Economical Computational Modeling of Layer and Staircase Formation and Evolution

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Layering in Atmospheres, Oceans, and Plasmas, KITP

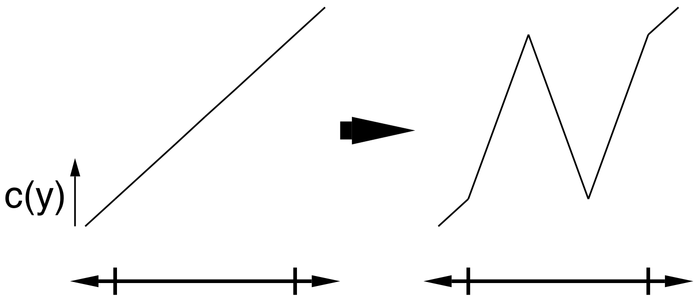
What are the minimal requirements to **resolve** turbulent convection on a vertical 1D domain?

To time advance ρ(z,t) [Boussinesq: use T], need:

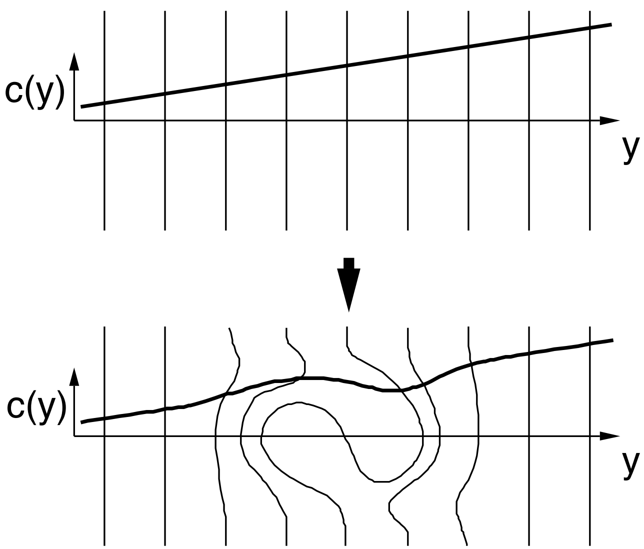
- Spatially resolved molecular (Fickian) transport of T
- Vertical advection
  - must overturn fluid
  - non-dilatational (1D analog of div u = 0)

Advection that is spatially local and continuous in time cannot satisfy these requirements, so advection by instantaneous rearrangements of vertical property profiles - *map-based advection* - is introduced

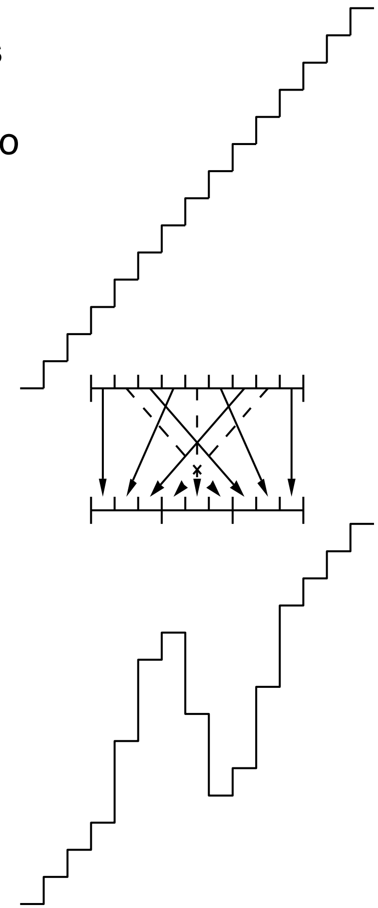
Turbulent motion is implemented as a sequence of *triplet maps* that preserve desired advection properties



The triplet map captures compressive strain and overturns, and causes no property discontinuities

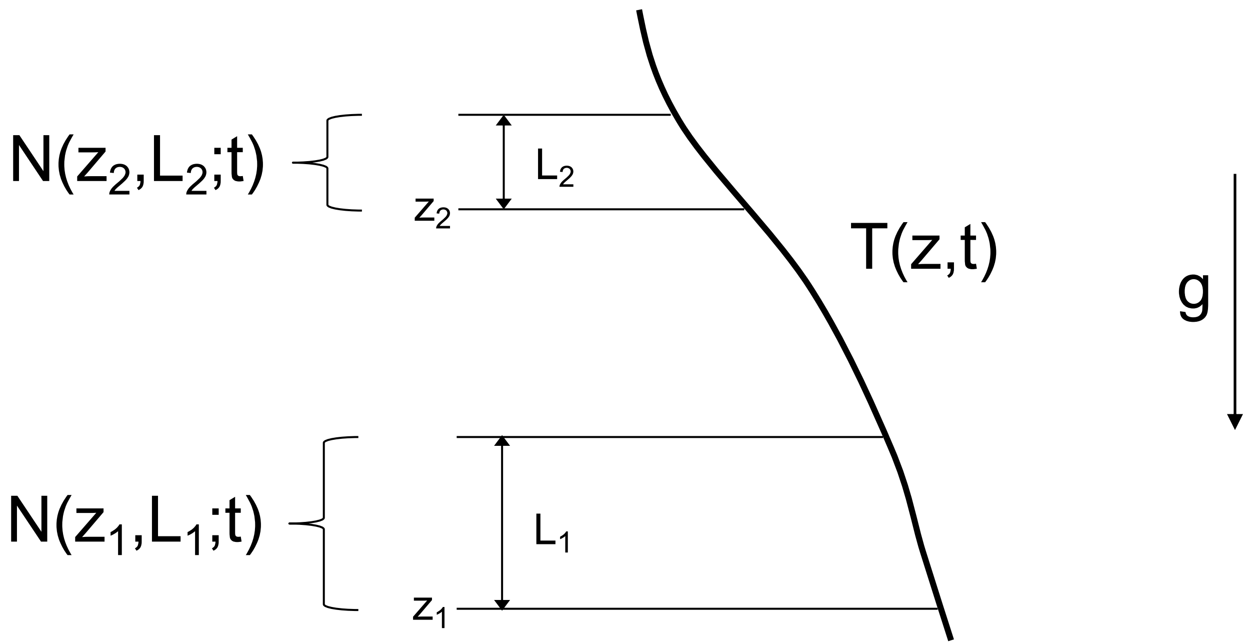


This procedure emulates the effect of a 3D eddy on property profiles along a line of sight



The triplet map is implemented numerically as a permutation of fluid cells (or on an adaptive mesh)

At every instant, the buoyancy frequency N can be evaluated for very possible map



Mapping *rate distribution*:

$$\lambda(z,L;t)\,dz\,dL\,dt \;=\; \text{const} * L^{-2}\,N(z,L;t)\,dz\,dL\,dt$$

Continual updating of λ is too costly, so use a **rejection method**

To introduce Pr dependence, impose a lower bound on N, yielding *Density Profile Evolution* (DPE)

If $L^2 N(z,L;t) / \nu$ < const, the map is forbidden because

viscous damping suppresses the incipient turnover

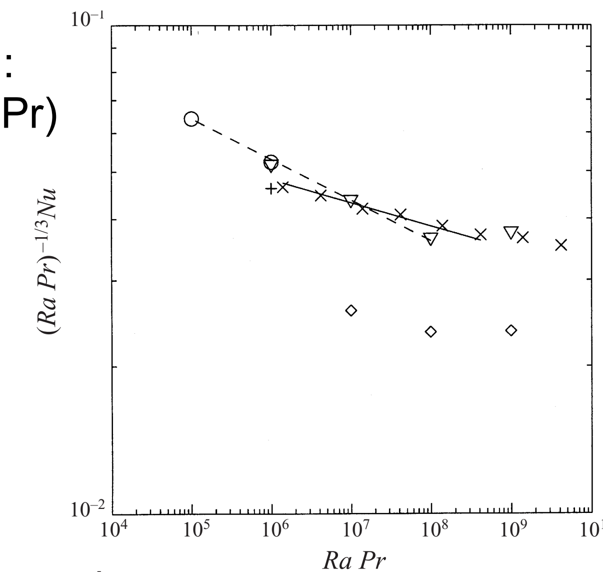
DPE (schematic):

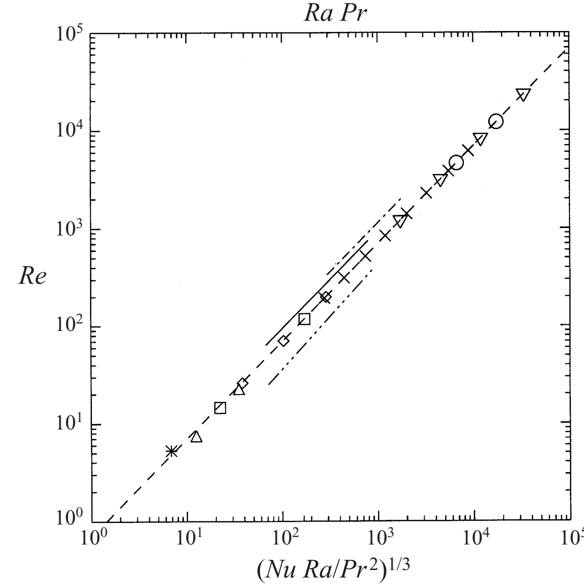
1. Sample a map at time t_{trial} as follows:
    a. Efficiently* sample the arguments of N(z,L)
    b. Decide whether to accept or reject this map
2. If accepted:
    a. Implement the map
    b. Time step the molecular transport PDE to time t_{trial}
3. Sample the new time t_{trial} of the next map attempt
4. Go to 1

*educated guess

Canonical results are reproduced

Rayleigh convection:
Nu(Ra,Pr) and Re(Ra,Pr)





Imposed unstable temperature gradient
(using jump-periodic boundary conditions)
yields *Bolgiano spectral scaling*

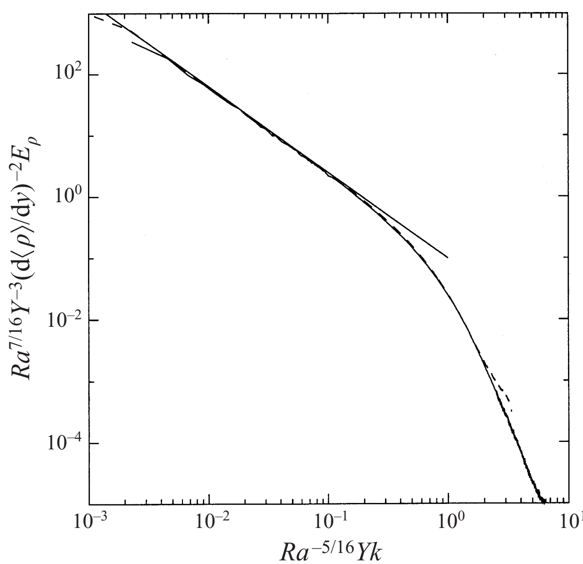


FIGURE 11. Computed power spectra of density fluctuations in stationary homogeneous buoyancy-driven turbulence, normalized to demonstrate the scaling of the high-wavenumber cutoff, for $Pr = 1$: ——, $Ra = 10^{11}$; - - - - -, $Ra = 10^{12}$. A line segment of slope $-\frac{7}{5}$ identifies the Bolgiano–Obukhov scaling regime.

A slow-diffusing stable species can cause layering of a convection process: *double-diffusive instability*

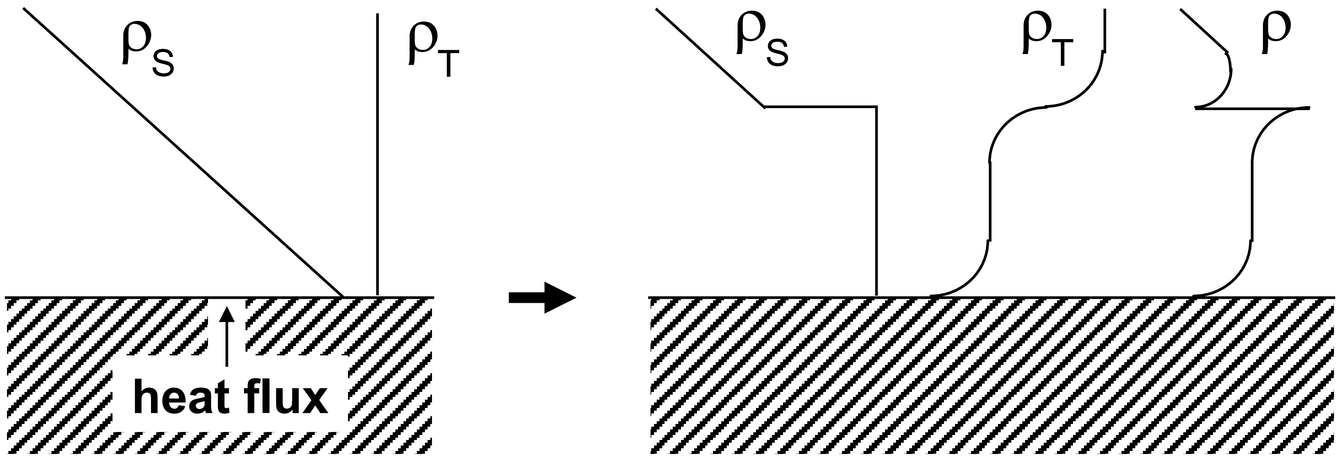
ρ_T **is the density variation due to temperature (T) variation**

ρ_S **is the density variation due to salinity (S) variation**

Initial state: constant temperature, salinity decreases with increasing height (stable, no motion)

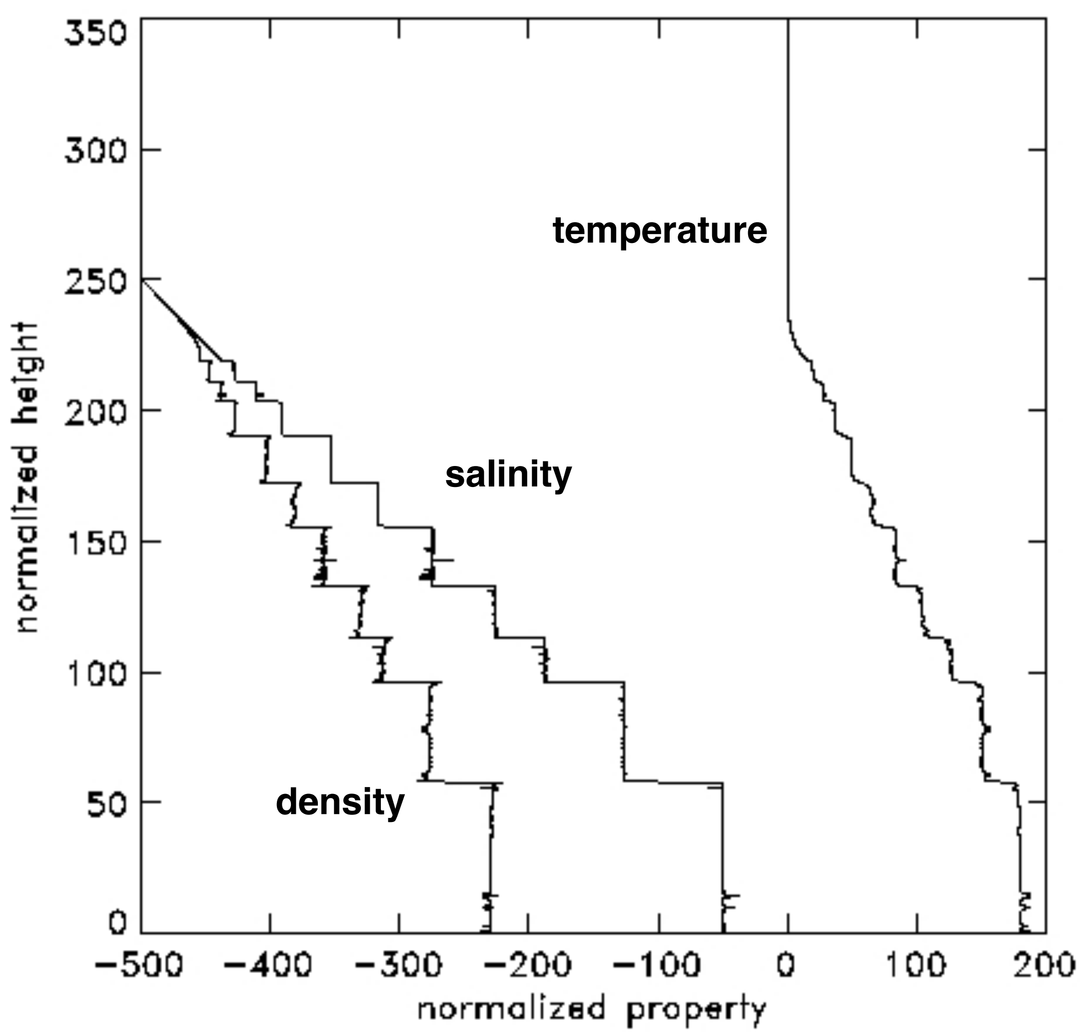
Forcing: heat from below causes gravitational instability leading to turbulent mixing

Role of molecular transport: salt diffusivity is negligible, so a stable jump forms, but heat diffuses across, initiating a new turbulent layer above the jump

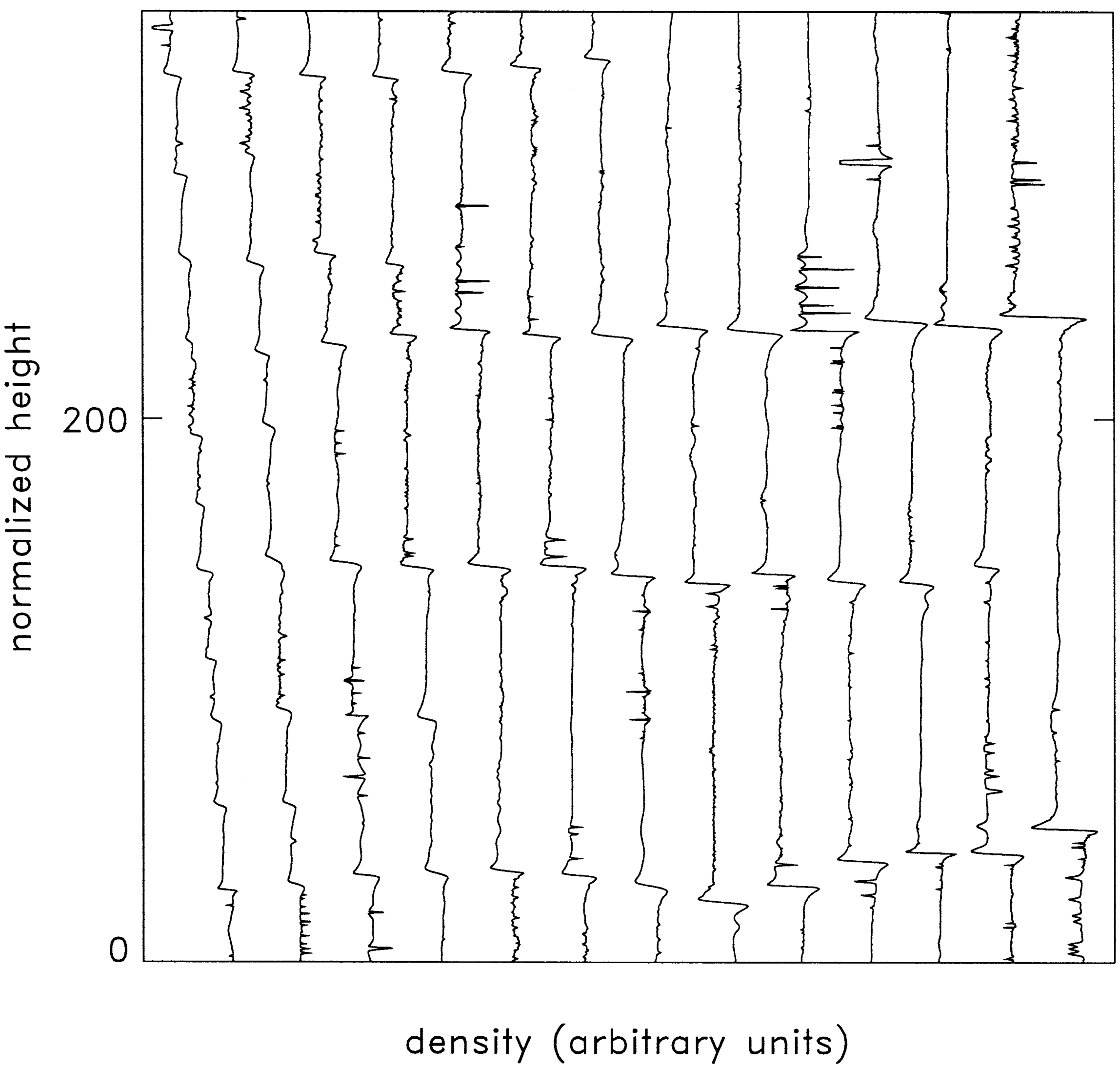


thermohaline staircase

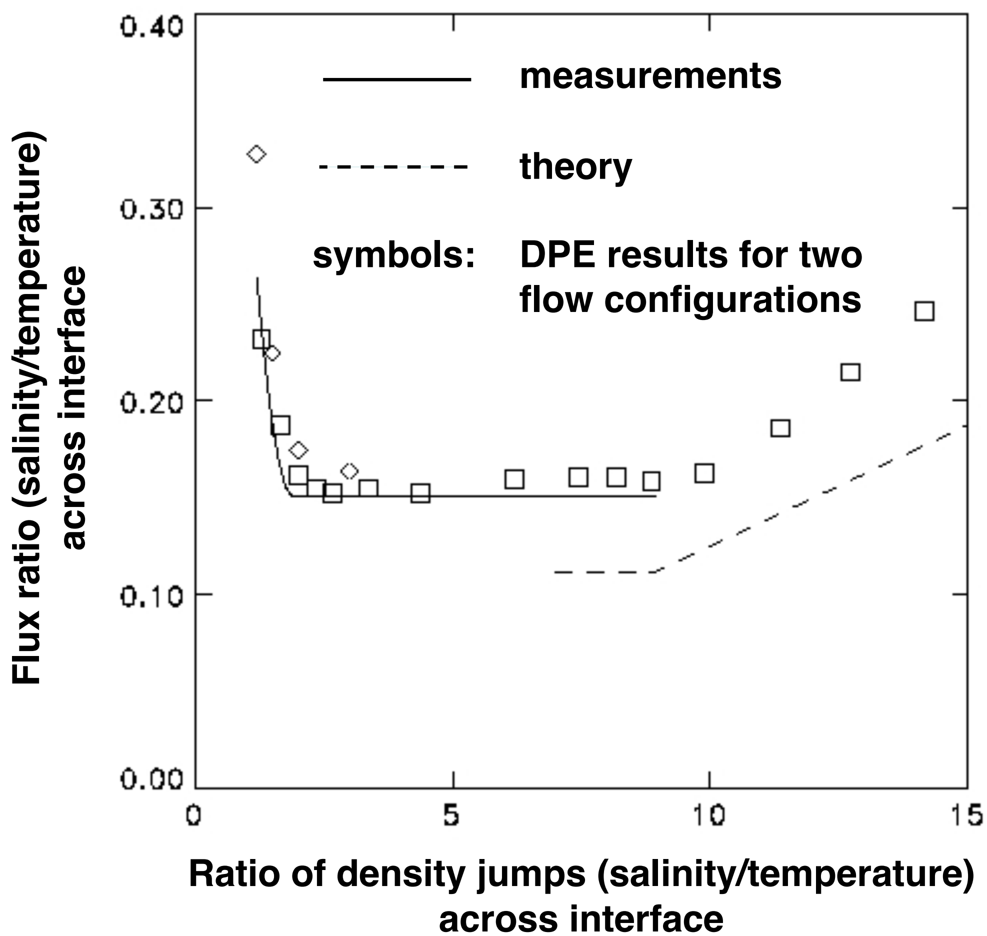
With the addition of the vertical salinity profile S, a staircase is obtained



In a homogeneous configuration (jump-periodic BCs) layers merge

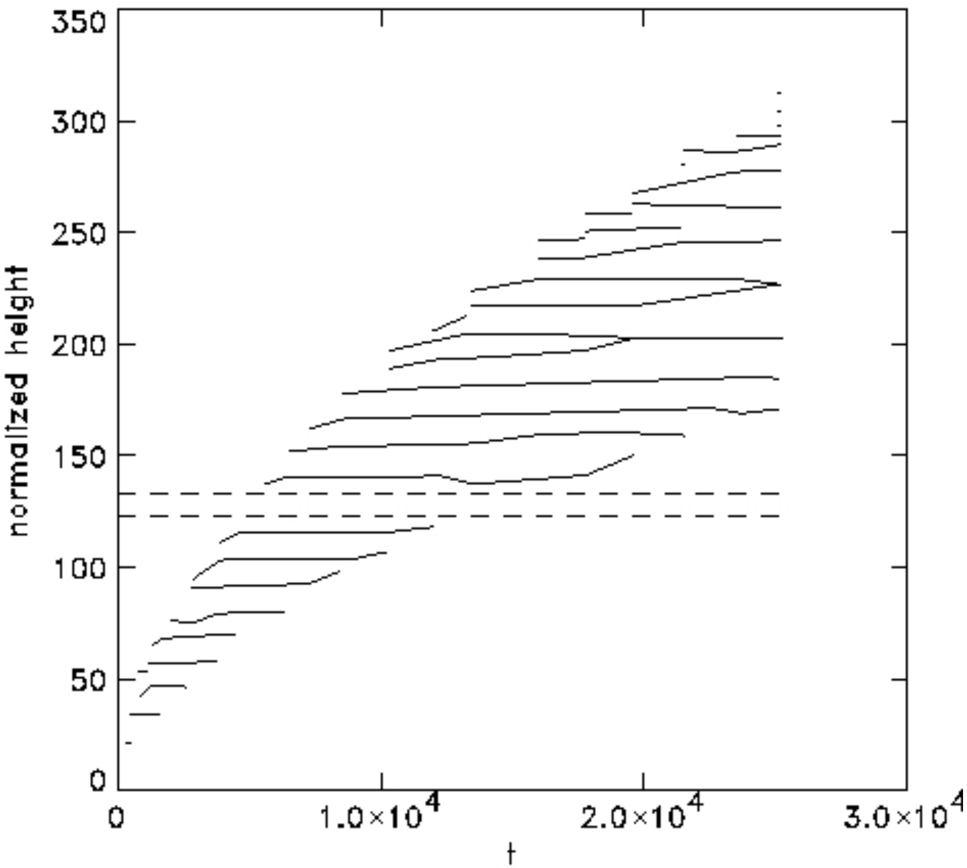


DPE reproduces observed regimes of interface structure

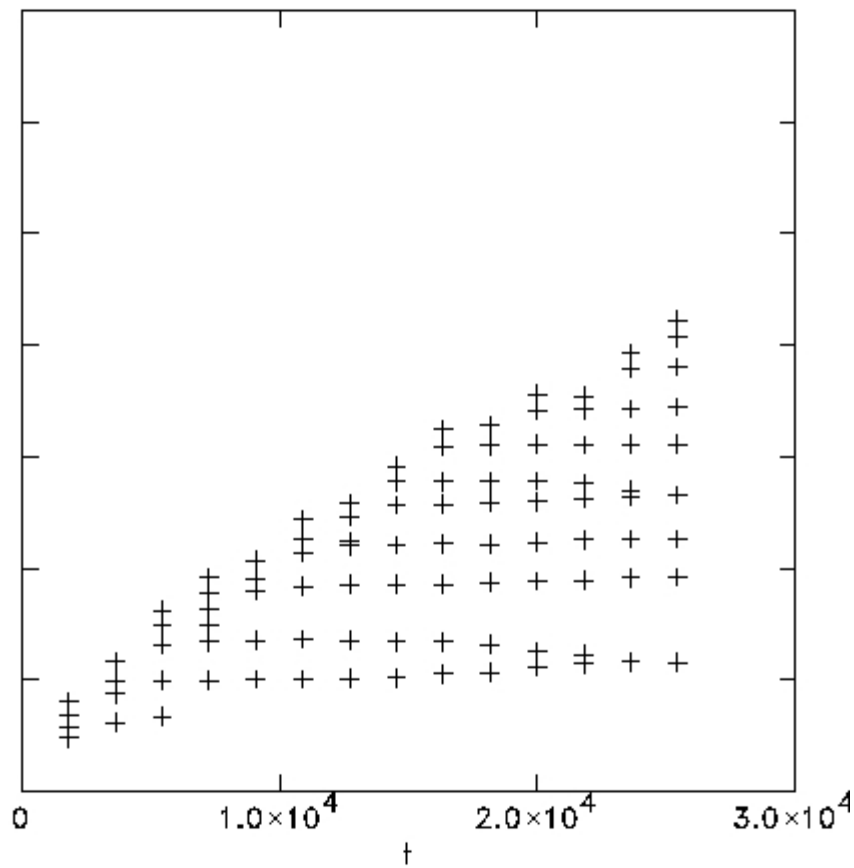


No velocity field, so P.E. is ‘dissipated’; need P.E. -> K.E. -> viscous dissipation

Experiment:
Huppert and Linden, 1979

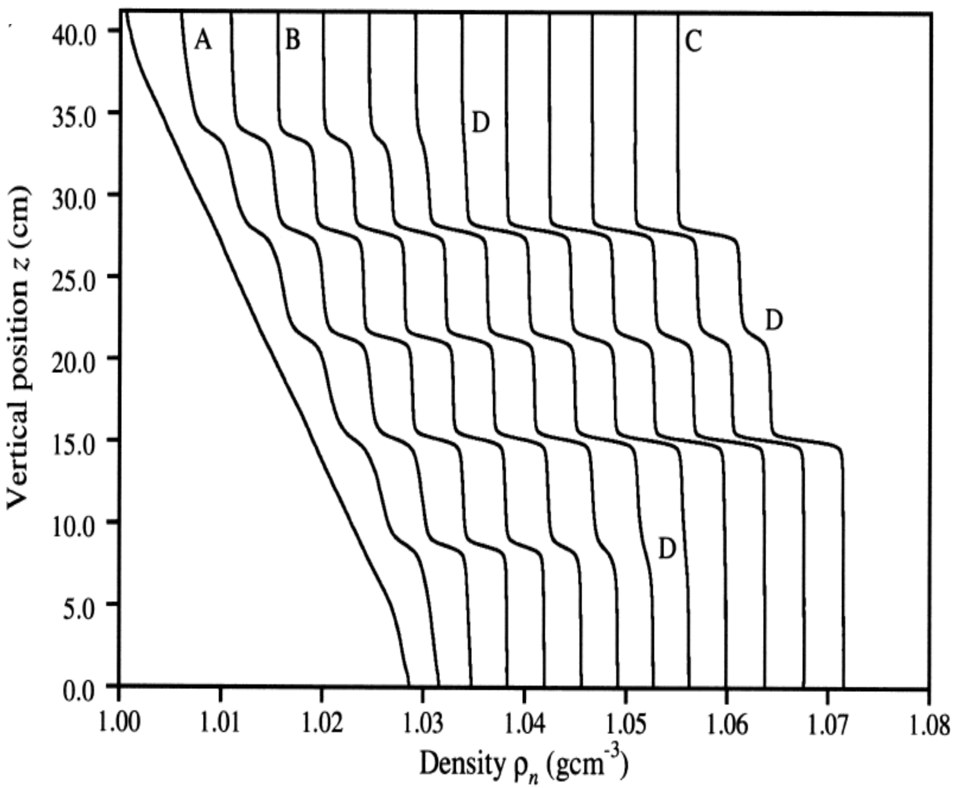


Density-Profile Evolution (DPE):
Kerstein, 1999

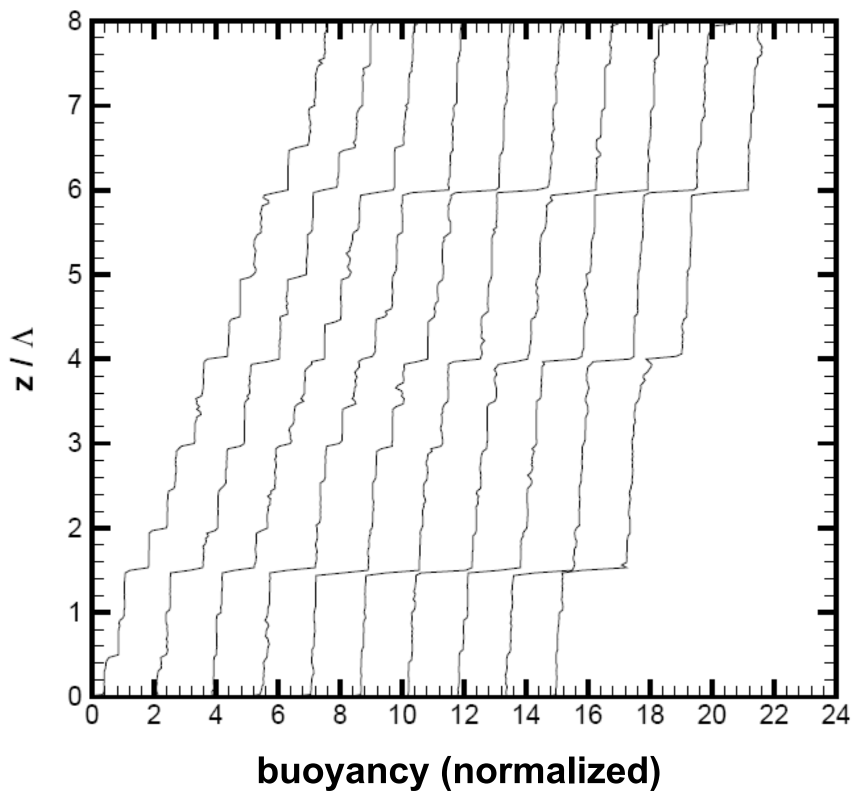


This extension, *One-Dimensional Turbulence* (ODT), produces layers in stirred stably stratified fluid

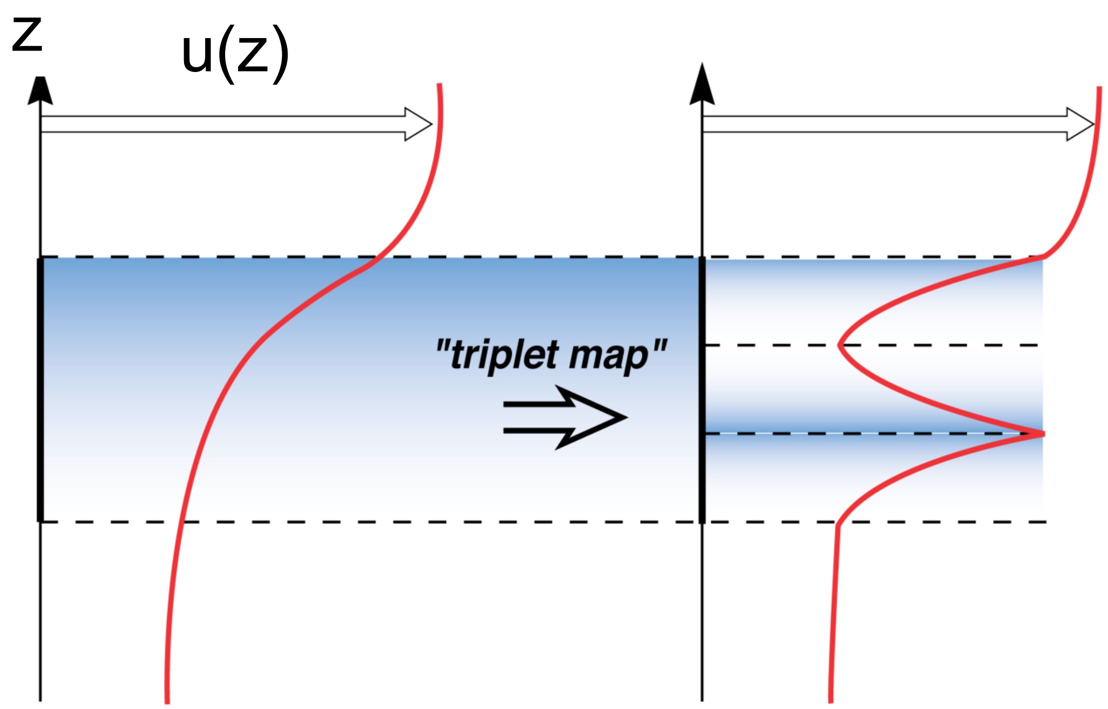
Experiment: Holford and Linden, 1999



ODT: Wunsch and Kerstein, 2001



In ODT, the eddy rate distribution λ includes shear as well as buoyancy contributions



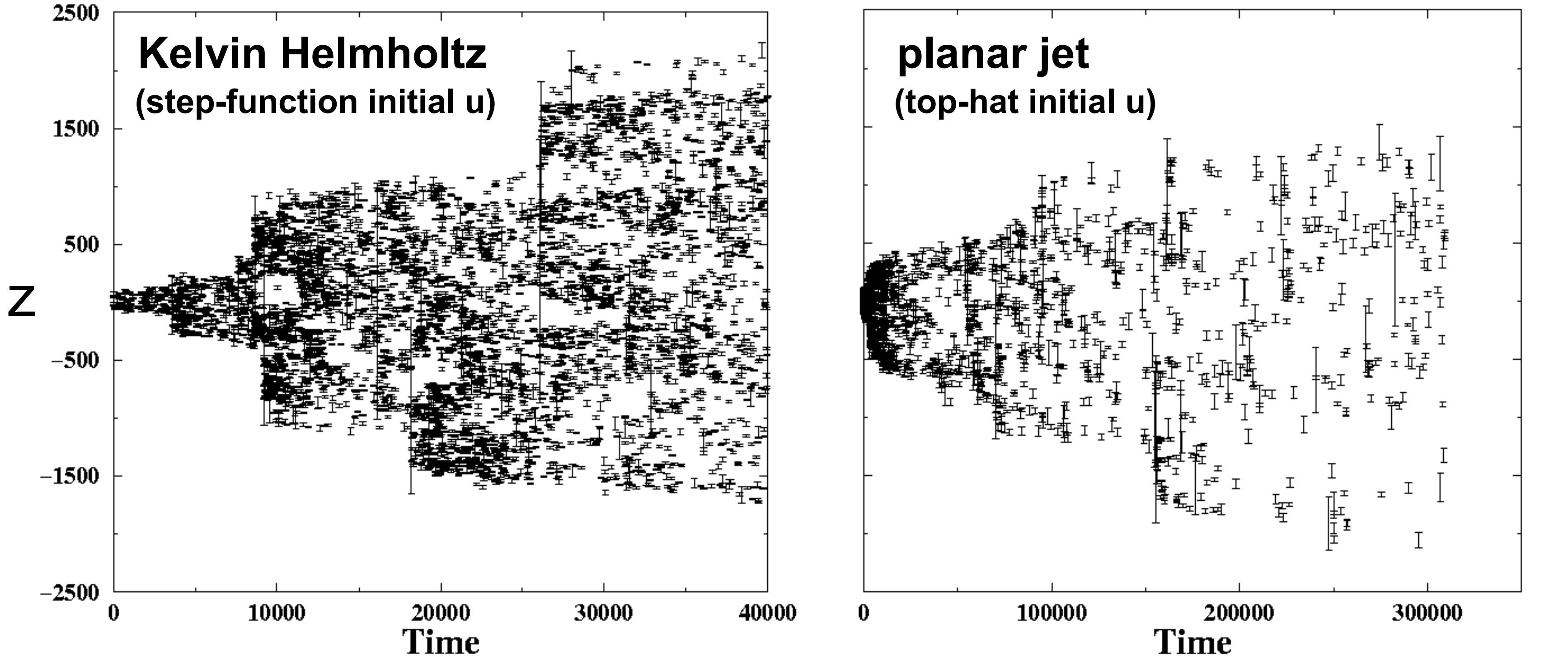
Eddy-induced shear amplification drives smaller eddies,

producing an <u>eddy cascade</u>

($k^{-5/3}$ energy spectrum in shear-dominated flows)

ODT simulations provide flow-specific representations of turbulence

These simulations are based on time advancement of $u_t = \nu u_{zz}$ with flow-specific initial u profiles (see below), plus eddies



- **Each vertical line shows the spatial extent of an eddy**
- **Horizontal location is its time of occurrence**
- **Units are arbitrary**

A full variable-density ODT formulation is compared to DNS of K-H for density ratios up to 8 (no buoyancy)

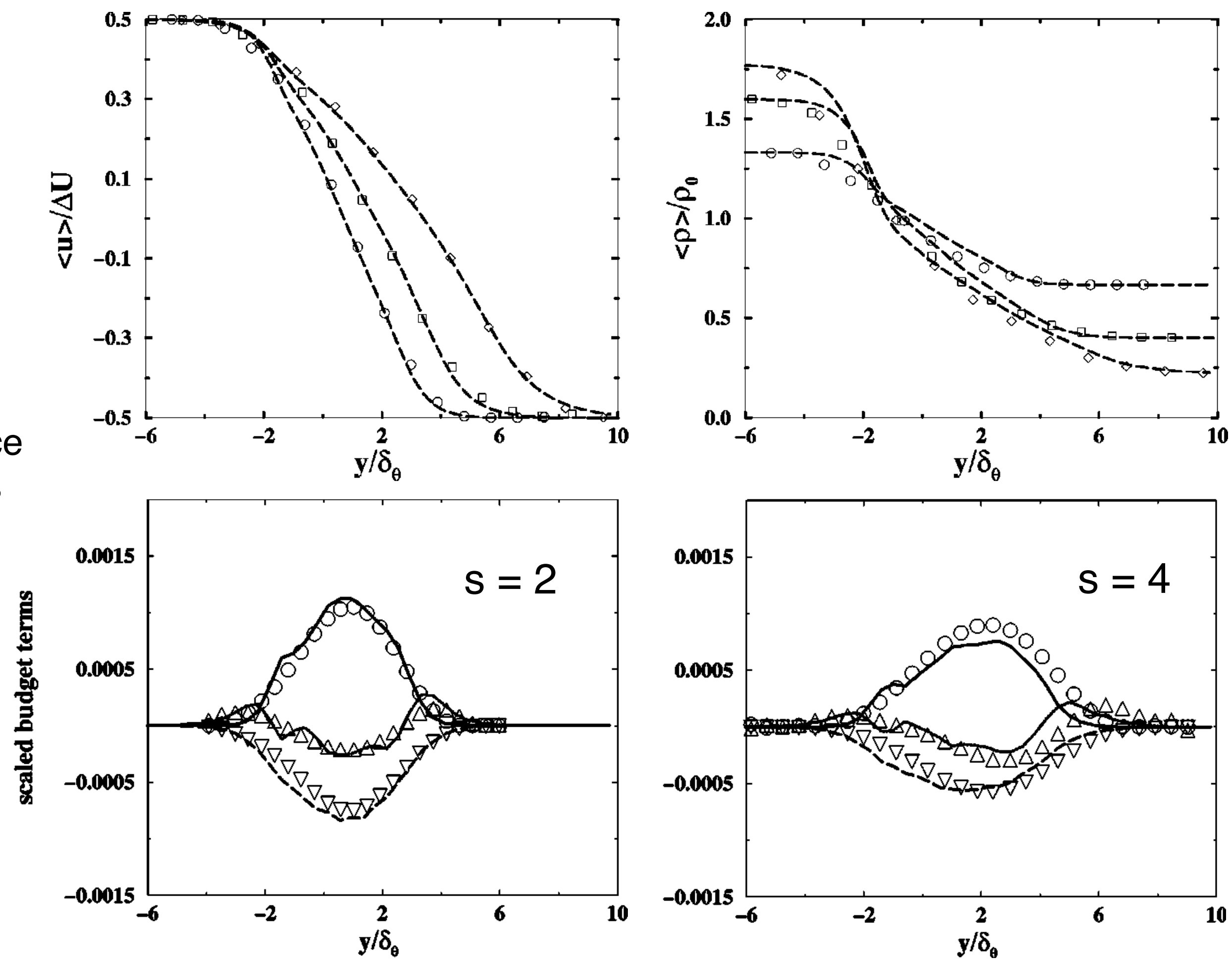
Plotted: lateral (y) profiles scaled by momentum thickness

Ma=0.7:
curves, ODT
(Ashurst and Kerstein 2005);
symbols, DNS
(Pantano and Sarkar 2002)

ΔU = free-stream velocity difference
ρ_0 = mean of free-stream densities

Free-stream density ratios (s) for mean profiles (top):
○, s=2; □, s=4; ◊, s=8

Energy budget terms (bottom):
○, production
Δ, transport
∇, dissipation



Eddy sampling is based on the set of time scales τ of possible eddies, generalizing the set of 1/N values

Principle: Enforce consistency of eddies and flow (velocity and density profiles)

Eddy: Eddy velocity $\sim l/\tau$ so eddy energy $\sim \rho\, l^3/\tau^2$ ($l =$ eddy size)

Flow: $P \equiv$ gravitational potential energy change caused by the eddy

$K \equiv$ maximum kinetic energy extractable by adding *kernels* to velocity components within the eddy interval l

Relation determining τ **for a given eddy at a given instant:**

$$\frac{\rho\, l^3}{\tau^2} = A\left(K - P - Z\frac{\mu^2}{\rho l}\right)$$

adjustable parameters (A, Z)

viscous penalty (imposes a threshold Reynolds number)

This approach resembles conventional mixing length theory

but

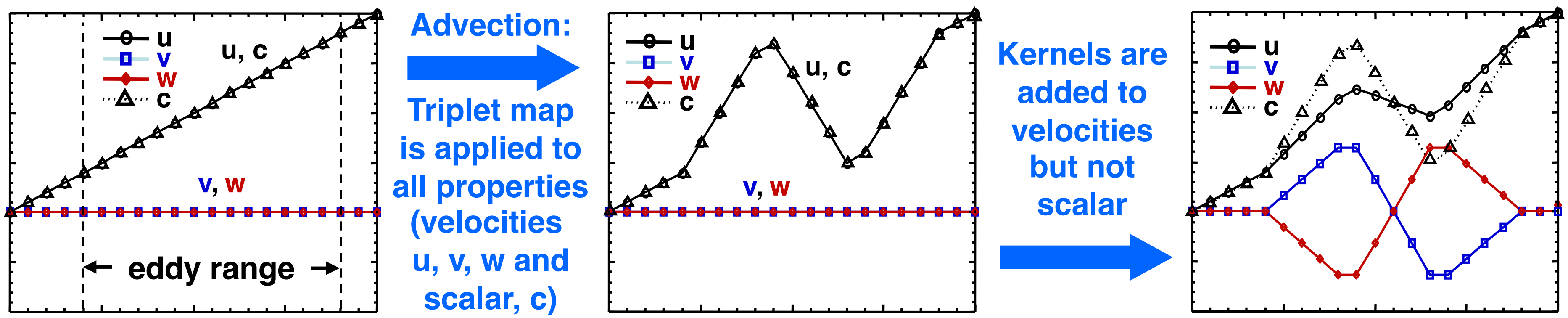
- The concept is applied to range of l values, not a single l value

- K and P are based on the instantaneous state, not an average state

- Alternation between eddies and molecular transport introduces strong coupling, thereby linking eddy dynamics to the flow configuration (ICs, BCs, body forces, fluid properties, etc.)

Velocity profiles determine the spatial distribution of kinetic energy, thereby influencing eddy occurrences, but velocity does not directly advect fluid

Energy conversion is implemented by an additional eddy operation



Kernels (analogous to wavelets) are applied to velocity profiles in order to

- Evaluate the kinetic-energy term in the expression for τ
- Redistribute kinetic energy among velocity components: ‘return to isotropy’
- Change kinetic energy in the eddy range by an amount equal and opposite to the map-induced change of gravitational potential energy

Representative applications of map-based advection

- Buoyant stratified flow
- Free shear flow
- Mixed convection
- Boundary layers
- Electrohydrodynamic turbulence
- Electromagnetic wave propagation in plasmas
- Frequency spectrum of jet noise
- Cloud aerosol microphysics (droplets and ice)
- Liquid jet breakup
- Combustion and other reacting flows
- Shock-flame interaction and transition to detonation
- Subgrid closure for CFD

Some possible contributions of the 1D approach to layering research

- Suite of staircase simulations for parameterization of fluxes and interface formation, migration, and merger
- Convection regime for high layer Ra
- Internal-wave effects on staircase formation and evolution
- Generalizations: Multiple species, radiative heat transport, multiphase, etc.
- ODT + Cahn-Hilliard
- Perturbation threshold for staircase initiation

An extensive single-interface parameter study using ODT yielded Nu and Re correlations

Simulations of unsheared interfaces with $R_\rho = 1.05$–6, $Ra = 10^6$–10^{10} and $Le = 0.01$ show that

$$Nu \sim \begin{cases} (Ra/R_\rho)^{0.37\pm0.03} & \text{when } Pr = 3\text{–}100 \\ (Ra/R_\rho)^{0.31} Pr^{0.22\pm0.04} & \text{when } Pr = 0.01\text{–}1, \end{cases} \tag{5.1}$$

$$Re \sim Ra^{0.45\pm0.04} R_\rho^{-0.12\pm0.05} Pr^{-0.58\pm0.03} \quad \text{when } Pr = 0.01\text{–}100. \tag{5.2}$$

A slight decrease of Nu with Pr is seen when $Pr \approx 10$–100, but it is not quantified since it is too small to accurately fit the available data.

Gonzalez-Juez, Kerstein, and Lignell 2011

Sheared interfaces were also investigated and trends were quantified

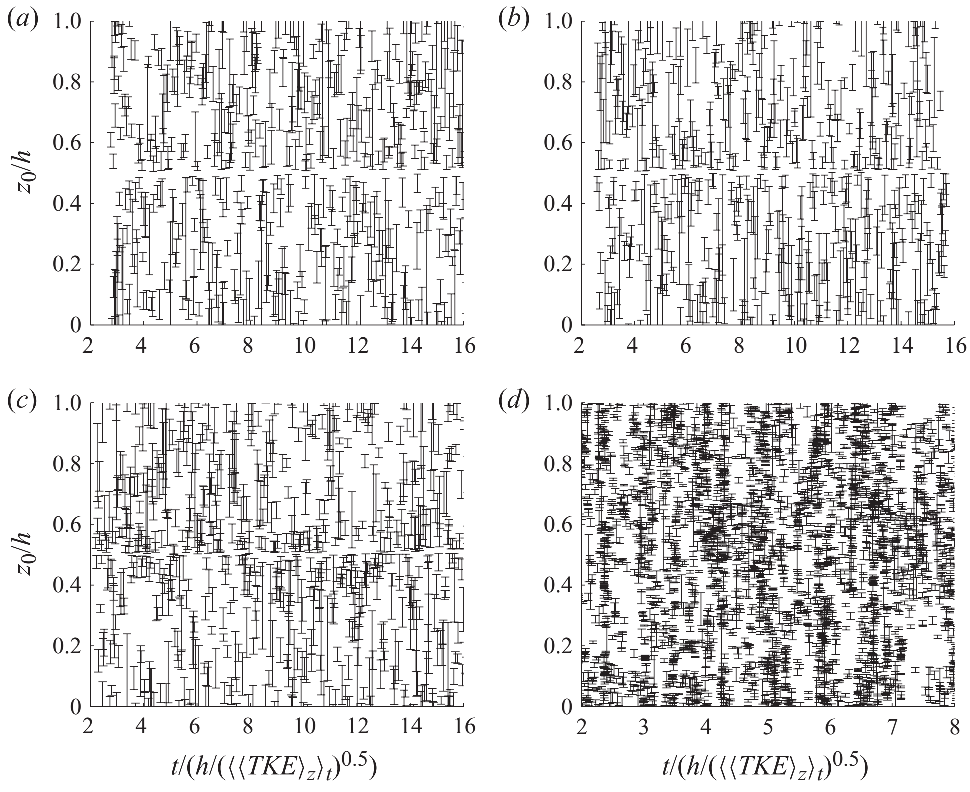
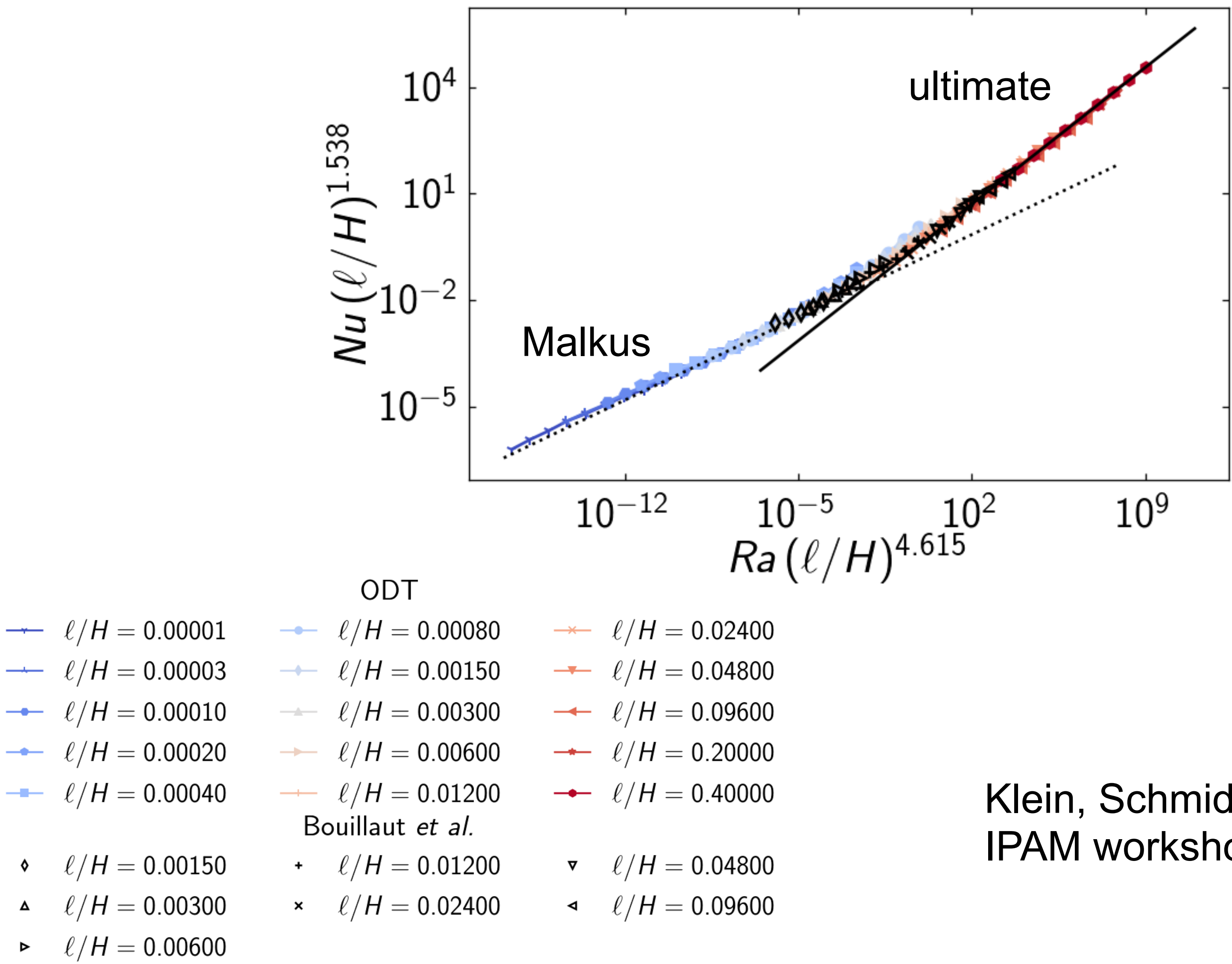


FIGURE 24. Temporal sequence of the locations z_0 and sizes l (vertical bars) of eddy events generated in an ODT simulation of double-diffusive convection with background shear. For clarity, not every eddy event implemented in the simulations is shown. Values of Ri are (a) ∞, (b) 794, (c) 7.94 and (d) 0.1. Other parameter values are $R_\rho = 6$, $Ra = 10^8$, $Le = 0.01$, $Pr = 7$, $C = 10$ and $Z = 1$.

Gonzalez-Juez, Kerstein, and Lignell 2011

Experimentally and with ODT, radiatively driven Rayleigh convection transitions to the ultimate regime



Klein, Schmidt, and Kerstein,
IPAM workshop, 2021

ODT captures fluctuation statistics as well as bulk properties of Rayleigh convection

Wunsch and Kerstein, 2005

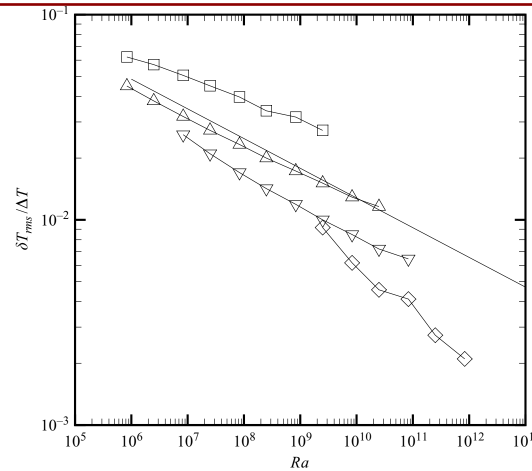


FIGURE 6. Magnitude of temperature fluctuations in the interior. Symbols are ODT simulation results for $ZC^2 = 10^4$ at □, $Pr = 0.025$; △, 0.7; ▽, 4; ◇, 1352; the solid line is $\delta T_{rms}/\Delta T = 0.37 Ra^{-0.145}$, a reported fit to $Pr = 0.7$ experimental data by Niemela *et al.* (2000).

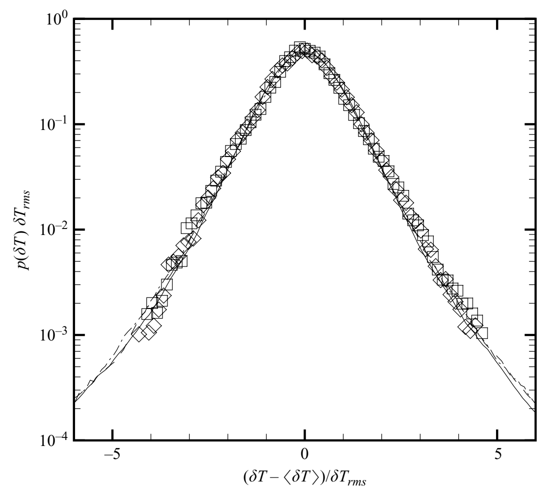


FIGURE 9. Rescaled probability density p of a temperature fluctuation δT (lines) for $Pr = 5.5$, $Ra = 2 \times 10^9$. The three lines correspond to ODT results for the three values of ZC^2: dash-dotted for $ZC^2 = 823$, dashed for $ZC^2 = 10^4$, and solid for $ZC^2 = 10^5$. The shape is independent of ZC^2. Here, $\langle \delta T \rangle = 0.5\Delta T$ and δT^2_{rms} is the variance of the p.d.f. For comparison, experimental data in two distinct cell geometries (□, cylindrical geometry; ◇, rectangular geometry) with the same Ra and Pr are also shown (Daya & Ecke 2001).

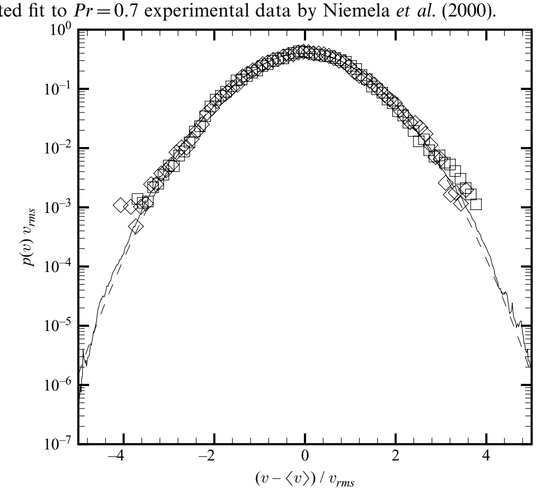


FIGURE 16. Rescaled probability density p of a core velocity fluctuation v. ODT simulation data (solid line) for $Pr = 5.5$, $Ra = 2 \times 10^9$ and $ZC^2 = 10^5$. Experimental data from the cell centre in two distinct geometries (□, cylindrical geometry; ◇, rectangular geometry) for the same Ra and Pr are shown for comparison (Daya & Ecke 2001). Also shown is a Gaussian p.d.f. (dashed line).

An internal wave can be idealized as sinusoidal vertical motion w = A sin(ωt) of the ODT domain

By the equivalence principle, this generalizes gravity to g – dw/dt in the potential-energy term of the expression for τ

Resources are available to learn more and use the model for research

MatLab package set up for staircase simulation –
Scott Wunsch

F77 code with detailed documentation, set up for channel flow simulation –
https://sites.google.com/site/odtresearch/codes

C++ code, efficient and easily customized –
https://github.com/ElsevierSoftwareX/SOFTX-D-20-00063