

A PBL-Turbulence Problem?



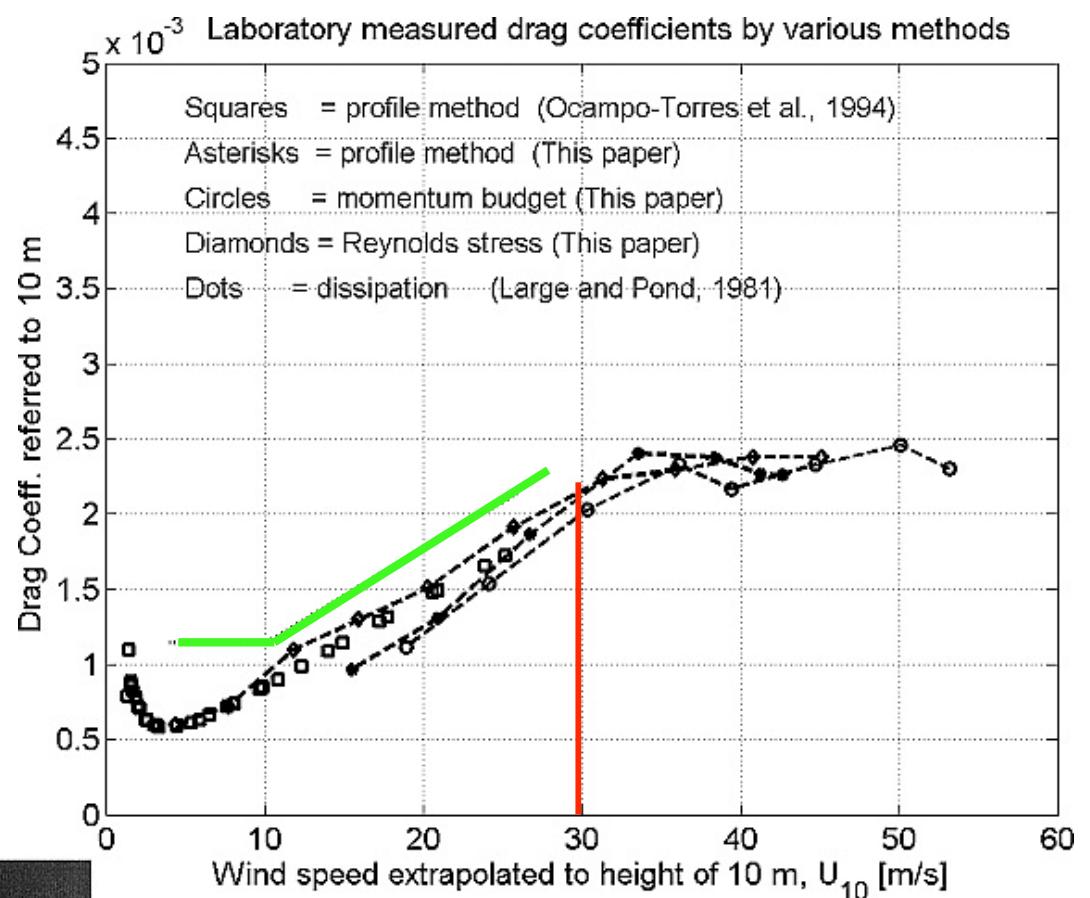
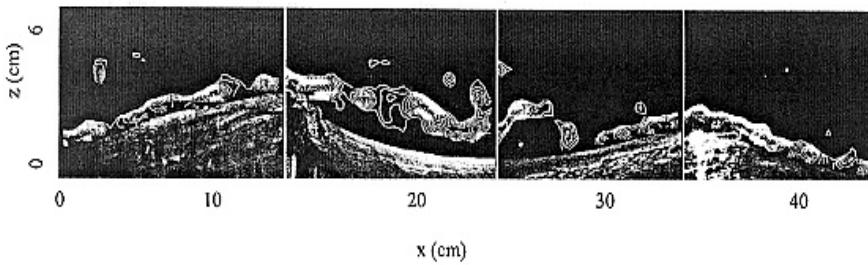
Courtesy NOAA

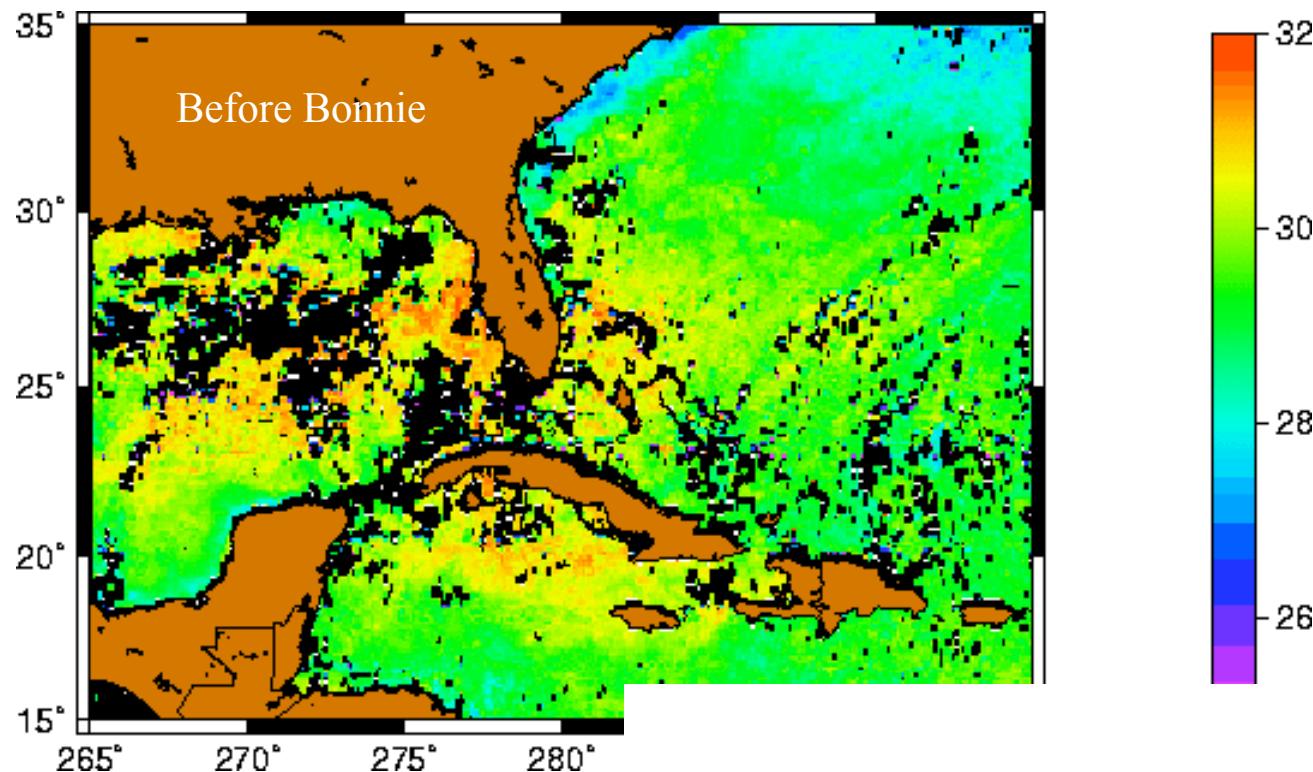
C_D Donelan et al, 2004

$$v_{max}^2 = \frac{T_s - T_o}{T_o} \frac{C_k}{C_D} (k_s^* - k)$$



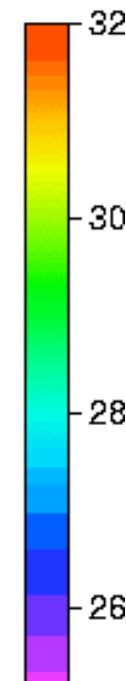
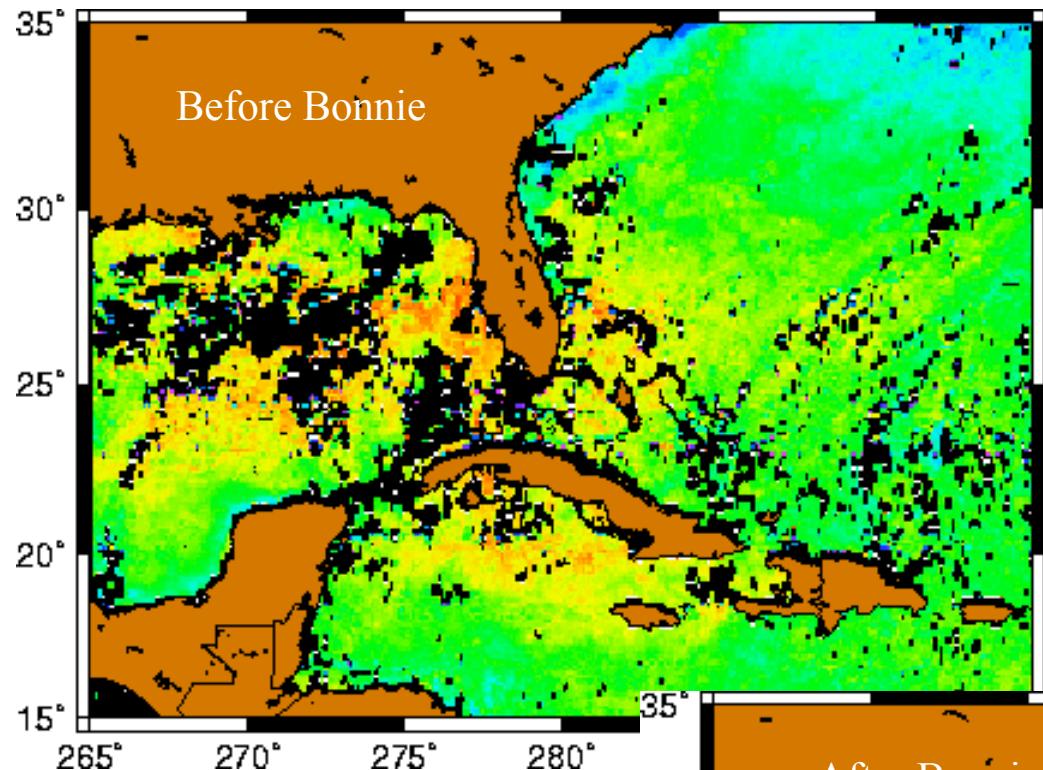
Maximum azimuthal wind speed (Emanuel, 2004)



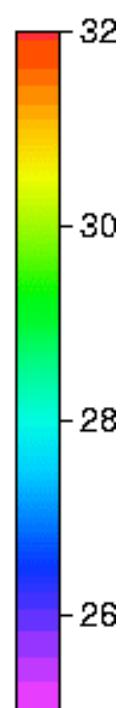
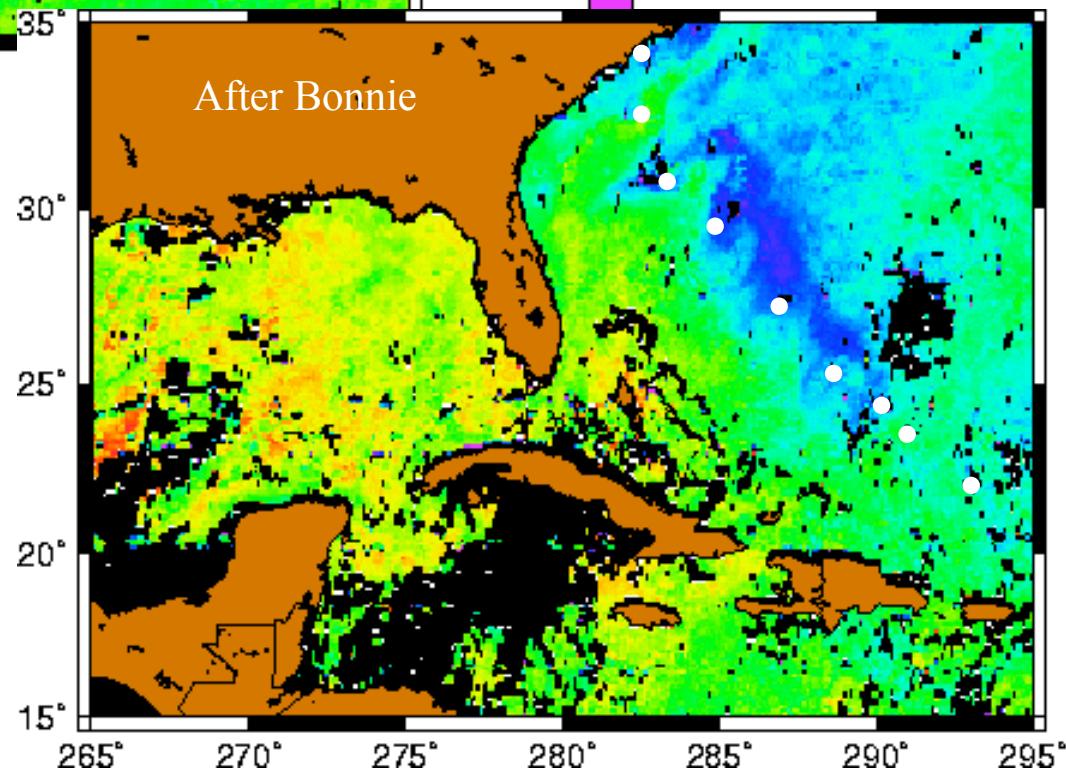


SST Variations, Ocean Mixing and Biology

Shuyi Chen,
RSMAS



SST Variations, Ocean Mixing and Biology



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ATMOSPHERIC BOUNDARY LAYER SIMULATION AND SUBGRID-SCALE DYNAMICS

1. An Introduction to Outdoor LES
2. Observations and SGS Model Equations
3. LES Applications

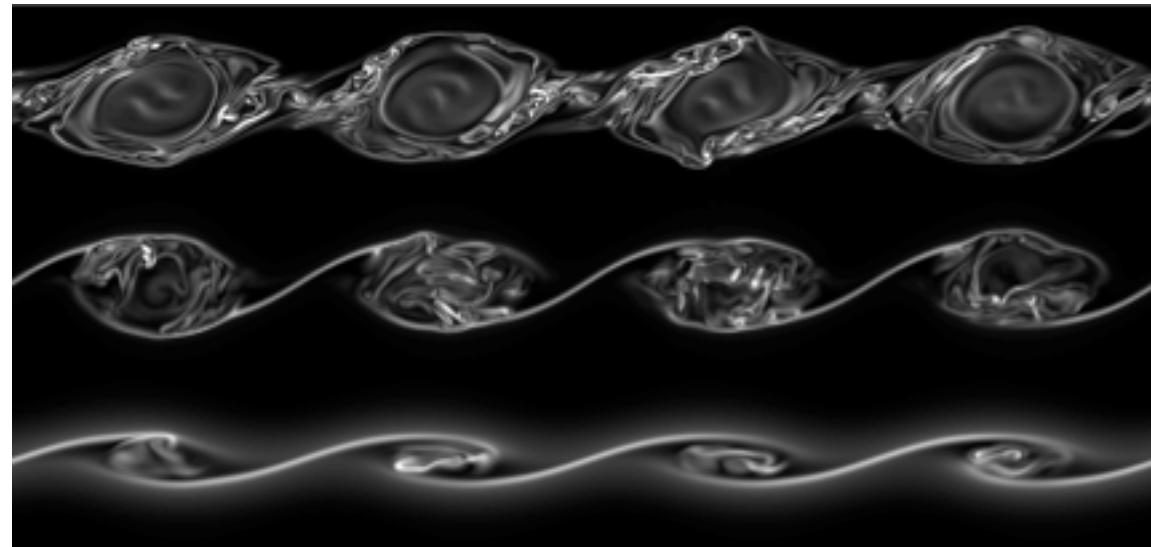
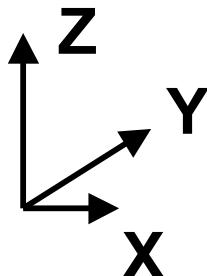
Peter P. Sullivan

National Center for Atmospheric Research

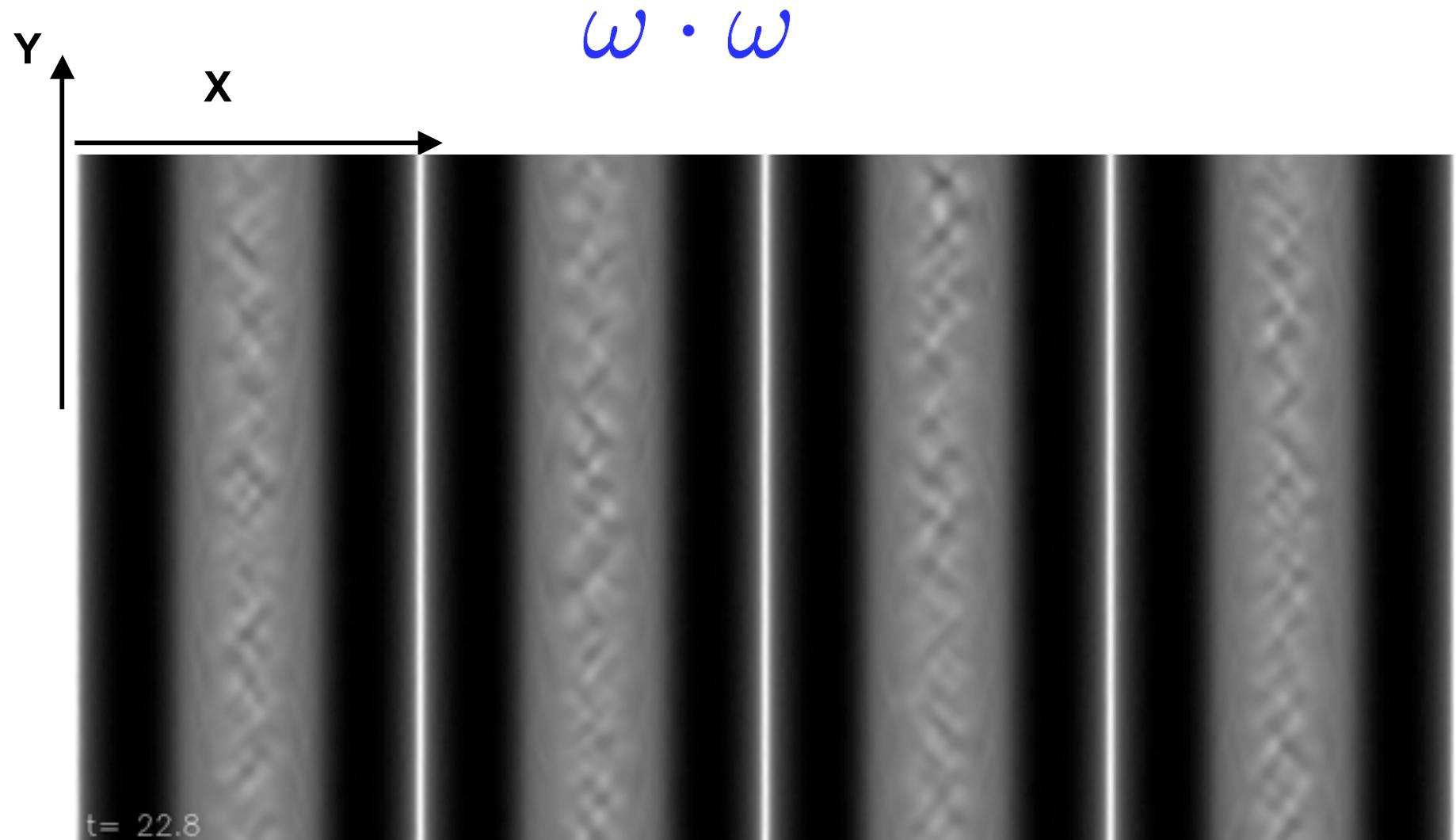
**“VIRTUAL” TURBULENCE,
EVIDENCE FROM DIRECT NUMERICAL SIMULATION
... NO EMPIRICISM**

DIRECT NUMERICAL SIMULATION (DNS) OF KELVIN-HELMHOLTZ FLOW

- Courtesy Joseph Werne Colorado Research Associates
- Solve 3D Navier Stokes with Boussinesq approximation
- Number of gridpoints (modes) $3000 \times 1500 \times 1500 = 6.7 \times 10^9$ 
- Reynolds number $Re = 2500$, varying stratification $Ri = [0.05, 0.15, 0.2]$
- 1500 processors



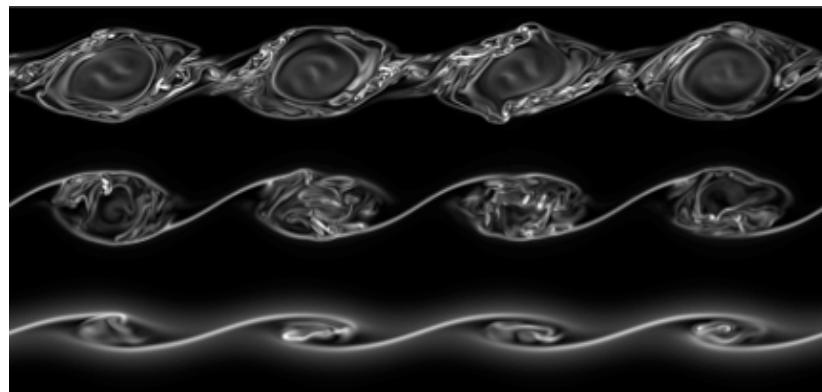
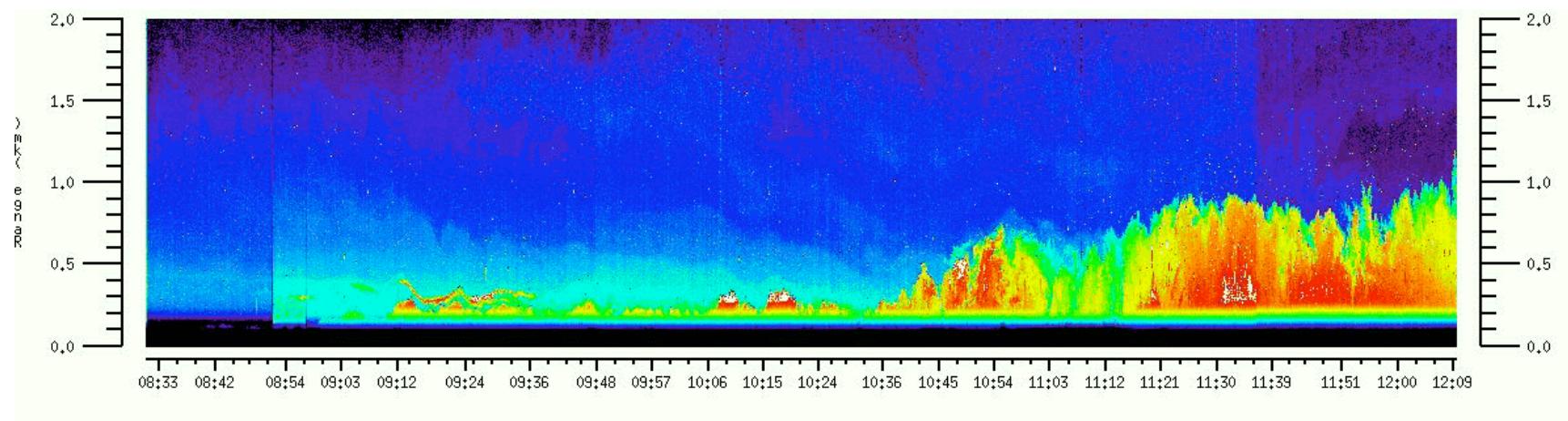
EVOLUTION OF ENSTROPY IN AN X-Y PLANE



steady \longrightarrow periodic \longrightarrow quasi-periodic \longrightarrow turbulent

“ ... We know what the PBL equations are ...
let's just use DNS?”

LIDAR OBSERVATIONS OF PBL DIURNAL EVOLUTION,
COURTESY SHANE MAYOR NCAR



LENGTH AND TIME SCALES OF HIGH-*Re* CONVECTIVE PBL TURBULENCE

- Energy-containing (large) eddies $\mathcal{L} \sim \mathcal{O}(z_i)$; $z_i \sim 1000\text{m}$
- Velocity scale of the (large) eddies $\mathcal{U} \sim (gQ_*z_i/\Theta_o)^{1/3}$; $\mathcal{U} \sim 1\text{m/s}$
- Large eddy turnover time $\mathcal{T} = \mathcal{L}/\mathcal{U}$; $\mathcal{T} = 1000\text{s}$
- Kolmogorov microscale $\eta = (\nu^3/\epsilon)^{1/4}$; $\eta \sim 1\text{mm}$
- Reynolds number $Re_{\mathcal{L}} = \mathcal{U}\mathcal{L}/\nu = 10^6$

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Amount of work (number of mode-steps) is

$$N^3 \cdot N_s \approx Re_{\mathcal{L}}^3$$

Therefore

$$N^3 \cdot N_s \approx 10^{18} \quad \text{for} \quad Re_{\mathcal{L}} = 10^6$$

**“ ... DNS is mighty useful, however we
don’t have enough IBM SP’s to get to a
PBL Reynolds number and resolve all
scales of a rough wall ... We need
something else ...”**

GEOPHYSICAL BOUNDARY LAYERS

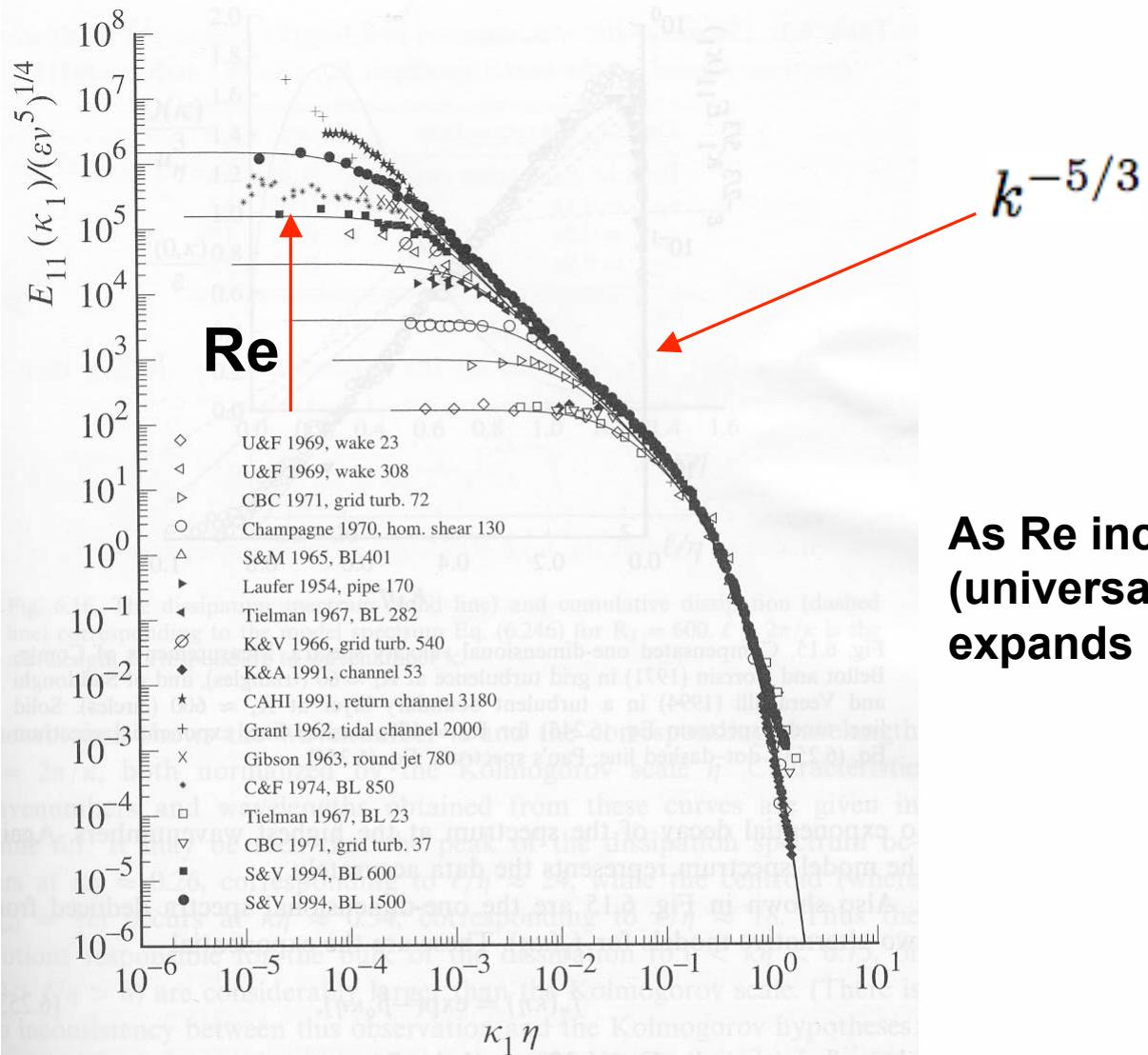
What makes turbulent PBLs unique?

- High Re
- Stratification (buoyancy) is always important
- Driven by large-scale forcings (*e.g.*, frictional drag, evaporation and transpiration, heat transfer, pollutant emission, terrain, diurnal cycling, ...)
- Interactions with interfaces
 - Rough high Re lower boundary (*e.g.*, terrain, vegetation, ...)
 - Time varying interface (surface waves, nonequilibrium, ...)
 - Stably stratified inversion/thermocline
- Clouds
- ...

HOW DO WE GET THERE?

- Spatially filter the full governing equations to eliminate small scale fluctuations
- Subgrid-scale (SGS) challenge
 - Spatial correlations of small scale fluctuations $\neq 0$
 - High Re limit, universality of small scales
 - Building equations for SGS correlations
- Coping with a rough wall boundary

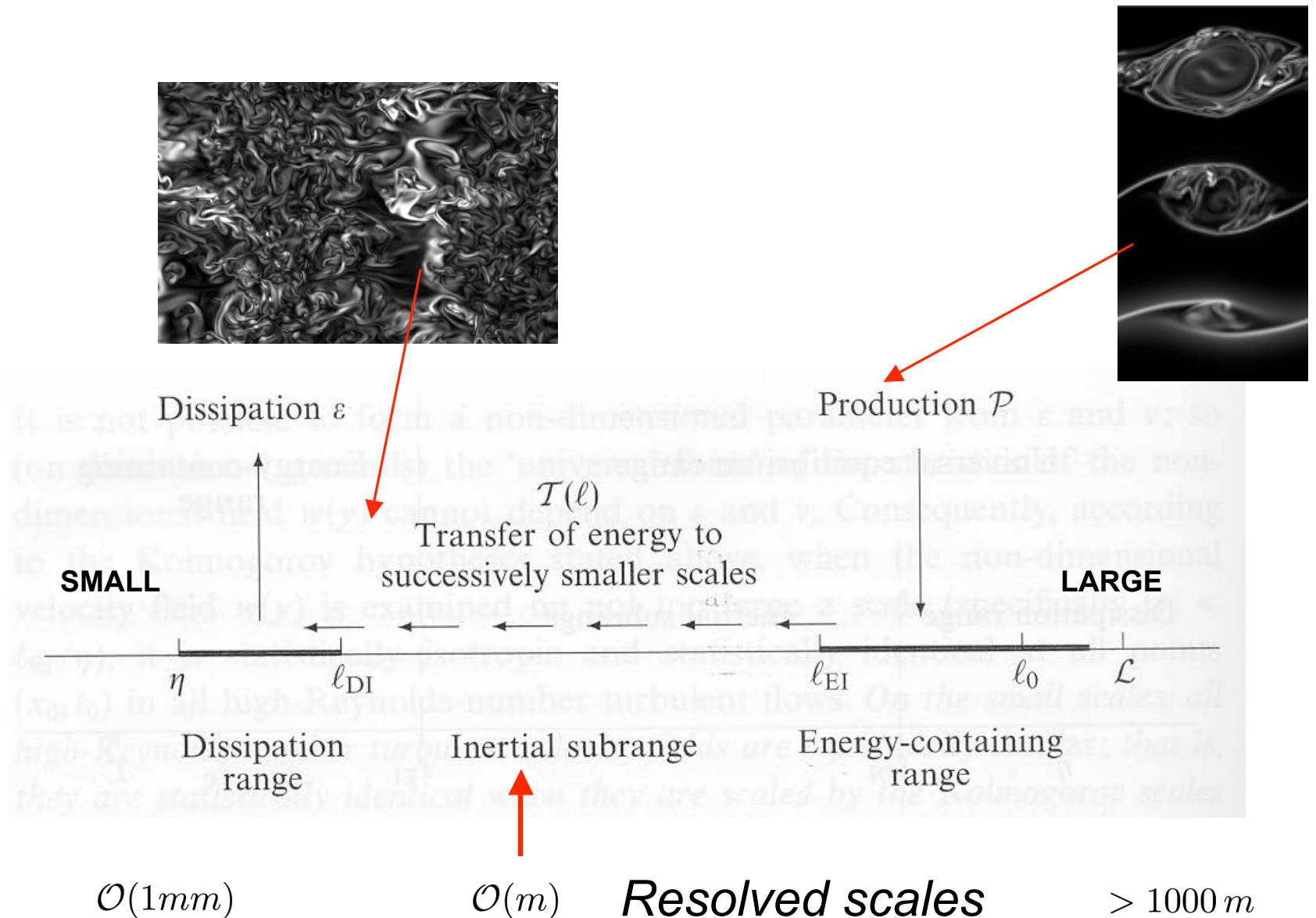
TURBULENCE ENERGY CASCADE CONCEPTS



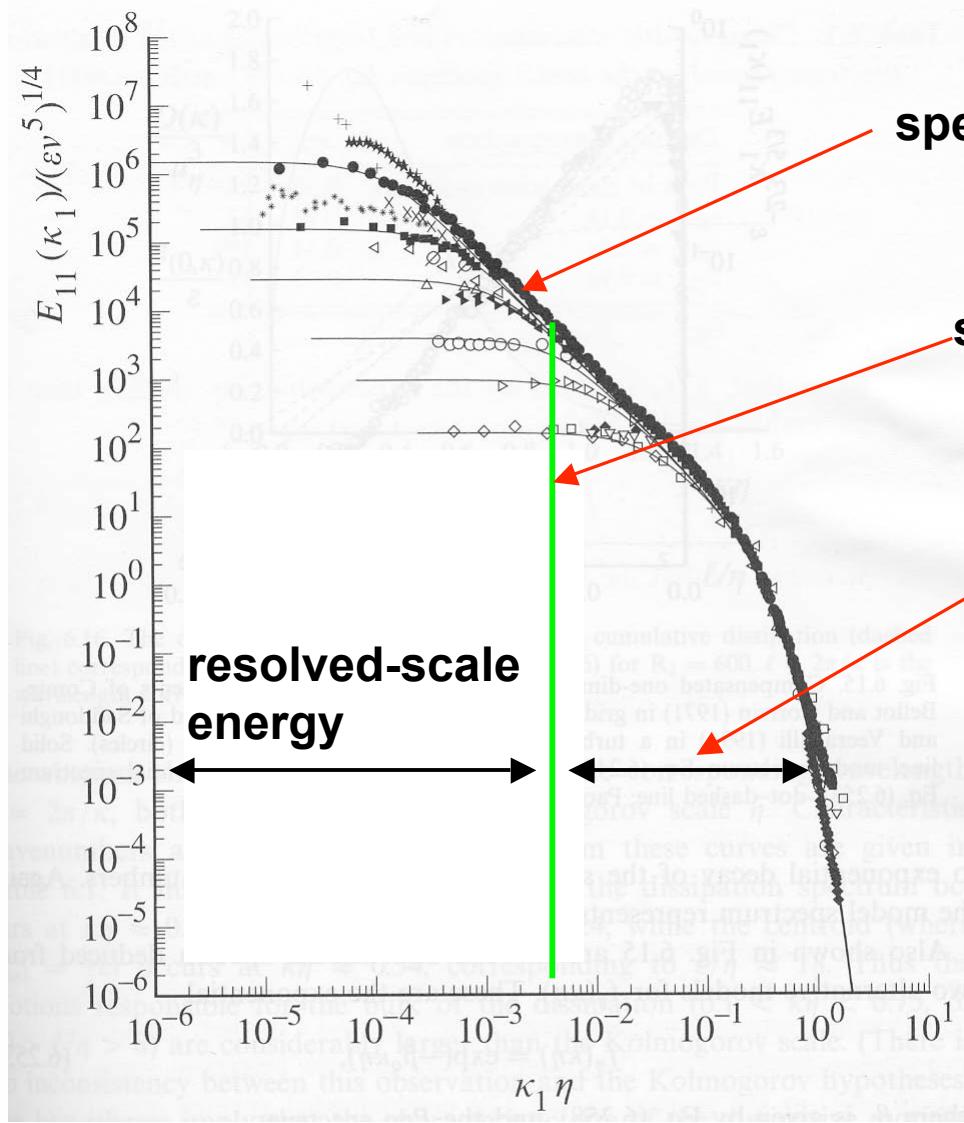
As Re increases the extent of the (universal) inertial subrange expands (Pope, 2000)

Fig. 6.14. Measurements of one-dimensional longitudinal velocity spectra (symbols), and model spectra (Eq. (6.246)) for $R_\lambda = 30, 70, 130, 300, 600$, and $1,500$ (lines). The experimental data are taken from Saddoughi and Veeravalli (1994) where references to the various experiments are given. For each experiment, the final number in the key is the value of R_λ .

TURBULENCE ENERGY CASCADE CONCEPTS



FILTERING IN THE INERTIAL RANGE



$$\text{spectrum } E(k) = \alpha \epsilon^{2/3} k^{-5/3}$$

$$\text{sharp filter cutoff } k_c = \pi/\Delta_c$$

$$e(k_c) = \int_{k_c}^{\infty} E(k) dk$$

$$\epsilon = C_{\epsilon} \frac{e^{3/2}}{\Delta_c}$$

EQUATIONS FOR DRY BOUSSINESQ ROTATING ATMOSPHERIC PBL

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\mathbf{f} \times \mathbf{u} - \nabla \pi + \hat{\mathbf{z}} g \frac{\theta'}{\theta_*} + \nu \nabla^2 \mathbf{u}$$

$$\frac{\partial \theta}{\partial t} + (\mathbf{u} \cdot \nabla) \theta = \alpha \nabla^2 \theta$$

Incompressible Boussinesq flow

$$\nabla \cdot \mathbf{u} = 0 \implies \nabla^2 \pi = s$$

see [Holton(2004)]

SPATIALLY FILTERED EQUATIONS FOR DRY BOUSSINESQ ROTATING ATMOSPHERIC PBL

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + (\bar{\mathbf{u}} \cdot \nabla) \bar{\mathbf{u}} = -\mathbf{f} \times \bar{\mathbf{u}} - \nabla \bar{\pi} + \hat{\mathbf{z}} g \frac{\bar{\theta}'}{\theta_*} + \nu \nabla^2 \bar{\mathbf{u}} - \nabla \cdot \mathbf{T}$$

$$\frac{\partial \bar{\theta}}{\partial t} + (\bar{\mathbf{u}} \cdot \nabla) \bar{\theta} = \alpha \nabla^2 \bar{\theta} - \nabla \cdot \mathbf{B}$$

$$\nabla \cdot \bar{\mathbf{u}} = 0 \implies \nabla^2 \bar{\pi} = \bar{s}$$

New terms! Subgrid-scale momentum and scalar fluxes

$$\begin{aligned} \mathbf{T} &= \overline{u_i u_j} - \overline{u_i} \overline{u_j} \\ \mathbf{B} &= \overline{u_i \theta} - \overline{u_i} \overline{\theta} \end{aligned}$$

see [Lilly(1967), Deardorff(1971), Leonard(1974), Moeng(1984)]

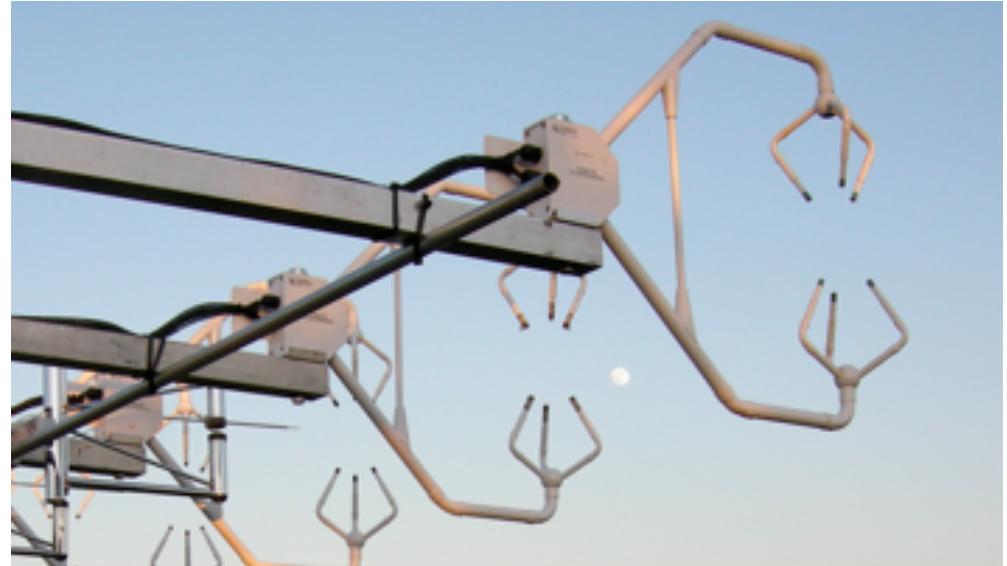
COMMENTS ON THE LES EQUATIONS AND THE SUBGRID SCALE STRESS TENSOR

$$\begin{aligned}\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} &= -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial}{\partial x_j} \left(\tau_{ij} - \nu \frac{\partial \bar{u}_i}{\partial x_j} \right) \\ \tau_{ij} &= \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j\end{aligned}$$

- The LES equations contain two parameters, Re and the filter properties (loosely the shape of the filter and its cutoff k_c)
- Solutions of the LES equations are *stochastic*, *i.e.*, \bar{u}_i is a random variable in (\mathbf{x}, t)
- τ_{ij} is unknown! It needs to be expressed in terms of known resolved fields \bar{u}_i
- Subgrid scale τ_{ij} is stochastic and depends on the filter. This makes \bar{u}_i also filter dependent.

SIMPLE (CHEAP) FILTERING EXAMPLE

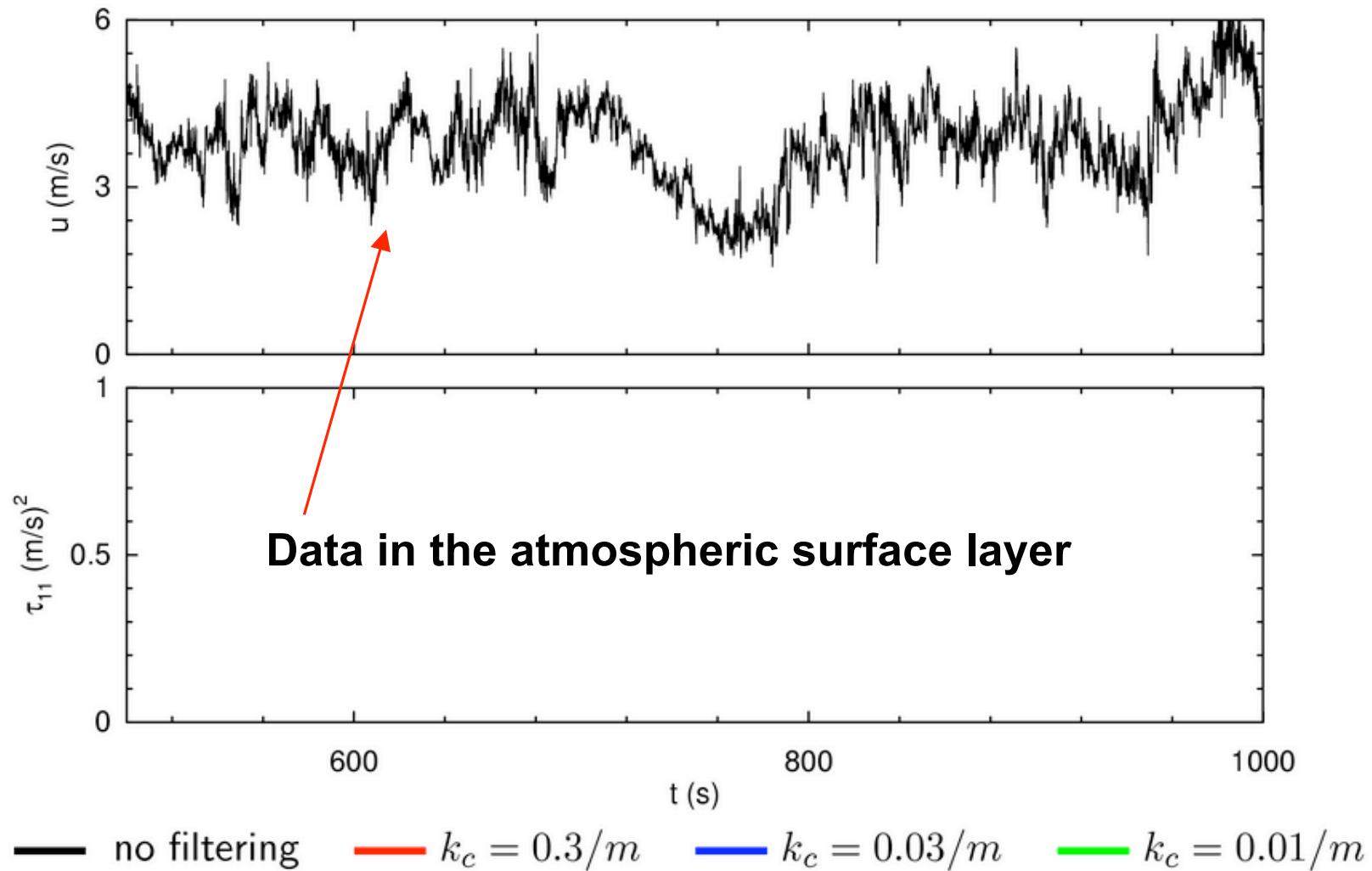
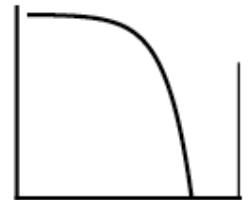
...



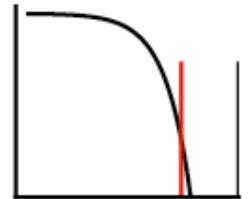
$$\tau_{11} = \overline{u_1 u_1} - \overline{u}_1 \overline{u}_1$$

MOVING BETWEEN DNS \leftrightarrow LES \leftrightarrow RANS

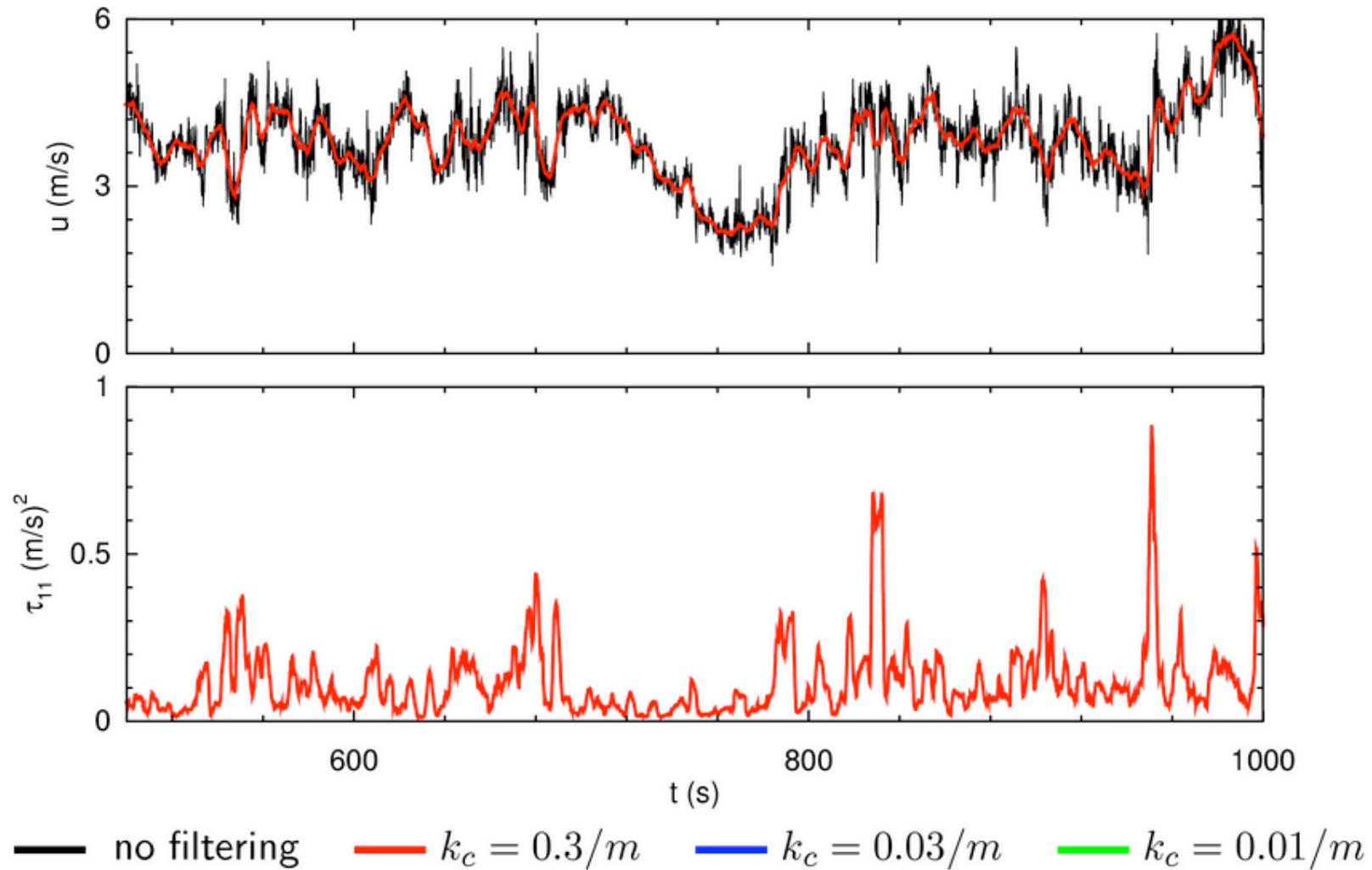
What happens to \bar{u}_i and τ_{ij} as we vary the filter cutoff k_c ?



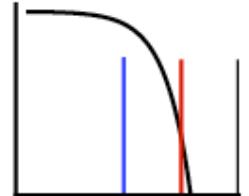
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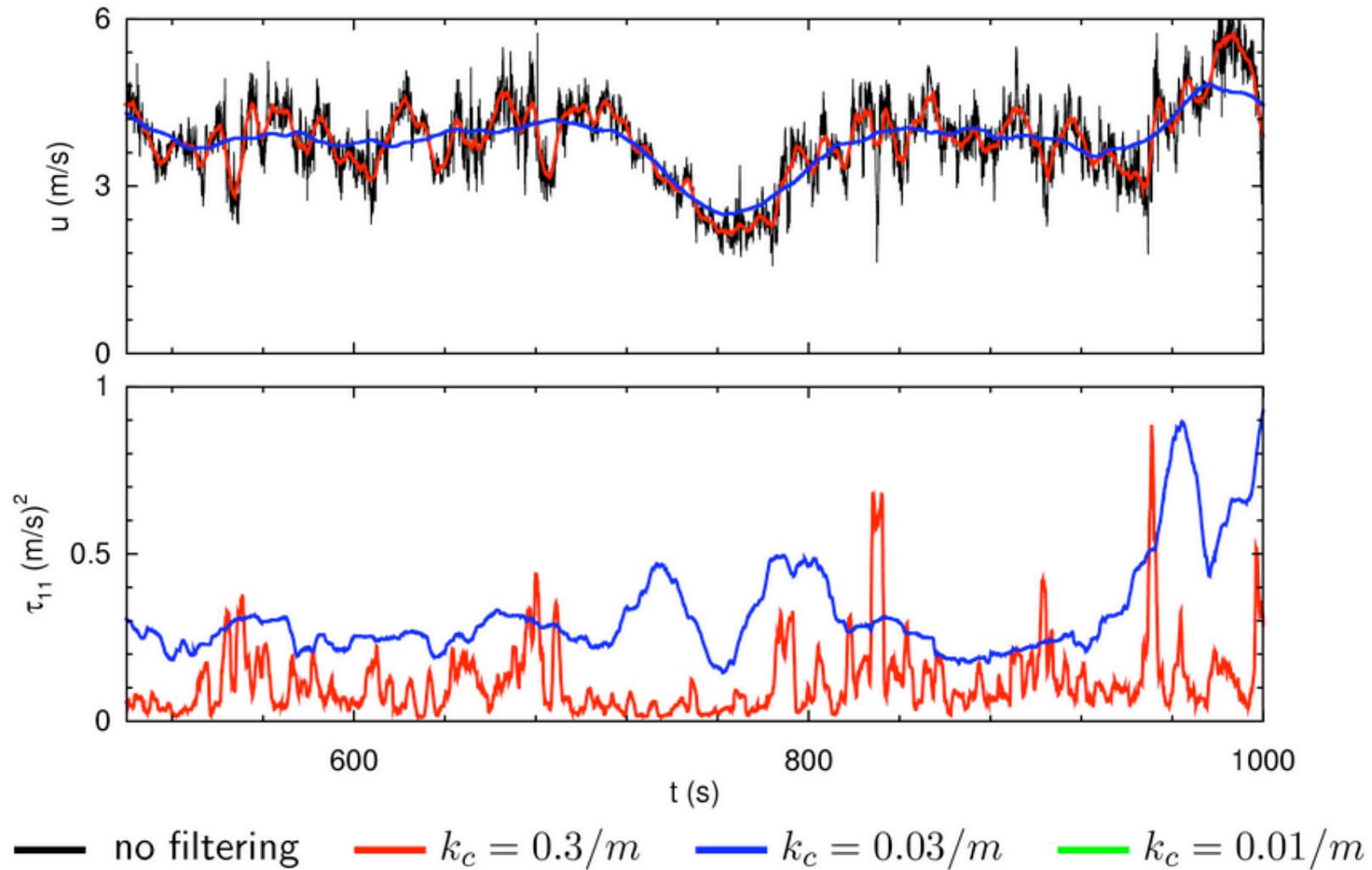
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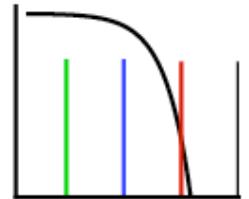
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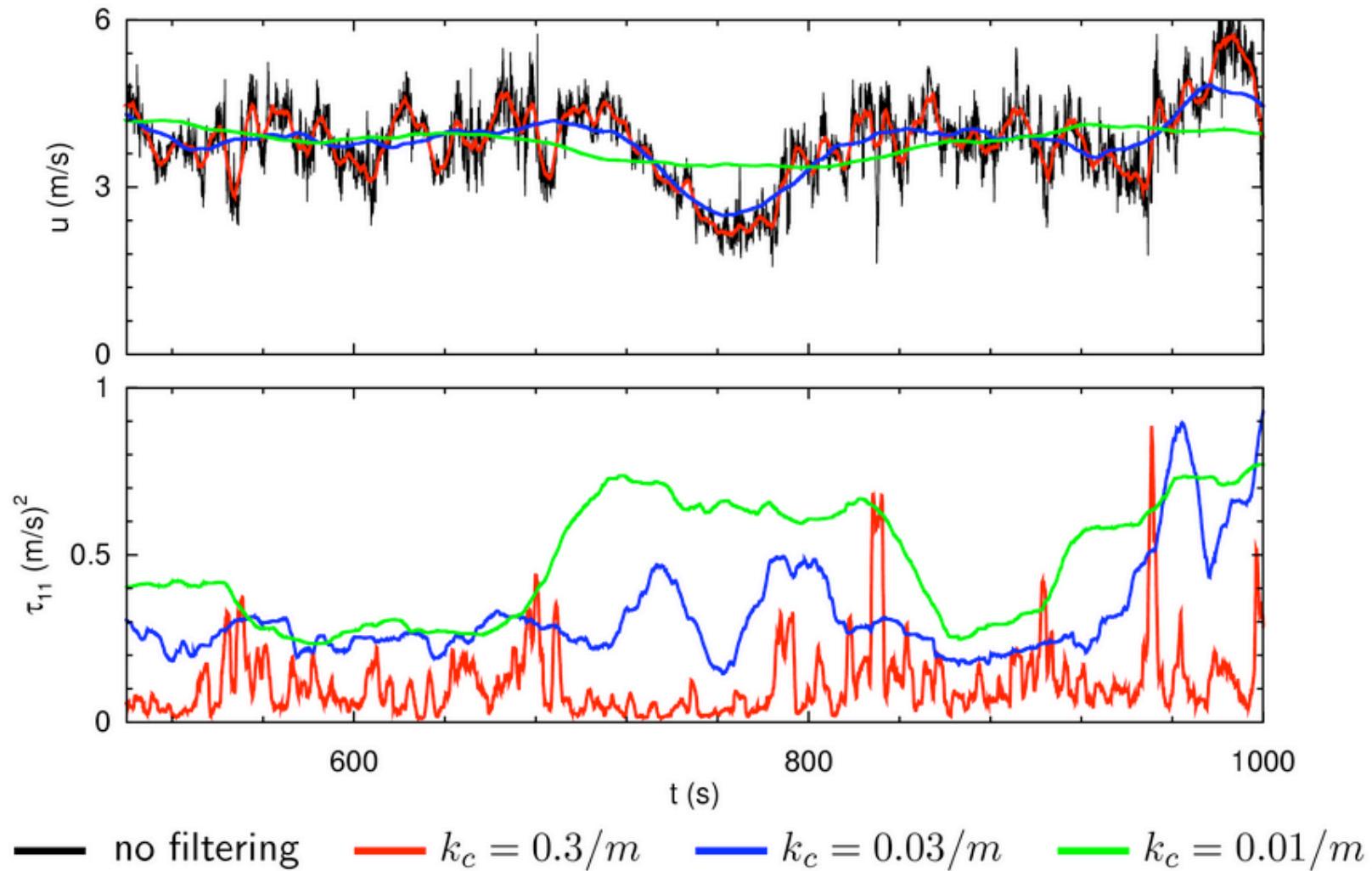
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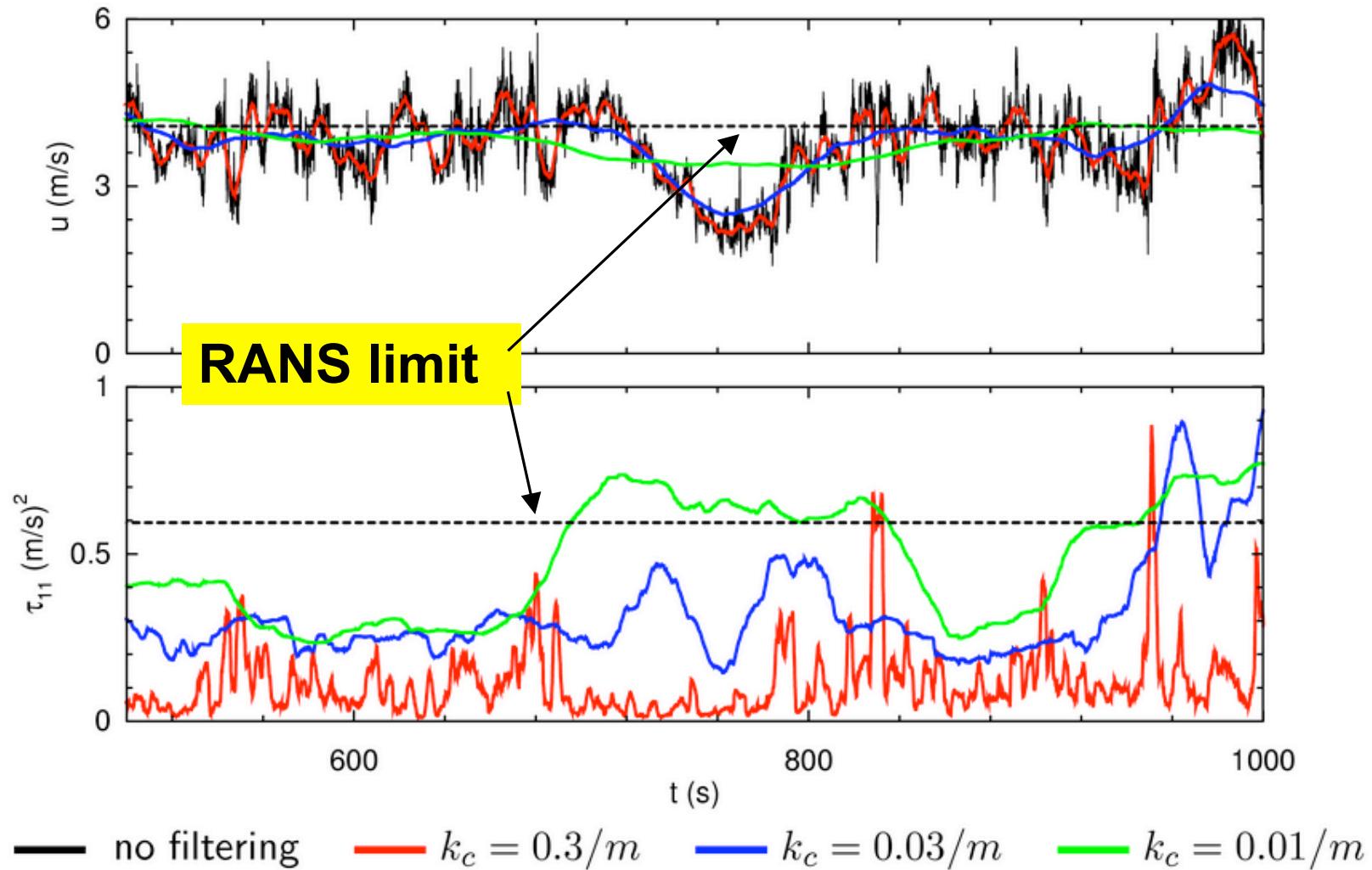


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MOVING BETWEEN DNS \leftrightarrow LES \leftrightarrow RANS

What happens to \bar{u}_i and τ_{ij} as we vary the filter cutoff k_c ?



SUBGRID SCALE TURBULENT KINETIC ENERGY

The SGS kinetic energy is

$$2e = \overline{u_i u_i} - \overline{u_i} \overline{u_i}$$

To get the “rate equation” for SGS e

$$\frac{\partial e}{\partial t} = \frac{1}{2} \left[\overline{u_i} \frac{\partial u_i}{\partial t} - \overline{u_i} \frac{\partial \overline{u_i}}{\partial t} \right]$$

SUBGRID SCALE TURBULENT KINETIC ENERGY

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Substitution steps:

$$u_i \frac{\partial u_i}{\partial t} = \overline{u_i} \mathcal{R}_i$$

$$\overline{u_i} \frac{\partial \overline{u_i}}{\partial t} = \overline{u_i} \overline{\mathcal{R}}_i$$

$$\frac{\partial e}{\partial t} = \frac{1}{2} [\overline{u_i} \mathcal{R}_i - \overline{u_i} \overline{\mathcal{R}}_i]$$

Algebra !

A NON-EQUILIBRIUM TKE SGS MODEL

SGS energy equation

$$\frac{\partial e}{\partial t} = -\bar{u}_i \frac{\partial e}{\partial x_i} - \tau_{ij} S_{ij} + \frac{g}{\theta_o} \tau_{i\theta} - \mathcal{T} - \epsilon$$

Production

Buoyancy

Transport

Model of viscous
dissipation

A NON-EQUILIBRIUM TKE SGS MODEL

SGS energy equation

$$\frac{\partial e}{\partial t} = -\bar{u}_i \frac{\partial e}{\partial x_i} - \tau_{ij} S_{ij} + \frac{g}{\theta_o} \tau_{i\theta} - \mathcal{T} - \epsilon$$

Parameterizations:

$$\tau_{ij} = -2\nu_t S_{ij} \quad \text{SGS momentum flux}$$

$$\tau_{i\theta} = -\nu_h \frac{\partial \bar{\theta}}{\partial x_i} \quad \text{SGS heat (scalar) flux}$$

$$\epsilon = C_\epsilon e^{3/2} / \Delta \quad \text{dissipation}$$

$$\nu_t = C_k e^{1/2} \Delta \quad \text{eddy viscosity}$$

$$\nu_h = \nu_t / Pr_t \quad \text{scalar diffusion}$$

“Constants” if Δ is in the inertial subrange [*Moeng and Wyngaard(1988)*]

$$C_\epsilon = 0.93, C_k = 0.1, Pr_t = 1/3$$

THE SMAGORINSKY MODEL

The model is of the form

$$\tau_{ij} = -2 \nu_t \bar{S}_{ij} \quad , \quad \bar{S}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

with eddy viscosity

$$\nu_t = C_k \sqrt{e} \Delta$$

In (2) we'll show how the eddy viscosity Smagorinsky model follows from SGS flux equations and test it against outdoor observations

In (2) we'll also examine ``Terra Incognita'' (Wyngaard, 2004) when the filter width $\sim O(L)$

In (3) we'll perform a grid convergence test of the PBL equations using the above TKE model

FLOW NEAR ROUGH BOUNDARIES

- Treatment of the lower boundary is the fundamental difference between Quasi-Direct Numerical Simulation (QDNS) [*Spalart et al.(1997)*]) and $1/Re \rightarrow 0$ LES [*Deardorff(1970)*])
- Impossible to resolve all separation points and wakes (at high Re) at a complex boundary, *e.g.*, the boundary might not even be defined!
- Numerical commutation errors [*Berselli et al.(2006)*] are mixed up with physical modeling
- Typical outdoor LES uses simple near wall models
 - Based on ensemble average ideas (Monin-Obukhov similarity theory)
 - Generate spatial fluctuations by applying MO on a point-by-point basis or using a linearization of the quadratic drag formula [*Moeng(1984)*])
- **Sometimes you don't get to choose where $1/\Delta_f$ sits!**
- There's work to be done near rough boundaries

FLOW OVER A ROUGH BOUNDARY

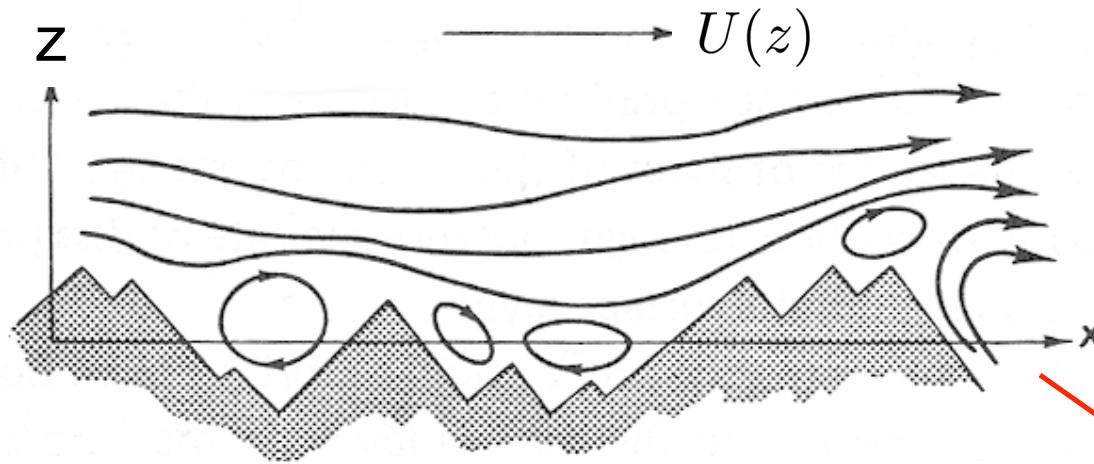
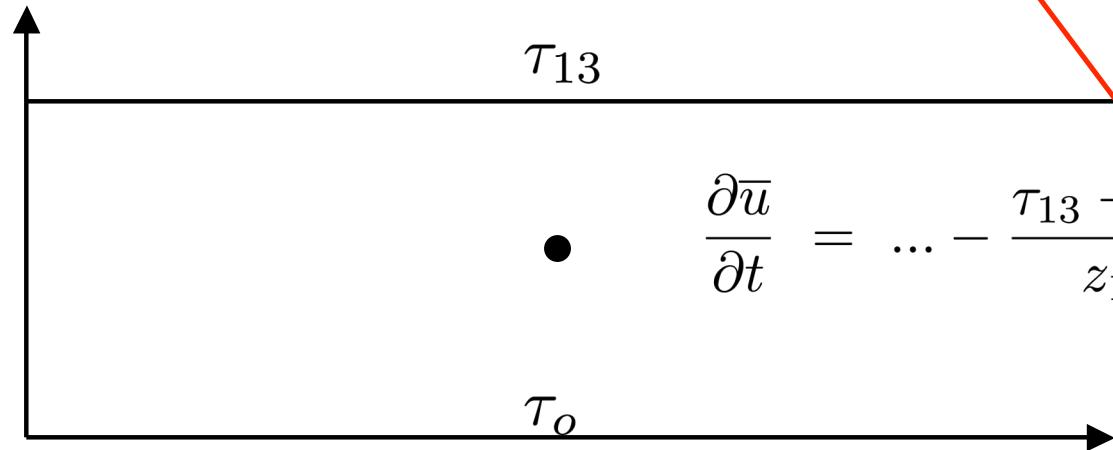


Figure 5.9. Flow over a rough surface.

$$\tau_o = f(z_o, \bar{u}, z_1, z_1/L)$$

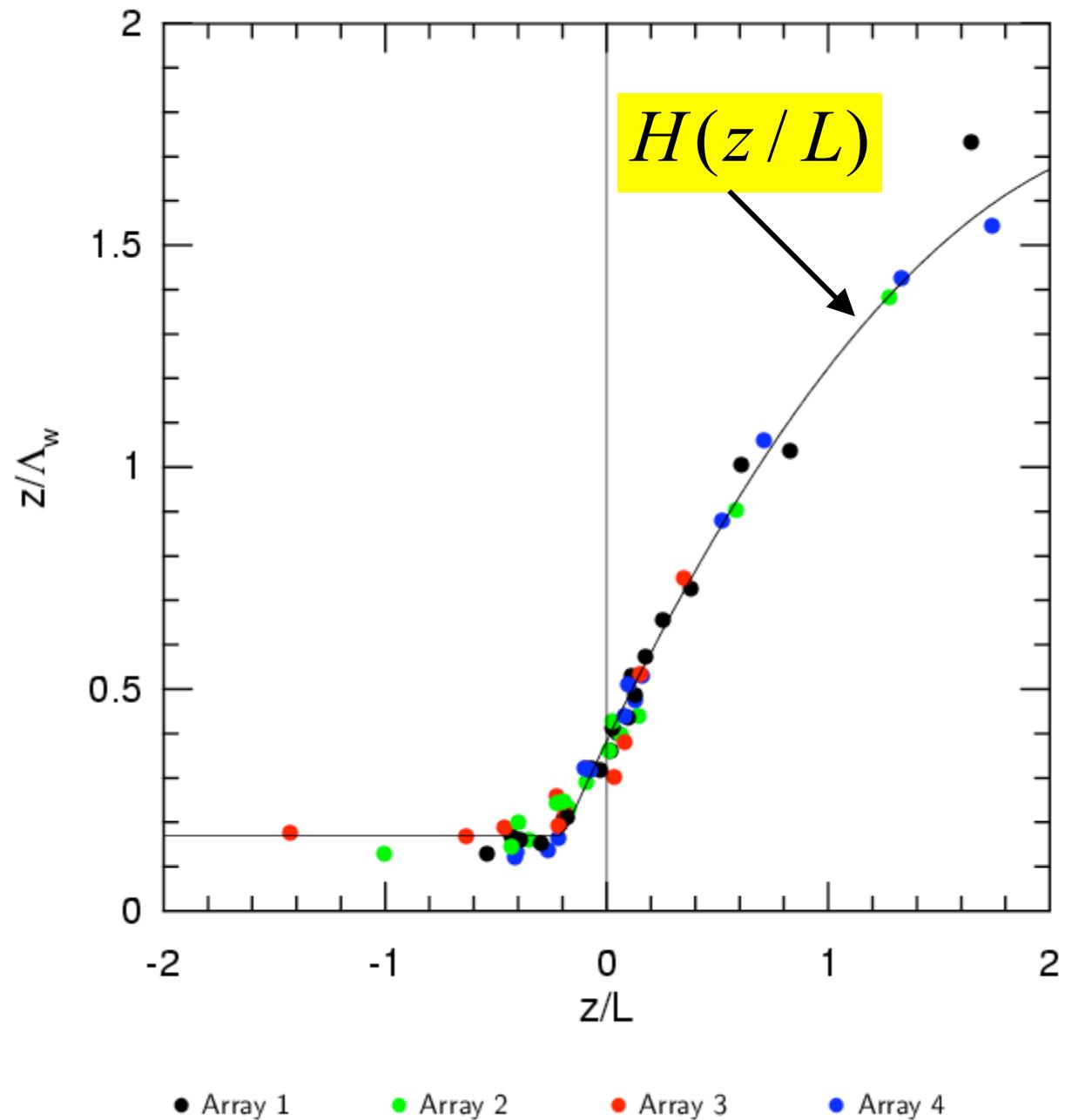


At a rough boundary all the flux is subgrid

SURFACE LAYER MEASUREMENTS AND LES: Λ_w/Δ_f AT FIRST GRID POINT OFF THE SURFACE

- $\Lambda_w \implies$ horizontal wavelength of the peak in the vertical velocity spectrum
 - w is least resolved in LES
 - Obeys MO scaling, *i.e.*, depends on (z, L)
- $\Delta_f \sim (\delta_x \delta_y \delta_z)^{1/3}$ the cell averaging volume

Dependence of Peak Wavelength on Stratification



RATIO OF PEAK WAVELENGTH TO FILTER WIDTH

The “peak” wavelength in the $w-$ spectrum is the empirical expression

$$\Lambda_w = \frac{\delta z}{H(\delta z/L)}$$

An estimate of the filter width is

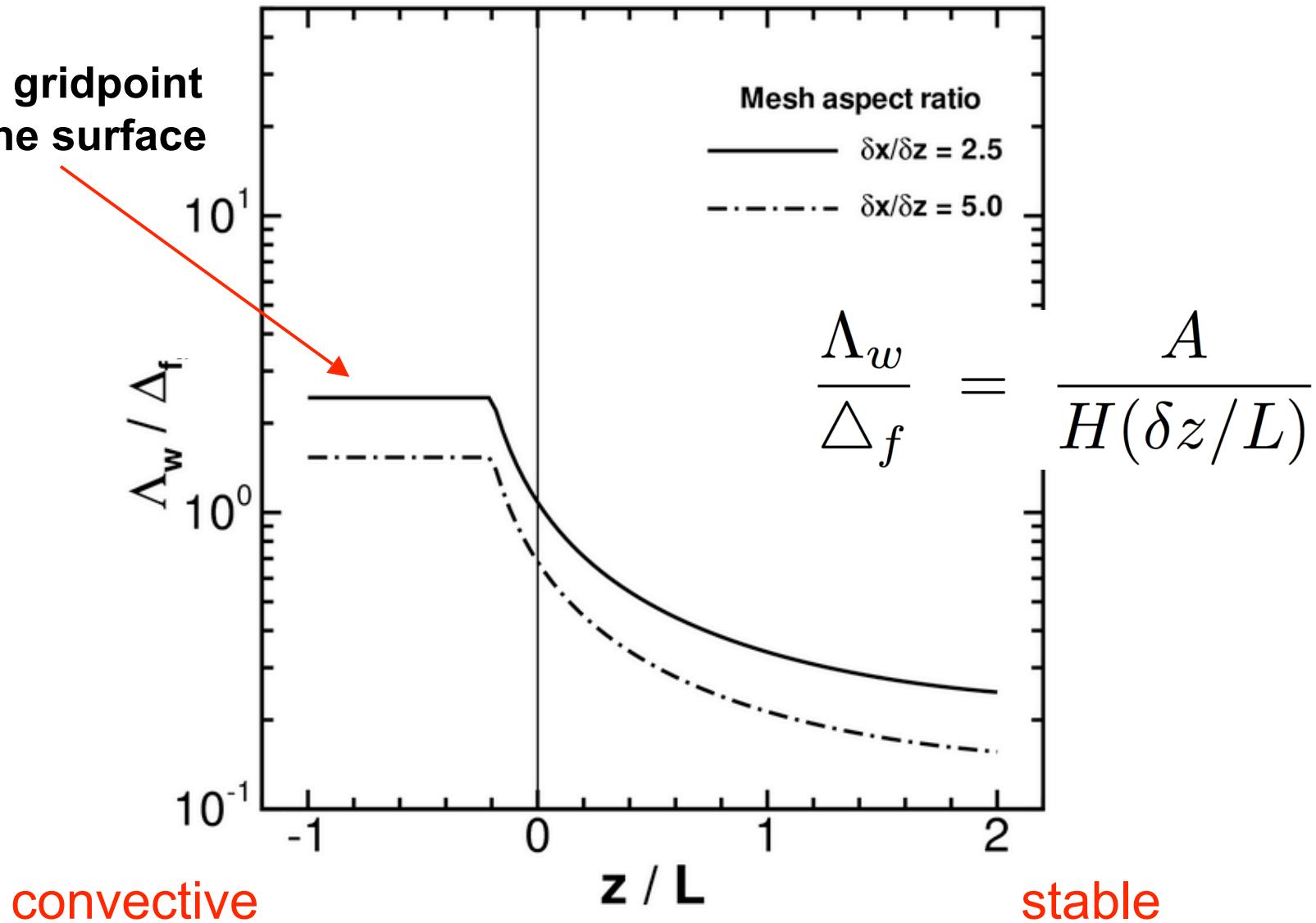
$$\begin{aligned}\Delta_f &= (\delta x \delta y \delta z)^{1/3} \\ &= \delta z / A\end{aligned}\quad \begin{matrix} \text{Mesh aspect ratio} \\ \leftarrow \end{matrix}$$

Then

$$\begin{aligned}\frac{\Lambda_w}{\Delta_f} &= \frac{\delta z}{\delta z} \frac{A}{H(\delta z/L)} \\ &= \frac{A}{H(\delta z/L)}\end{aligned}$$

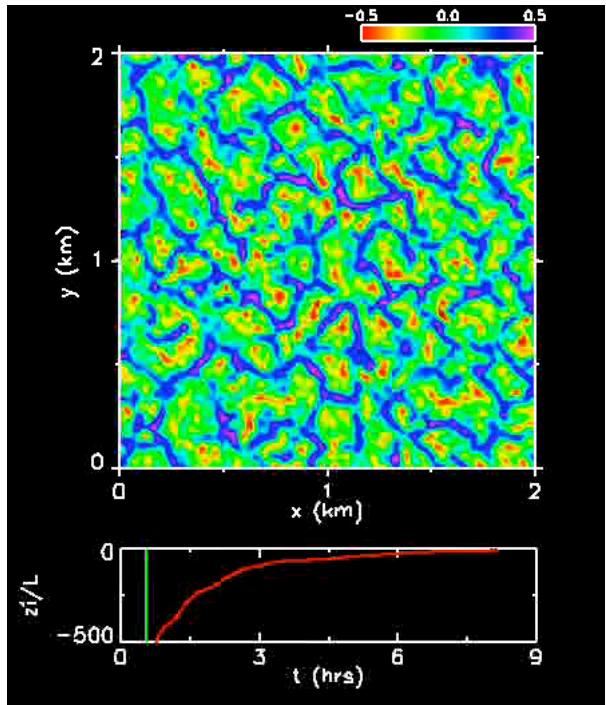
RATIO OF TURBULENCE LENGTH SCALE TO FILTER WIDTH AT FIRST LES GRIDPOINT $z = \delta_z$

First gridpoint
off the surface

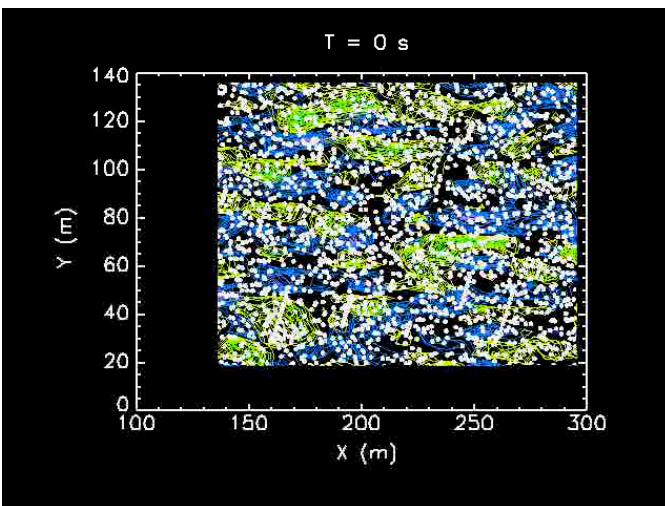


NUMERICAL ALGORITHM AND OPTIONS

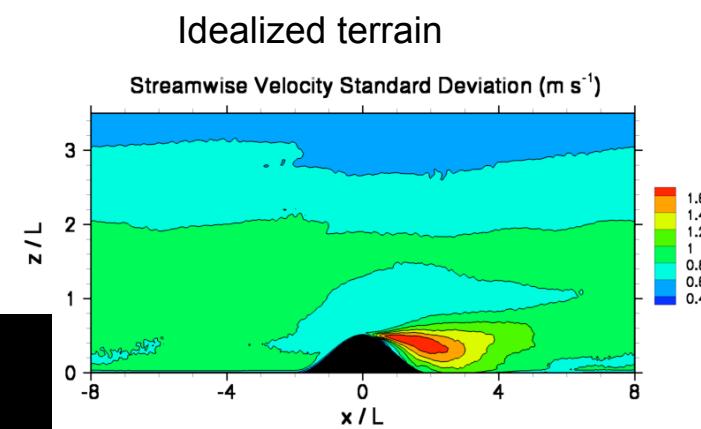
- Spatial discretization, pseudospectral in $x - y$, second-order finite difference in z , staggered in z
- Time stepping 3rd order Runge-Kutta with a fixed CFL number
- SGS model non-equilibrium TKE with surface layer corrections
- Explicit dealiasing using 2/3-rule in $x - y$ planes
- M-O wall functions
- Radiation upper boundary condition
- Variants allow surface fitted coordinate system using colocated variables
- Coupling with land surface model and vegetation
- Upside down version for ocean boundary layers with wave effects
- Highly parallelized using as many as 16,384 processors



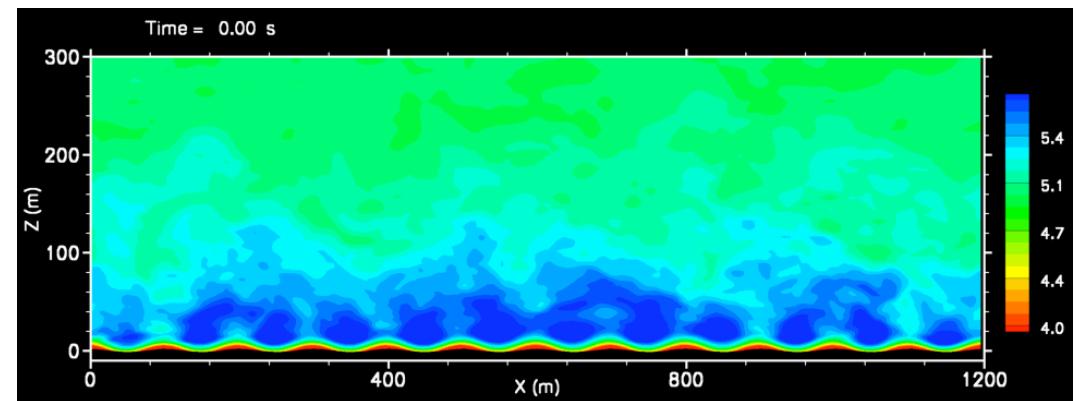
PBL driven by time varying geostrophic winds



Langmuir circulations and stochastic wave breaking in the OBL



Stable boundary layers $z_i/L \sim 1.2$



Non-equilibrium winds and waves

02468

P.D. Thompson

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THE REPRESENTATION OF SMALL-SCALE TURBULENCE
IN NUMERICAL SIMULATION EXPERIMENTS

• turbulence
• numerical simulation
• experiments
• representation
• models
• mixing

D. K. Lilly 201A

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Boulder, Colorado



Workshop on Micrometeorology

Niels E. Busch

Joost A. Businger

James W. Deardorff

Coleman duP. Donaldson

M. A. Estoque

Hans A. Panofsky

H. Tennekes

John C. Wyngaard

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7

Three-Dimensional Numerical Modeling of the Planetary Boundary Layer

JAMES W. DEARDORFF

National Center for Atmospheric Research,¹ Boulder, Colo.

7.1. INTRODUCTION

It is becoming more and more apparent that the study of micrometeorology cannot be confined to the "constant-flux" layer near the surface. One wishes to know how to relate the wind and temperature at "anemometer" level to externally imposed conditions; to know at what rates the heat and momentum fluxes are decreasing with height within the "constant-flux" layer; to explain the presence of a vanishing potential temperature gradient at heights as low as 50 m; to understand the cause of fluctuations of long period associated with unseen turbulent structures extending well up into the planetary boundary layer (PBL); and to understand the manner in which the scale of the dominant eddies increases with height up past the top of the surface layer. For reasons such as these, the surface layer and the remaining bulk of the PBL should be studied as a single entity.

The numerical modeling of turbulence in three dimensions (3-D) is becoming competitive with other methods of its study, in the writer's opinion. The more advanced digital computers are now sufficiently speedy to allow explicit treatment of scales of turbulence down to roughly 5% of the maximum scale of the problem. Until recently this was not possible, and numerical modelers were restricted to two dimensions. At about the same as 3-D modeling was being considered, it

¹The National Center for Atmospheric Research is sponsored by the National Science Foundation.

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