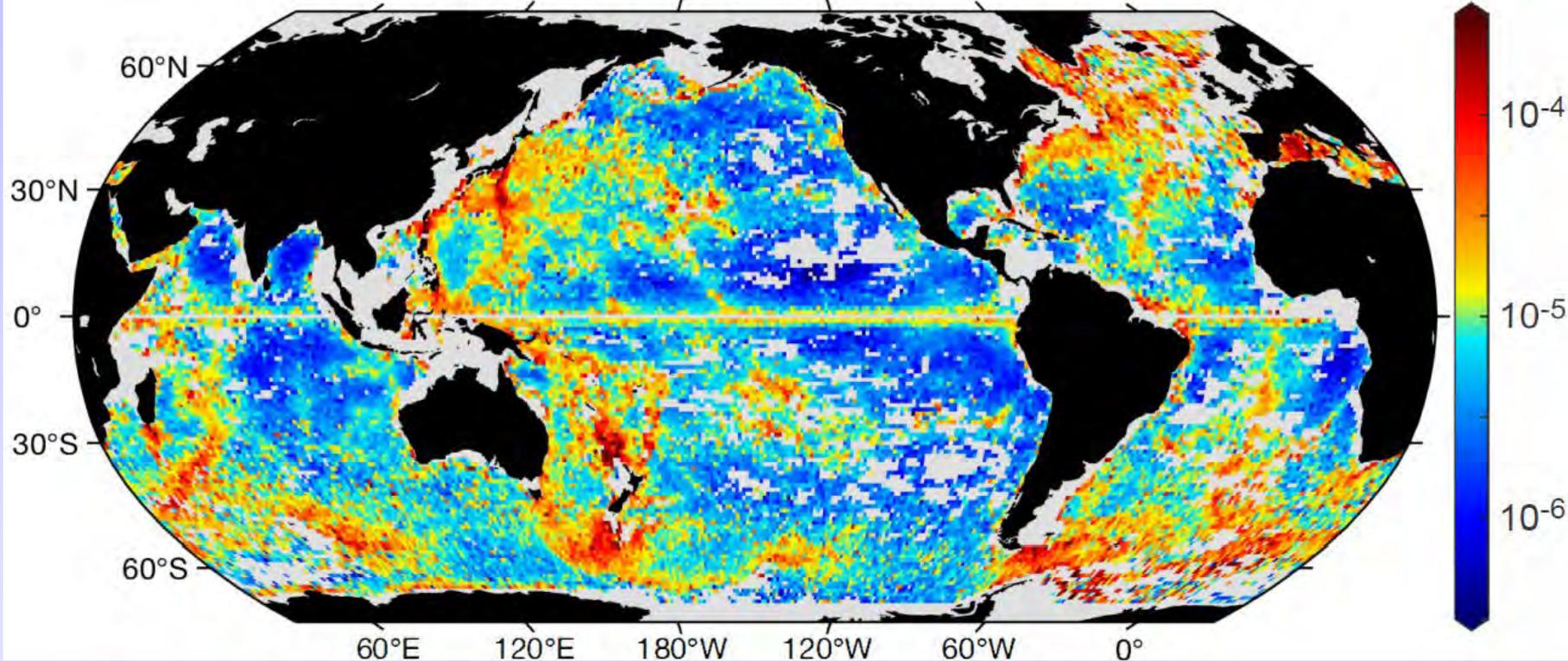


# The Osborn Relationship can be used to Estimate Diffusivities from Observed small-scale Dissipation

Estimated Ocean Diffusivity Based on ARGO Observations

$$\kappa = \frac{\Gamma \varepsilon_{Obs}}{N_{Obs}^2}$$

Average Diffusivity 250-1000m ( $\text{m}^2\text{s}^{-1}$ )



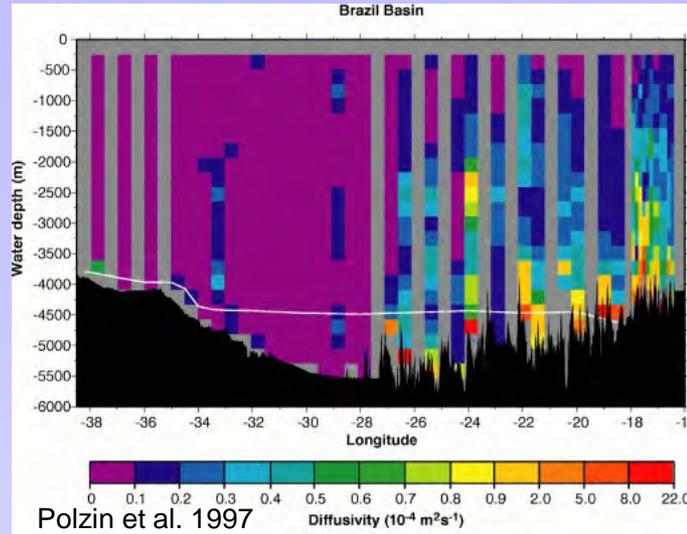
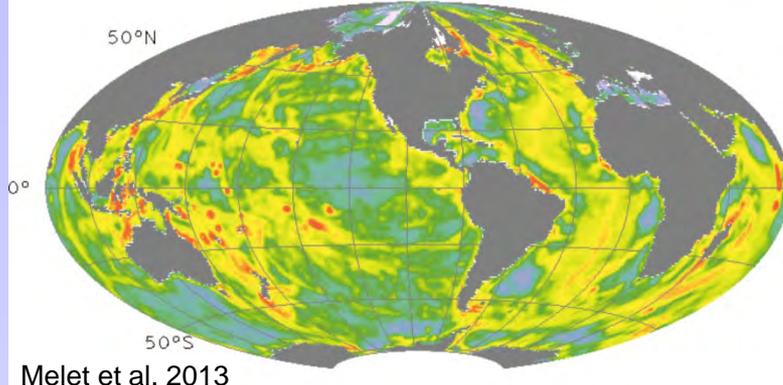
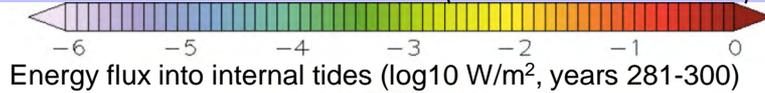
Bindoff et al. (2019) (IPCC SROCC, Ch. 5)

Updated from Whalen, Talley and MacKinnon, GRL 2012



# Parameterizing breaking high-mode internal tides

$$E(x, y) = \frac{1}{2} \rho N_{Bot} k h^2 \left\langle U_{bot,model}^2 + u_{Tide}^2 \right\rangle$$



map of internal tide generation from model's evolving  $U_{bot}$  &  $N_{bot}$

vertical structure based on wave-wave interaction physics (St Laurent et al 2002 or Polzin 2009)

Osborn relationship:

$$\kappa = \frac{\Gamma \varepsilon}{N^2}$$

dissipation rate (related to diffusivity through mixing efficiency)

$$\varepsilon = \frac{qE(x, y)F(z)}{\rho}$$

% of energy that dissipates locally

$$\Gamma \equiv \frac{R_f}{1 - R_f} \leq \sim 0.2$$



# The Osborn Relationship Leads to Energetic Consistency ... *Approximately*

Ocean models must calculate diffusion implicitly for numerical stability:

$$\frac{\theta^{n+1} - \theta^n}{\Delta t} = \frac{\partial}{\partial z} \left( \kappa \frac{\partial \theta^{n+1}}{\partial z} \right)$$

The Osborn relationship diffusivity is usually calculated explicitly:

$$\kappa = \frac{\Gamma \varepsilon}{N^{2,n}} \quad N^{2,n} = -\frac{g}{\rho} \left( \alpha \frac{\partial \theta^n}{\partial z} + \beta \frac{\partial S^n}{\partial z} \right)$$

but the realized buoyancy flux is  $\kappa N^{2,n+1}$

Energetic consistency is lost because  $N^{2,n+1} \neq N^{2,n}$

The Osborn relationship is generally problematic whenever  $N^2 \approx 0!$

Why does this energetic inconsistency matter?

Murphy's Law: *“Whatever can go wrong will go wrong.”*

The ocean-modeler's corollary to Murphy's Law:

*“Ocean models are Murphy's Law machines.”*



# Mixing in a stratified water columns takes energy.

- Osborn Relationship:  $\kappa = \frac{\Gamma \varepsilon}{N^2}$   $\Gamma \equiv \frac{R_f}{1 - R_f} \leq \sim 0.2$ 

Turbulent Kinetic Energy supplies the local potential energy change due to the local buoyancy flux.
- New Implicit Energetics approach:

Turbulent Kinetic Energy supplies the potential energy changes throughout the entire water column integrated over a timestep due to the local diffusivity.

These are the same in the limit where  $\Delta t \rightarrow 0$ .



# Potential Energy of a Hydrostatic Column (Exact)

$$\begin{aligned} PE &= \int_{-D}^{\eta} \rho g (z' + D) dz \\ &= - \int_{p_D}^0 (z + D) dp \\ &= \int_0^{p_D} \int_p^{p_D} R \frac{dp'}{g} dp \\ &= \int_0^{p_D} R \frac{1}{g} p dp + \left[ p \int_p^{p_D} R \frac{1}{g} dp \right]_{p=0}^{p_D} \end{aligned}$$

$$PE = \int_0^{p_D} R \frac{1}{g} p dp$$

- Linear in specific volume
- Fixed bounds of integration in pressure

Specific Volume:  $R \equiv \frac{1}{\rho}$

Hydrostatic Balance:

$$\frac{dp}{dz} = -g\rho$$

Height above the bottom ( $D$ ) as a function of pressure:

$$\begin{aligned} z(p) &= -D + \int_{p_D}^p \frac{dz}{dp} dp' \\ &= -D - \int_{p_D}^p \frac{R}{g} dp' \end{aligned}$$

Integration by parts:

$$\int u dv = uv - \int v du$$



# PE Change from Mixing & Conversion to TKE

Change in potential energy due to diffusivity  $\kappa_k$  at interface  $k$ :

$$\frac{d\dot{P}E}{d\kappa_k} = \int_0^{p_D} \frac{d\dot{R}}{d\kappa_k} \frac{1}{g} p dp$$

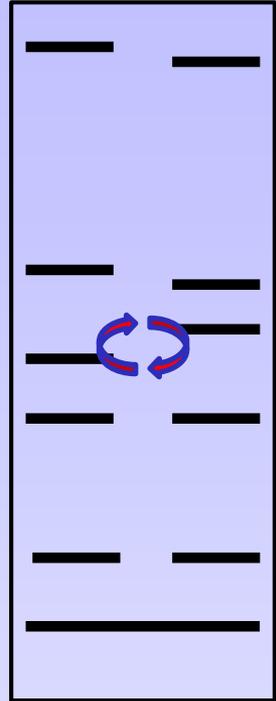
A fraction  $n^* \approx 0.07$ ? of released PE is available to drive more mixing, but energy released by contraction of the column radiates as gravity waves:

$$\frac{dTKE}{d\kappa_k} = - \left[ \int_0^{p_D} \frac{d\dot{R}}{d\kappa_k} \frac{1}{g} p dp - \min \left( 0, \frac{p_D}{g} \int_0^{p_D} \frac{d\dot{R}}{d\kappa_k} dp \right) \right] \begin{pmatrix} 1 & \frac{dTKE}{d\kappa} < 0 \\ n^* & \frac{dTKE}{d\kappa} > 0 \end{pmatrix}$$

Mixing is done for conservative temperature and salinity:

$$\int_0^{p_D} \frac{d\dot{R}}{d\kappa_k} \frac{1}{g} p dp = \int_0^{p_D} \left( \frac{\partial R}{\partial \theta} \frac{d\dot{\theta}}{d\kappa_k} + \frac{\partial R}{\partial S} \frac{d\dot{S}}{d\kappa_k} \right) \frac{1}{g} p dp$$

The tridiagonal equations for the total implicit evolution of  $\theta$  and  $S$  profiles can be differentiated with  $\kappa_k$  and integrated over all the layers above & below without having to re-traverse the water column.





# Vertically Integrated Potential Energy Change due to Diffusion

$$\frac{dPE}{d\kappa_{k-1/2}} = \int_0^{p_D} \left( \frac{\partial R}{\partial \theta} \frac{d\dot{\theta}}{d\kappa_{k-1/2}} + \frac{\partial R}{\partial S} \frac{d\dot{S}}{d\kappa_{k-1/2}} \right) p \frac{1}{g} dp$$

$$\Delta_{\Delta\kappa_{k+1/2}} PE = \frac{1}{\Delta t} \sum_{j=1}^K \left( \frac{\partial R}{\partial \theta_j} \Delta_{\Delta\kappa_{k+1/2}} \theta_j + \frac{\partial R}{\partial S_j} \Delta_{\Delta\kappa_{k+1/2}} S_j \right) \frac{1}{g} \bar{p}_j \Delta p_j$$

$$\Delta_{\Delta\kappa_{k+1/2}} PE = \frac{W_{k+1/2}}{A} \frac{(\Delta\kappa_{k+1/2} \Delta t / \Delta z_{k+1/2})}{A + B(\Delta\kappa_{k+1/2} \Delta t / \Delta z_{k+1/2})}$$

$$A \equiv h_k^\downarrow h_{k+1}^\uparrow + \frac{\kappa_{k+1/2}^{prev} \Delta t}{\Delta z_{k+1/2}} (h_k^\downarrow + h_{k+1}^\uparrow)$$

$$B \equiv h_k^\downarrow + h_{k+1}^\uparrow$$

$$W_{k+1/2} \equiv \left( h_{k+1}^\uparrow \frac{\partial PE}^{\downarrow}}{\partial \theta_k} - h_k^\downarrow \frac{\partial PE}^{\uparrow}}{\partial \theta_{k+1}} \right) (h_k^\downarrow h \tilde{\theta}_{k+1}^\uparrow - h_{k+1}^\uparrow h \tilde{\theta}_k^\downarrow) +$$

$$\left( h_{k+1}^\uparrow \frac{\partial PE}^{\downarrow}}{\partial S_k} - h_k^\downarrow \frac{\partial PE}^{\uparrow}}{\partial S_{k+1}} \right) (h_k^\downarrow h \tilde{S}_{k+1}^\uparrow - h_{k+1}^\uparrow h \tilde{S}_k^\downarrow)$$

$$\frac{\partial PE}^{\downarrow}}{\partial \theta_k} = \frac{1}{g} \bar{p}_k \Delta p_k \frac{\partial R}{\partial \theta_k} + q_{k-1/2}^\downarrow \frac{\partial PE}^{\downarrow}}{\partial \theta_{k-1}}$$

$$\frac{\partial PE}^{\uparrow}}{\partial \theta_k} = \frac{1}{g} \bar{p}_k \Delta p_k \frac{\partial R}{\partial \theta_k} + q_{k+1/2}^\uparrow \frac{\partial PE}^{\uparrow}}{\partial \theta_{k+1}}$$

A properly written tridiagonal solver for the implicit finite volume tracer diffusion equation:

$$a_{k+1/2} \equiv \frac{\kappa_{k+1/2} \Delta t}{\Delta z_{k+1/2}}$$

$$(h_k + a_{k+1/2} + a_{k-1/2}) T_k^{n+1} = h_k T_k^n + a_{k-1/2} T_{k-1}^{n+1} + a_{k+1/2} T_{k+1}^{n+1}$$

$$h_k^\downarrow = h_k + Q_{k-1/2}^\downarrow a_{k-1/2}$$

$$q_{k+1/2}^\downarrow = \frac{a_{k+1/2}}{h_k^\downarrow + a_{k+1/2}}$$

$$Q_{k+1/2}^\downarrow \equiv 1 - q_{k+1/2}^\downarrow = \frac{h_k^\downarrow}{h_k^\downarrow + a_{k+1/2}}$$

$$\tilde{T}_k^\downarrow = \frac{h_k T_k^n + a_{k-1/2} \tilde{T}_{k-1}^\downarrow}{h_k^\downarrow + a_{k+1/2}}$$

...

$$T_k^{n+1} = \tilde{T}_k^\downarrow + q_{k+1/2}^\downarrow T_{k+1}^{n+1}$$

$$h \tilde{T}_k^\downarrow \equiv h_k T_k^n + a_{k-1/2} \tilde{T}_{k-1}^\downarrow$$

$$h \tilde{T}_k^\uparrow \equiv h_k T_k^n + a_{k+1/2} \tilde{T}_{k+1}^\uparrow$$

$$h_k^\downarrow \equiv h_k + Q_{k-1/2}^\downarrow a_{k-1/2}$$

$$h_k^\uparrow \equiv h_k + Q_{k+1/2}^\uparrow a_{k+1/2}$$

- The buoyancy frequency does not appear anywhere in these expressions!
- The only approximations here are hydrostatic balance and that the thermal expansion and haline contraction coefficients of a layer don't change much over a timestep.



## Fully implicit expression for PE change:

$$\Delta_{\Delta\kappa_{k+1/2}} PE = \frac{W_{k+1/2}}{A} \frac{(\Delta\kappa_{k+1/2} \Delta t / \Delta z_{k+1/2})}{A + B(\Delta\kappa_{k+1/2} \Delta t / \Delta z_{k+1/2})}$$

$$A \equiv h_k^\downarrow h_{k+1}^\uparrow + \frac{\kappa_{k+1/2}^{prev} \Delta t}{\Delta z_{k+1/2}} (h_k^\downarrow + h_{k+1}^\uparrow)$$

$$B \equiv h_k^\downarrow + h_{k+1}^\uparrow$$

$$W_{k+1/2} \equiv \left( h_{k+1}^\uparrow \frac{\partial PE^\downarrow}{\partial \theta_k} - h_k^\downarrow \frac{\partial PE^\uparrow}{\partial \theta_{k+1}} \right) (h_k^\downarrow h \tilde{\theta}_{k+1}^\uparrow - h_{k+1}^\uparrow h \tilde{\theta}_k^\downarrow) + \left( h_{k+1}^\uparrow \frac{\partial PE^\downarrow}{\partial S_k} - h_k^\downarrow \frac{\partial PE^\uparrow}{\partial S_{k+1}} \right) (h_k^\downarrow h \tilde{S}_{k+1}^\uparrow - h_{k+1}^\uparrow h \tilde{S}_k^\downarrow)$$

Solve for  $\Delta\kappa_{k+1/2}$  given  $\Delta PE$ : 
$$\Delta\kappa_{k+1/2} = \frac{\Delta z_{k+1/2}}{\Delta t} \frac{A^2 \Delta PE_{k+1/2}}{W_{k+1/2} - AB \Delta PE_{k+1/2}} \quad \text{for } \Delta PE_{k+1/2} < \frac{W_{k+1/2}}{AB}$$

Simplified to mixing between 2 layers, with a linear eqn of state & 1 state variable...

$$\Delta_{\kappa_{3/2}} PE = \frac{W_{3/2}}{h_1 h_2} \frac{\Delta\kappa_{3/2} \Delta t}{h_1 h_2 \Delta z_{3/2} + (h_1 + h_2) \Delta\kappa_{3/2} \Delta t}$$

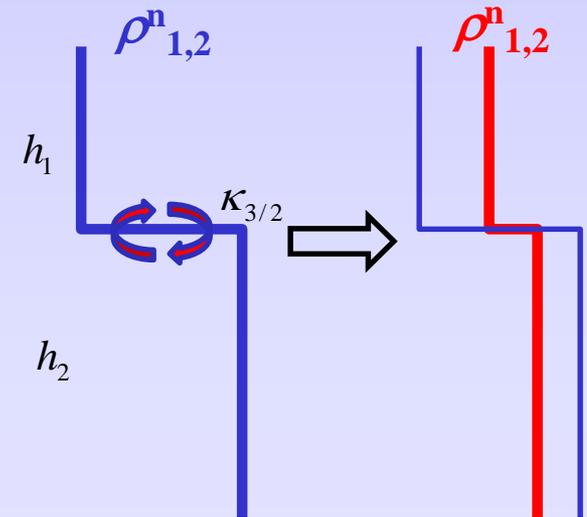
$$W_{3/2} = \rho \frac{\partial R}{\partial \theta} h_1^2 h_2^2 (\bar{p}_1 - \bar{p}_2) (\theta_2^n - \theta_1^n) \quad \Delta z_{3/2} = \frac{1}{2} (h_1 + h_2)$$

$$\approx \frac{1}{2} g h_1^2 h_2^2 (h_1 + h_2) \frac{\partial \rho}{\partial \theta} (\theta_1^n - \theta_2^n)$$

$$\Delta_{\kappa_{3/2}} PE = \frac{1}{2} g (\rho_1^n - \rho_2^n) h_1 h_2 \frac{2 \Delta\kappa_{3/2} \Delta t}{h_1 h_2 + 2 \Delta\kappa_{3/2} \Delta t}$$

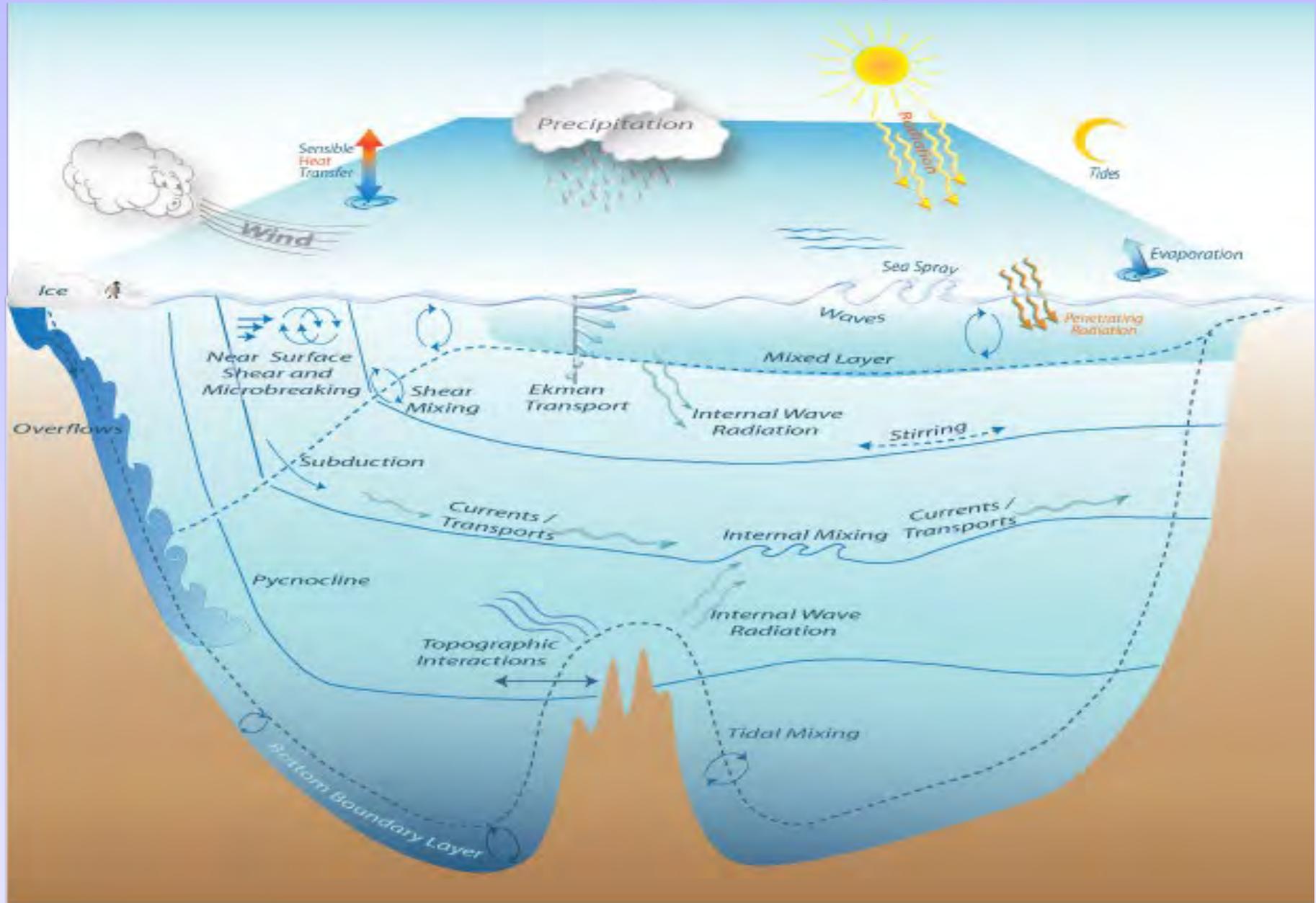
$$\Delta_{\kappa_{3/2} \rightarrow \infty} PE = \frac{1}{2} g (\rho_1^n - \rho_2^n) h_1 h_2$$

$$\Delta_{\kappa_{3/2} \rightarrow 0} PE = g (\rho_1^n - \rho_2^n) \kappa_{3/2} \Delta t$$





Energetic considerations can be used with the new integrated approach to parameterize many of the mixing processes in the ocean.





# An 'ePBL' Framework: The energetics concept of a Kraus-Turner-Niiler boundary layer scheme with a KPP-like finite diffusivity

**Kraus-Turner-Niiler Bulk Mixed Layer:** Integrated energetics is used to determine the boundary layer depth ( $h$ ) or entrainment rate ( $w_E$ ).

Mixing	Mechanical	Convection
$\frac{h}{2} g' \max(w_E, 0) + \frac{h}{2} \max(B_0, 0) = m_* u_*^3 - n_* \frac{h}{2} \min(B_0, 0)$		

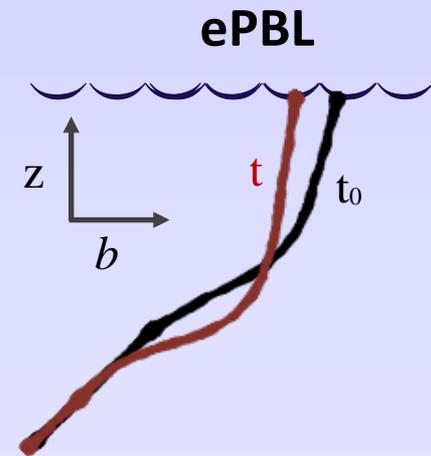
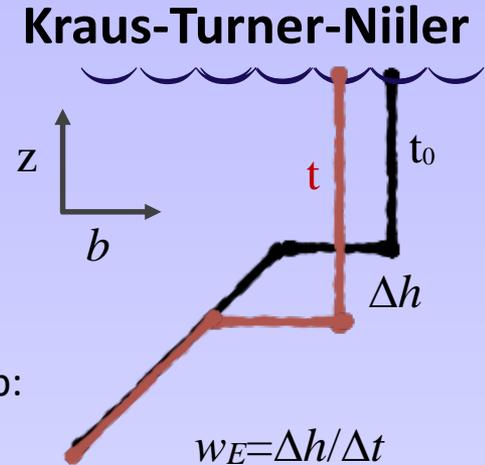
**ePBL:** Similar integrated energetics concept, but with finite turbulent mixing coefficients (diffusivity & viscosity);  $H_{bl}$  is the depth at which the TKE is used up:

Mixing	Mechanical	Convection
$\int_{-H_{bl}}^0 \max(N^2 K(z), 0) dz = m_* u_*^3 - n_* \int_{-H_{bl}}^0 \min(N^2 K(z), 0) dz$		
<p>This uses the shorthand: <math>N^2 K(z) \equiv \frac{1}{\rho_o} \int_0^{K(z)} \left( \int_0^{p_D} \frac{d\dot{R}}{d\kappa_z} \frac{1}{g} pdp \right) d\kappa_z</math></p>		

**Mixing Coefficients:**  $K_\lambda(z) = C_\lambda w(z) L(z)$

**Mixing Length:**  $L(z) = (z_0 + |z|) \max \left[ \frac{l_b}{H_{bl}}, \left( \frac{H_{bl} - |z|}{H_{bl}} \right)^\gamma \right]$

**Velocity Scale:**  $w(z) = C_{w_*} \left( \int_z^0 \overline{w'b'} dz \right)^{1/3} + C_{u_*} u_* \left[ 1 - a \cdot \min \left( 1, \frac{|z|}{H_{bl}} \right) \right]$



See Reichl and Hallberg (2018, *Ocean Modelling*) for full details.  
 See also Li, Reichl, et al., (2019, *JAMES*) for an Intercomparison.

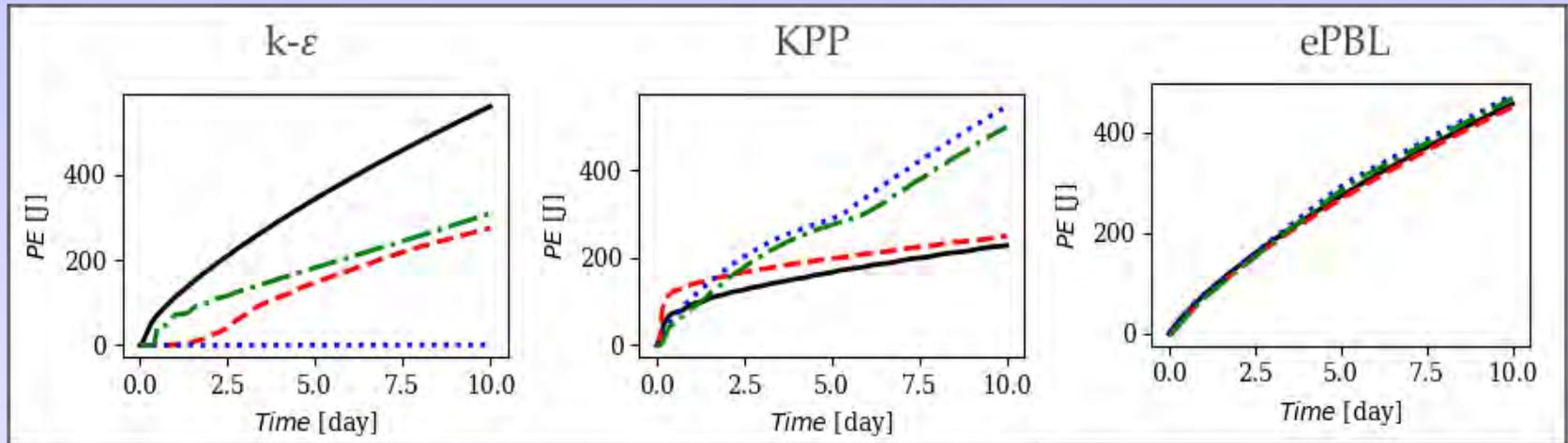


# Energetics Planetary Boundary Layer (ePBL) numerics: Robust model solution to grid resolution and time-step

A simple wind-driven test case of mixing into a stratified water column demonstrates the very weak dependence on vertical resolution and timestep arising from the integrated energetics approach.

1-d Wind-driven Simulations  $\tau = 0.25 \text{ N/m}^2$

$$f = 2\Omega \sin(60) \text{ s}^{-1}$$



$\Delta Z=1 \text{ m}, \Delta T=30 \text{ s}$

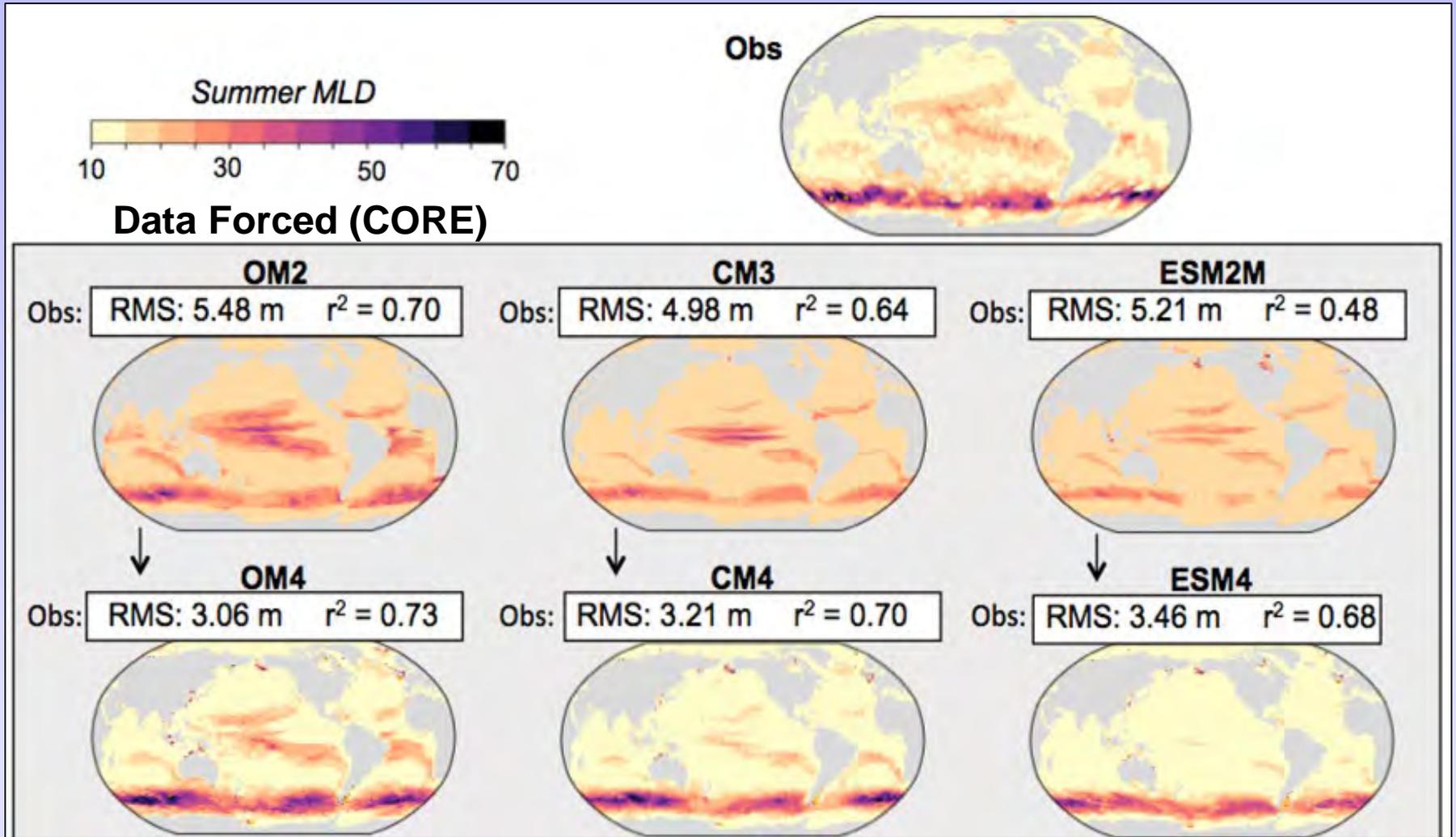
$\Delta Z=20 \text{ m}, \Delta T=30 \text{ s}$

$\Delta Z=1 \text{ m}, \Delta T=7200 \text{ s}$

$\Delta Z=20 \text{ m}, \Delta T=7200 \text{ s}$



# Results: ePBL (here with modifications for Langmuir Turbulence) contributes to improved Mixed Layer Depths in climate models



Adcroft et al. (2019, *JAMES*)

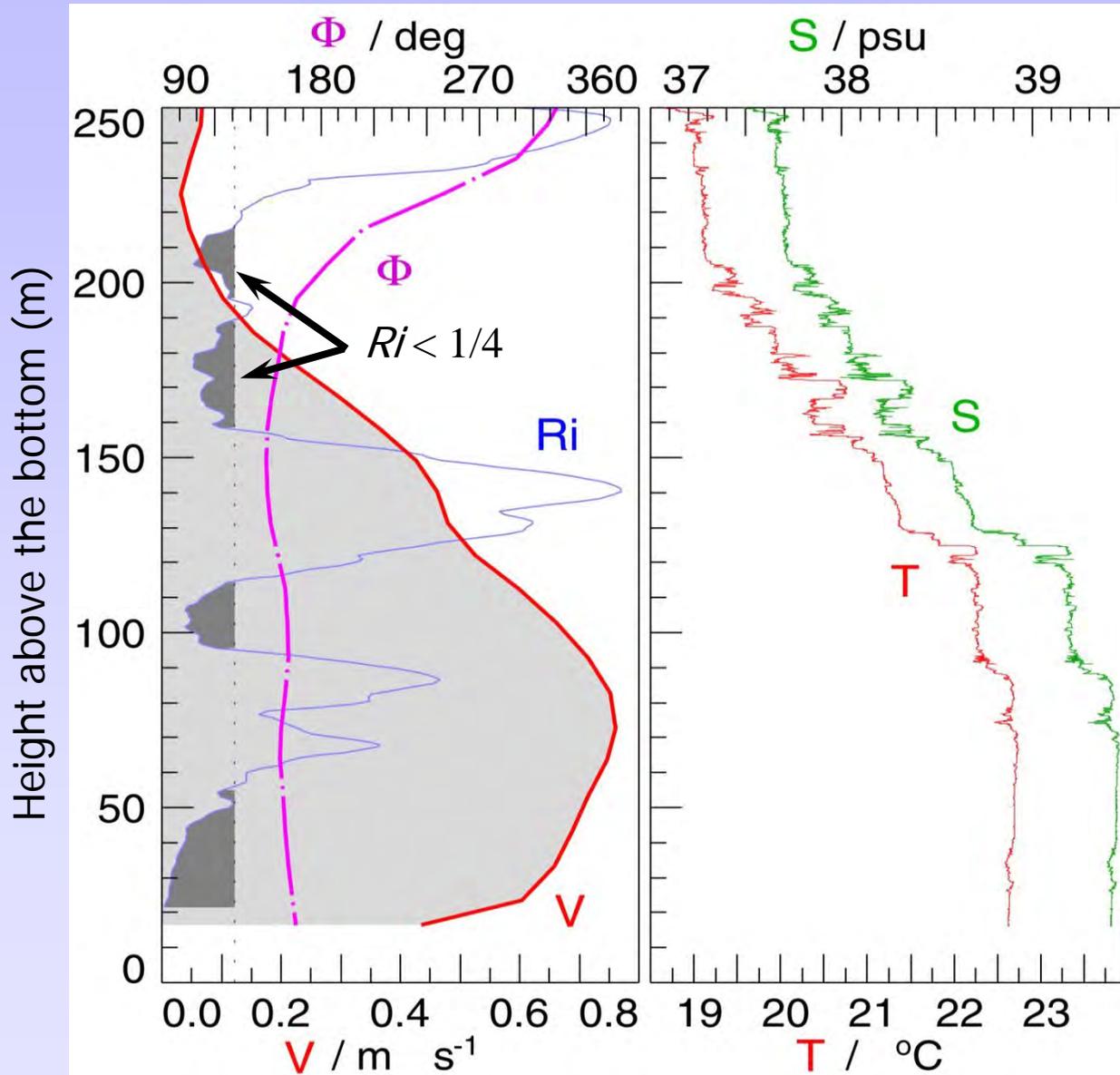
Held et al. (2019, *JAMES*)

Dunne et al. (2020, *JAMES*)



# Shear-driven Mixing in a (Bottom) Boundary Layer

## Observed profiles from the Red Sea outflow plume



$$\|Sh\|^2 = \left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2$$

$$N^2 = -\frac{g}{\rho} \frac{\partial \rho}{\partial z}$$

$$Ri = \frac{N^2}{\|Sh\|^2}$$

Actively mixing  
Interfacial Layer

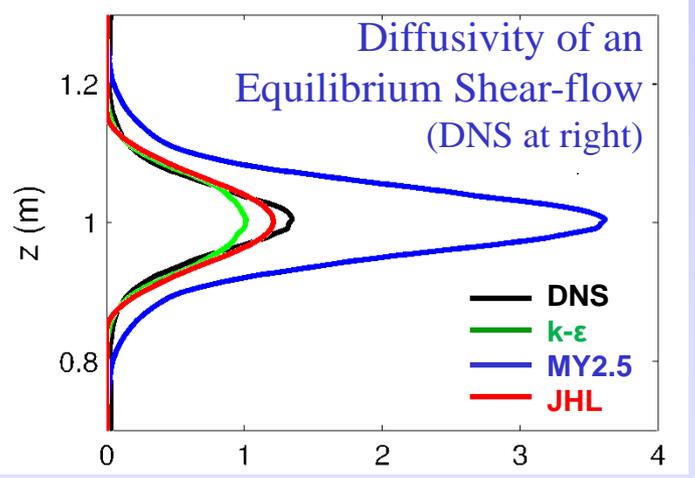
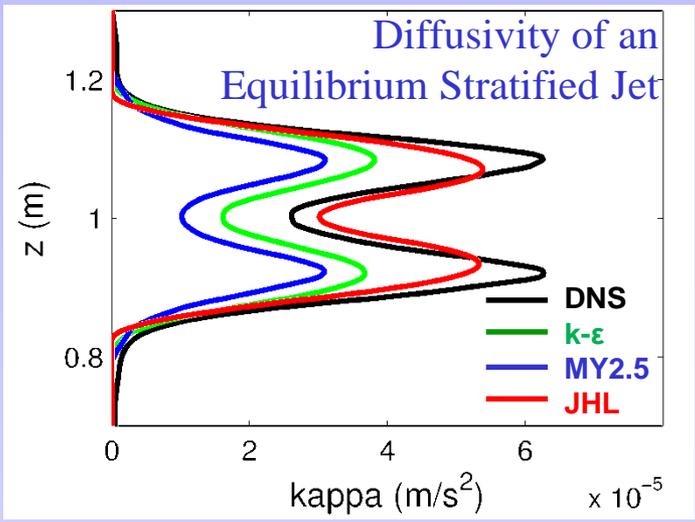
Shear  $Ri \#$  Param.  
Appropriate Here.

Well-mixed  
Bottom Boundary  
Layer

Courtesy H. Peters, see  
Peters et al., (2005, *JPO*)



# The Jackson et al. (2008, *JPO*) Parameterization of Shear Instability



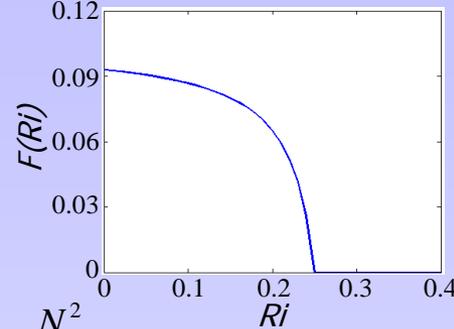
**DNS** – Results of 3-D DNS  
**k-ε** – GOTM standard (~2008) k-ε closure (untuned)  
**MY** – Mellor Yamada level 2.5 closure (untuned)  
**JHL** – Jackson, et al, 2008 parameterization (tuned)

$$\frac{\partial}{\partial z} \left( (\kappa + \nu_o) \frac{\partial Q}{\partial z} \right) + \kappa \|S\|^2 \left( -\kappa N^2 \right) - (c_N N + c_S \|S\|) Q = 0 \quad \left( = -\frac{DQ}{Dt} \right)$$

*Term being reimplemented with new implicit expressions*

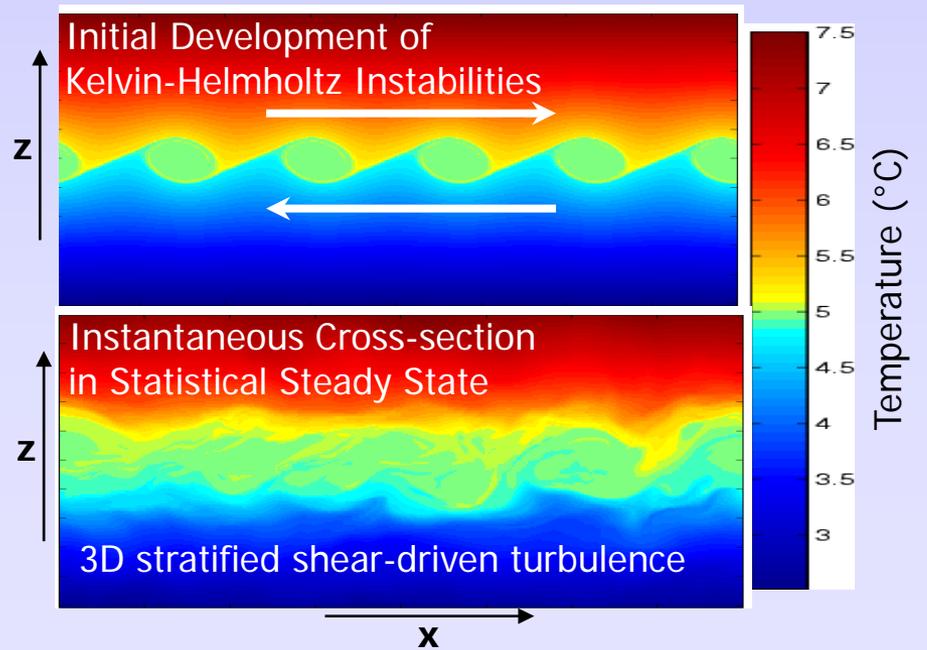
$$\frac{\kappa}{L_D^2} - \frac{\partial^2 \kappa}{\partial z^2} = 2 \|S\| F(Ri)$$

$\kappa$ : Turbulent diapycnal diffusivity and viscosity [ $m^2 s^{-1}$ ]  
 $Q$ : TKE per unit mass [ $m^2 s^{-2}$ ]



$$\|S\|^2 = \left( \frac{\partial u}{\partial z} \right)^2 + \left( \frac{\partial v}{\partial z} \right)^2 \quad N^2 = -\frac{g}{\rho_0} \frac{\partial \rho}{\partial z}$$

$$Ri = \frac{N^2}{S^2} \quad L_D^{-2} = \frac{N^2}{\lambda^2 Q} + \frac{f^2}{Q} + \frac{(z_{Top} + z_{Bot})^2}{z_{Top}^2 z_{Bot}^2} \approx \frac{N^2}{\lambda^2 Q}$$





# Using integrated energetics to convert energy input into diffusivities in parameterizations...

A novel physical parameterization should provide:

- Energy dissipation rate ( $\Gamma\epsilon$ ) as a function of location or a surface or bottom energy flux ( $u^{*3}$ )
- A maximum diffusivity (e.g., law of the wall or limit on the vertical gradient of diffusivity)
- What to do with excess energy (dissipate it, shuffle it up or down, or a mixture)

Energy input from parameterizations of separate mixing processes are used to increment diffusivities in successive upward and/or downward passes.

Each pass takes  $O(N)$  calculations – roughly the cost of a tridiagonal solver.

This approach works well for integrated boundary layer parameterizations, including overlapping top & bottom boundary layers.

This approach constitutes a convenient framework for consistently adding new energy-based mixing parameterizations to MOM6 and CESM.



# Discussion

What new diapycnal mixing processes should we try to include in CESM3 and/or MOM6?

- *Do they have a clear energy budget associated with these processes?*
- *When energy is not fully consumed, where should it go?*
- *What limits are there on the magnitude of a diffusivity or its gradients (e.g., law-of-the-wall, auto-diffusion, etc.)?*