Large Eddy Simulations of Planetary Boundary Layers

Turbulence-Resolving Modeling of Self-Organized Turbulence

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Lecture Contents

- Motivation
- Concepts
- Mathematical foundations
- Turbulence closure
- Boundary conditions
- Structure of PBL turbulence
- Portraits of the most energetic eddies
- Role of turbulence selforganization
- Toward turbulence parameterization: LES versus Single-Column Models
- Conclusions



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Motivation



- The best observatories collect data only in the lower PBL (e.g. Obninsk 315 m meteorological mast, Russia, left panel) while PBL thickness often exceed 500 m (sodar data from Obninsk, IEM, April 2007, right panel).
- Accuracy is not very high due to transitional effects, site location
- Comprehensive meteorological measurements are very rare (exception e.g. May 1998 SHEBA)

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Motivation

- Simulations may help
- Observations difficult, expensive and cannot be repeated
- DNS resolve all scales but it is now feasible only up to Re ~ 10³
- DNS are still in the range of Re-dependent statistics
- Environmental Re ~ 10⁹
- Geoscientists are also interested in meteorological micro-physics
- Micro-physics simulations are costly

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Motivation

- Atmospheric and ocean physicists are looking for a techniques **much** more comprehensive than RANS but **much** less costly than DNS
- Fortunately the high Re turbulence exhibits properties, which allows us to construct such a technique in a semi-rigorous way



Phenomenological Concept I

- Turbulence in inertial interval of scales is universal and could be modeled statistically
- Inaccuracy in modeling of Kolmogorov's turbulence could be large but it does not matter as its total energy is small
 ~ k -5/3

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Phenomenological Concept II

In isotropic
 turbulence 95% of
 TKE on resolved
 scales could be
 reached with only
 100 nodes in each
 direction



Figure 6. Required ratio of L/Δ as function of Re_{λ} (with a = 2) for different levels of subfilter energy, i.e. $E_{sgs}/E = 1\%$ (—) and $E_{sgs}/E = 5\%$ (—), respectively. (-·) $\Delta = \eta$; (···) respective asymptotes according to (30).

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Next Aim of LES



Aim of Turbulence-Resolving Modeling at high Re

- At the high-frequency end of the spectrum:
- Energy decrease

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- Correlations deteriorate
- Energy cascade is predominantly directed to small, dissipative scales
- In the inertial sub-range model statistic approaches an intermediate asymptote
- The aim is to recover this asymptote as accurate as possible in resolved-scales of the LES (S. Pope, 2004)



Figure 2. Variation of the model Q^m for that statistic Q as a function of the turbulence resolution length scale Δ (on a log scale): Q_0^m is the DNS limit as Δ tends to zero; Q_I^m is the intermediate asymptote in the inertial subrange.

Next Mathematical Foundations



Mathematical Foundations I

- There are many approaches to derive LES equations ranging from ad hoc filtering (grid-filtered model of Deardorff, 1970) to statistical conditional modeling (perfect LES of Langford and Moser, 1999)
- The aim is to obtain a mathematical guidance on construction of low-dimensional models and their closures

$$\partial_t u + u \cdot \nabla u + \nabla p - \operatorname{Re}^{-1} \Delta u = f, \quad in \quad Q_T$$
$$\nabla \cdot u = 0, \quad in \quad Q_T$$
$$u\Big|_{\Gamma} = 0 \text{ or periodic}$$
$$u\Big|_{t=0} = u_0, \quad Q_T = \Omega \not\subset \Gamma \times (0,T)$$

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Mathematical Foundations II

- The formidable mathematical problem in high Re LES is imparity of energy balance between TKE generation and dissipation
- Energy just accumulate at the cut of scale (aliasing)

 $\text{Re} \rightarrow \infty$

$$\partial_t E + u \cdot \nabla E = P, \quad in \quad Q_T$$

 $\int (u \cdot \nabla u) \cdot u = 0, \quad in \quad Q_T$

• Hence there is no loss of energy and information in the infinite Re system

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Mathematical Foundations III

$$\partial_t E + u \cdot \nabla E = P, \quad in \quad Q_T$$

 $\int (u \cdot \nabla u) \cdot u = 0, \quad in \quad Q_T$

• Exact filtering becomes possible with **Germano** differential filter

$$\overline{u} - l_{cut}^2 \Delta \overline{u} = u$$

- So that the complete solution can be restored on the basis of a filtered (large-scale) solution
- Thus no closure problem in filter-based derivations of LES (Germano, Adams, Carati, Winkelmans etc)

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Next Regularization



Mathematical Foundations IV

- To overcome the difficulty with aliasing, the original NSE must be perturbed (regularized)
- Aliasing piling up of the energy at the smallest resolved scale
- Leray's (1934) regularization idea can be expressed as large-scale velocity field transports small-scale velocity field
- Similar in some sense to the idea of *the Rapid Distortion Model* (or RTD by J.C.R. Hunt)

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• Related to NSE-alpha model (Foias et al., Chen et al.)

$$\partial_t u + (\nabla \times u) \times \overline{u} + \nabla (p + \frac{1}{2}u^2) = \overline{f}, \nabla \cdot u = 0.$$



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Mathematical Foundations V

$$\partial_t u + (\nabla \times u) \times \overline{u} + \nabla (p + \frac{1}{2}u^2) = \overline{f}, \nabla \cdot u = 0.$$

- With Germano-Helmholtz differential filter
- Result in a closed, dissipative LES model

Use:
$$\overline{u} = (I - l_{cut}^2 \Delta)^{-1} u$$

$$\partial_{t}\overline{u} + \overline{u} \cdot \nabla \overline{u} = \nabla \cdot (-pI + T), \nabla \cdot \overline{u} = 0,$$

$$T = 2l_{cut}^{2} (\partial_{t}S + \overline{u} \cdot \nabla S + S\Omega - \Omega S),$$

$$S = \frac{1}{2} (\nabla \overline{u} + (\nabla \overline{u})^{T}), \quad \Omega = \frac{1}{2} (\nabla \overline{u} - (\nabla \overline{u})^{T}).$$

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Next Leray model test



Leray Model Test

- Has a semi-rigorous model constructed?
- Not exactly!
- Leray LES filters out small scales at equation level
- Leray model do not demonstrate any superiority (Liu et al., 2006)
- Just opposite, Leray model is numerically illconditioned and therefore less stable than others



Fig. 3. Energy spectra for decaying isotropic turbulence.







Mathematical Foundations VI

- Another regularization approach is taken in Ladyzhenskaya-Kaniel model (LKM)
- O. A. Ladyzenskaja (1969) introduced the secondorder stress term into dissipation
- This term accounting for large velocity gradients in non-linear fluid
- This term is consistent with the Smagorinsky model (important for the following understanding)
- Finally, she proved the existence, uniqueness and convergence (to the NSE) theorem for such a regularized system

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Mathematical Foundations VII

$$\partial_t u + u \cdot \nabla u = \nabla \cdot (-pI + T^*), \nabla \cdot u = 0,$$

Leonard equality :
 $u \cdot \nabla u = \nabla (u \otimes u) = \nabla (\overline{u} \otimes \overline{u}) + \nabla (u \otimes u - \overline{u} \otimes \overline{u})$
 $T = 2l_{cut}^2 (\partial_t S + \overline{u} \cdot \nabla S + S\Omega - \Omega S) \Leftrightarrow T^* = 2l_{cut}^2 |S|S$

• Since the system has additional viscosity concentrated on small-scales, the following is satisfied

$$\overline{u} \to u$$
, if $\delta_x >> l_{cut}$





Next: Conservation Laws and symmetries



Symmetry and Conservation Laws I

- Any particular conservation law is a mathematical identity to certain symmetry of a physical system
- Mathematically expressed through **Noether theorem**
- Energy conservation time shift symmetry
- Linear momentum conservation – space shift symmetry
- Angular momentum conservation – rotation shift symmetry
- Kolmogorov energy cascade
 scaling transformations



FIG. 10. (a,b) Images of the convective pattern (observed from above) in the cell with a ramp on the bottom plate, for $\varepsilon = 0.012$ and $\varepsilon = 0.046$, respectively. In both experiments, $\Omega = 3.93$. (c,d) Structure functions associated with (a) and (b), respectively. Image processing has been required to obtain these pictures (see text).

Guarino, A. and Vidal, V., 2004:Hexagonal pattern instabilities in rotating Rayleigh-Bénard convection of a non-Boussinesq fluid: Experimental results, *Phys. Rev. E*, **69**



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Symmetry and Conservation Laws II

Model Type	Translations	Rotations and reflections	Scaling transfor mations*	Material indiffer ence**
Smagorinsky (Smagorinsky, 1963; Lilly, 1967)	Y	Y	Ν	Υ
Dynamic Smagorinsky (Germano, 1986; Lilly, 1992; Vreman et al., 1994; Meneveau et al., 1999)	Y	Y	Y	Y***
Structure function (Metais and Lesieur, 1992)	Y	Y	N	Ν
Gradient (Clark et al., 1979)	Y	Y	N	N
Scale-Similarity (Bardina et al., 1980)	Y	Y	Y	Y*
Lund-Novikov tensor diffusivity (1992)	Y	Y	N	N
Kosovic or non-linear Lund- Novikov model (Kosovic, 1997)	Y	Y	N	N

* To held scaling invariance, **the length** scale should not appear in the model explicitly

** in the limit of 2D flow in simply connected domain

*** under special conditions on the filter core, **neither Gaussian nor box filters satisfy**

Razafindralandy D., and Hamdouni, A., 2006: Consequences of symmetries on the analysis and construction of turbulence models, *Symmetry, Integrability and Geometry: Methods and Applications*, 2, 052, 20 pp.

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Mathematical Foundations: Summary

- Regularization introduces physical filtering which eliminates small-scales form equations (no need to filter model fields)
- LKM is simpler and more stable than Leray's models
- Popular and reliable Smagorinsky sub-grid model is consistent with LKM
- Symmetry considerations however demand elimination of explicit length scale in sub-grid model
- It could be done through Germano Identity
- Mathematical analysis of NSE and symmetries gives a valuable guide for model closure development
- Of more than 100 sub-grid closures proposed over the last 30 years none satisfy all mathematical restrictions



Next: Turbulence Closure and Germano Identity



Turbulence Closure Problem I

- Start with Ladyzhenskaya-Kaniel model (LKM)
- Remember that the Smagorinsky sub-grid closure satisfies LKM conditions but do not follow from them
- Use Leonard equality to separate resolved and unresolved scales

$$\partial_t \overline{u} + \overline{u} \cdot \nabla \overline{u} = \nabla \cdot (-\overline{p}I + (\overline{u} \otimes \overline{u} - u \otimes u) - T^*),$$
$$\nabla \cdot \overline{u} = 0,$$
$$T^* = 2l_{cut}^2 |\overline{S}| \overline{S}$$

- To make the model consistent, express the regularization parameter (filter scale) through resolved quantities
- To do this apply Germano Identity

$$\overline{\overline{u}^{h}\otimes\overline{u}^{h}}^{H}-\overline{\overline{u}^{h}}^{H}\otimes\overline{\overline{u}^{h}}^{H} = \left(\overline{\overline{u\otimes u}}^{h}-\overline{\overline{u}^{h}}^{H}\otimes\overline{\overline{u}^{h}}^{H}\right)-\overline{T^{*}}^{H}$$

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Next: How does it works



Turbulence Closure Problem II

Figure 6. The predictions $Q^{mA}(\Delta)$ and $Q^{mB}(\Delta)$ of the statistic Q obtained from LES models A and B as functions of the turbulence resolution length scale Δ for the case in which Q and the processes affecting it are confined to the energy-containing range.

Figure 8. For the given model A, and the dynamic model D, a sketch of the resolved contribution $Q^w(\Delta)$ and of the modelled residual contributions $Q^{rA}(\Delta)$ and $Q^{rD}(\Delta)$ to the model predictions $Q^{mA}(\Delta)$ and $Q^{mD}(\Delta)$ of a large-scale statistic Q. The dynamic model selects the model coefficient c_Q so that $Q^{mD}(\widetilde{\Delta})$ equals $Q^{mD}(\overline{\Delta})$.

- Germano Identity does not give unique closure
- Closures based on GI called DYNAMIC closures
- Aim of the LES is to recover the intermediate asymptote in turbulent statistics (Figure 6)
- Dynamic procedure optimize this recovery as it provide the largest decrement of the error $||Q_{LES}(\Delta)-Q||_{L2}$ within the asymptotic range (Figure 8, Pope, 2004)

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Next: Dissipation on small scales

Turbulence Closure Problem III

- The asymptotic behavior of statistics is a characteristic of high Re flow
- Dynamic procedure maintain high Re by shifting dissipation to high-frequency end of the resolved spectrum
- The best recovery of the asymptotic statistics is the reason behind the dynamic closures success

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Next: DMM

Turbulence Closure Problem IV: Dynamic Mixed Model

- Dynamic Mixed Model (DMM) is the most straightforward implementation of a consistent LKM-LES
- Originally by Bardina et al. (1983) scale-similarity arguments
- Improved by many authors, Vreman et al. (1997) form reads

$$T_{DMM} = (\overline{u}^{h} \otimes \overline{u}^{h} - \overline{u \otimes u}^{h}) - T^{*} = L - 2(C_{s}^{2}\Delta^{2})|\overline{S}^{h}|\overline{S}^{h}$$
$$\frac{l_{cut}^{2}}{\Delta^{2}} = C_{s}^{2} = \frac{1}{2}\frac{(L_{ij} - H_{ij})M_{ij}}{\|M_{ij}\|_{2}^{2}},$$

 $= \frac{1}{h}H$

 $C_{\rm s}$ - Smagorinsky constant, Δ - effective filter size of the mesh

Takes the main burden of calculations in the optimization process

$$M = 2\left|\overline{S^{h}}\right|\overline{S^{h}}^{H} - \alpha^{2} 2\left|\overline{\overline{S^{h}}}^{H}\right| \overline{\overline{S^{h}}}^{H}, \alpha = \frac{\overline{\overline{\Delta}}^{h}}{\overline{\Delta}^{h}},$$
$$H = \left(\overline{\overline{\overline{u^{h}}}^{H} \otimes \overline{\overline{u^{h}}}^{H}}^{H} - \overline{\overline{\overline{u^{h}}}^{H}}^{H} \otimes \overline{\overline{\overline{u^{h}}}^{H}}^{H}\right) - \left(\overline{\overline{\overline{u^{h}}} \otimes \overline{\overline{u^{h}}}^{h}}^{H} - \overline{\overline{\overline{u^{h}}}^{h}} \otimes \overline{\overline{\overline{u^{h}}}^{h}}^{H}\right),$$
$$L = \overline{\overline{u^{h}} \otimes \overline{\overline{u^{h}}}^{H}} - \overline{\overline{u^{h}}}^{H} \otimes \overline{\overline{u^{h}}}^{H}$$

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Next: Filters

Turbulence Closure Problem V

- For actual numerical simulations one have to construct a set of filters
- Most popular are Gaussian and Box filters
- Both filters are identical under second-order numerical schemes
- Both filters do not satisfy symmetry constrains
- It result in numerical instability of the dynamical procedure
- Ad hoc engineering modification either by limiters, e.g. l_{cut}>0, or by balance equations in Largangian formulation, e.g. TKE(x,t)>0.

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Turbulence Closure VI

- As the most consistent model, DMM was extensively studied with observational data HATS, Campbell Tracks and other campaigns (Porte-Agel et al., 2001; Sullivan et al., 2003; Kleissl et al., 2004)
- It identify relative importance of different terms in the sub-grid closure (near surface)

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Next: Cs variability

Turbulence Closure VII

- In unbounded shear flow determination of the subgrid closure is difficult
- It is also computationally expensive, consuming >30% of time and >70% of memory
- Task is even more complicated in stratified and rotating PBL with variable background shear

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Turbulence Closure VIII Dynamic Model of Heat Diffusion

- Dynamic model for heat/scalar diffusion could be derive quite in the same way as for the momentum (Porte-Agel et al., 2004)
- Dynamic mixed model is however less stable for heat transport than for momentum, hence DMM is not applied in known LES

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SGS dissipations. Squares (left axis) are obtained using Deardorff's

correction. Results are averages over three values obtained using 8-min

subperiods. The error bars for the open circles show the approximated

standard deviation associated with those three samples.

atmospheric

$$T_{Q}^{*} = \left(\frac{l_{Q}}{\Delta}\right)^{2} \Delta^{2} \left| \overline{S}^{h} \right| \nabla \overline{Q}^{h} \qquad \qquad \frac{l_{Q}}{\Delta} = \frac{C_{s}}{Sc^{1/2}},$$
Dynamic coefficient as function of stability by
Porte-Agel et al. (2001), Evaluation in
Campbell Track field experiment, CA

$$Sc \equiv \Pr: Q = \theta$$

$$\left(\frac{l_{Q}}{\Delta}\right)^{2} = \frac{K_{i}X_{i}}{\left\|X_{i}\right\|_{2}^{2}},$$

$$X = 2\left(\left|\overline{S}^{h} \right| \overline{\nabla Q}^{h}^{H} - \alpha^{2} \left|\overline{S}^{h}^{H} \right| \overline{\nabla Q}^{h}^{H}\right),$$

$$K = \overline{u}^{h}\overline{Q}^{h}^{H} - \overline{u}^{h}^{H} \overline{Q}^{h}^{H}$$
PORE Agel et al. (2001), Evaluation in
Campbell Track field experiment, CA

$$Sc \equiv \Pr: Q = \theta$$

$$\int_{S} \frac{1}{12} \int_{S} \frac{1$$

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Turbulence Closure IX

- If Cs is dynamical, than sub-grid Pr should be fairly constant with very little effect on resolved scales
- Intercomparisons demonstrate little sensitivity of simulations to sub-grid Pr
- Simulated with LESNIC Pr = 0.8 + 5 Ri at Ri < 1 Pr = 2 Ri at Ri > 10
- Prescribed in LESNIC
 Pr = 1 + 7 Ri
- Good deal of self-correlation is probably in this function but
- Mixing efficiency independence of closure results in automatic recovery of Monin-Obukhov similarity in boundary conditions

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Next: Closure summary

Turbulence Closure: Summary

- Dynamic mixed model (DMM) satisfies mathematical requirements provided the correct filter choice
- DMM produces optimal recovery of the auto-model interval in the turbulence statistics provided that such interval exists (high Re flow)
- DMM shifts dissipation toward smallest resolved scales thus large eddies evolve (almost) without dissipation
- DMM seems to flexible enough to take care of stratification in PBL so that variability of sub-grid Pr is not important for simulations
- DMM is able to cure numerical errors at the smallest resolved scales as the dissipation increase does not distinguish physical or numerical energy cascade

Next: Boundary Conditions

Boundary Conditions I

- Boundary conditions on large-scale fields in LES are non-trivial
- Observations of wind gusts and tornado (right, 1999 F5 Tornado in Oklahoma) reveals that vortices can slip over impenetrable rough surfaces
- Even more problematic to impose boundary conditions for heat and scalars

Next: General numerical requirements

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Boundary Conditions II

- Numerical schemes require prescription of fluxes as boundary conditions
- Fluxes close to impenetrable walls are always **unresolved**
- In Prandtl's boundary layer, the vicinity of the wall is where turbulence is thought to be produced
- Unresolved production Garbage simulations
- Nature is friendly for us however

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Boundary Conditions III

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- Direct cascade helps to justify walllaw boundary conditions
- Detached (large-scale) eddies formerly considered "inactive" in Townsend and Bradshaw but indeed proven to be "active"

Figure 1. Sketch of a typical high Reynolds number boundary layer; $h \approx 1-2$ km, $\ell_s \approx 100-200$ m, $\ell_e \approx 10-20$ m, the roughness length z_0 is less than 0.1 m over a field, less than 1 m over a typical city.

Energy cascade towards dissipative scales

Direct transfer of energy towards dissipative scales

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(a)

(b)

Boundary Conditions IV

Figure 6. The scale parameter A of the expression $\Lambda_{\text{max}} = Au_*/f_c$ plotted against height. Data from: 'Laban's mills' (Högström, 1992), Δ ; Lövsta (Högström, 1990), \bigcirc ; Östergarnasholm (cf. Smedman et al., 1999), *. Note that each symbol represents a mean over many measurements from each site and measuring height.

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- Detached eddies originate in the shear motions immediately above the surface layer
- Eddies are of the PBL scale, descend and impinge onto the surface
- Supported by atmospheric observations (right, Hoegstroem et al., 2002)
- Supported by LES (left, Esau)
- Theory explain how PBL depth may influence (through large-eddies) surface fluxes

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Boundary Conditions V

- Theory predicts the log-law (in neutral PBL) for the velocity profile
- Neglecting velocity rotation, flux variability. and pressure gradients. the law reads

$$\tau_0^{1/2} = \frac{\kappa |u_{z \to 0}|}{\ln \frac{z}{z_0}} \frac{u}{|u|}$$

- Stratification corrects the log-law with Monin-Obukhov similarity function of the flow stability
- The MO function is simply a reflection of the turbulence mixing efficiency in stratified flow (Pr vs Ri)
- Thus, correct Pr vs Ri in LES should result in recovery of the nondimensional velocity gradients and hence fluxes **automatically**
- DATABASE64 LES show it (right)

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Boundary Conditions VI

$$\tau_0^{1/2} = \frac{\kappa |u_{z\to 0}|}{\ln \frac{z}{z_0}} \frac{u}{|u|} \qquad \begin{array}{c} \kappa = 0.34 - 0.55, \\ M(\kappa) = 0.41 \end{array}$$

- Important issues are determination of z_0 and κ
- $\begin{tabular}{ll} \hline κ cannot be determined independently of z_0 in data \end{tabular}$
- Semi-analytical analysis based on the structure function in sheared flow (Lvov et al., 2005) $\kappa = 0.42$
- Constant may depend on flow Re
- Lab exp. (Jinyin et al., 2002) and LES (Cai et al., 1996): Re increase, constant increase
- PBL (SHEBA) data (Andreas et al., 2006) suggests directly opposite

 $\kappa = -1.48 \cdot 10^{-2} \ln \text{Re}_* + 0.427$

Large-Eddy Simulations for Turbulence-Resolving Modeling

- Large-eddy Simulation (LES) resolve only large, presumably non-universal eddies in fluid flow
- The resolved scales in LES defined by Nyquist theorem (min 2 grid nodes per wave length)
- It has sense if such large eddies indeed dominate the turbulent mixing
- In this sense, LES is a science about turbulence self-organization

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Surface-Layer Turbulence Patterns in Neutral PBL LES

- Structure of resolved-scale turbulence stress (right)
- Its surface (the first resolved layer) imprint in a selected domain
- Self-organization of the instant turbulence stress and up to some degree imprints are visible

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Structure of Thermally-Driven Turbulence I

- Potential vorticity in fluid is a conservative quantity
- It drives free convection self-organization into vortex rings
- Lord Raylegh (1921) found the vortex ring as a fastest growing modal perturbation in shear-free convection
- Rings, multiplied and distorted, compact themselves into cellular convection patterns

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Structure of Thermally-Driven Turbulence II

 Rings, multiplied and distorted by secondary flow instabilities, compact themselves into cellular convection patterns

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Structure of Thermally-Driven Turbulence III

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Heterogeneous Convection

• Cloudiness build up over dryer and hotter terrain

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In shear-driven PBL, the most energetic structure is a vortex pair aligned (?) with the mean flow direction

Left panel – schematic picture of the flow structure adopted after lab. experiments [Fric & Roshko, 1989: Structure in the near field of the transverse jet Proc. 7th Symp. on Turbulent Shear Flows (no. 6-4. Stanford, August)]
Right panel – the most energetic vortex pair structure computed with POD analysis from LES data (Esau, JoT, 2003)

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Structure of Shear-Driven Turbulence II

Observed very often as structures of the cloudiness organization, fog density in the atmosphere Langmuir circulation in the ocean mixed layer

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Shear to Convective Transition I Leads

- Temperature difference generate convection
- Convection generate shear
- Shear enhances convections

Conclusions

- Turbulence-resolving simulations are suitable and flexible tool to study
- Complex, selforganized turbulence on meteorological scales
- With realistic variability of boundary conditions and microphysical phenomena

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