USING HATS DATABASES TO EVALUATE SUBFILTER-SCALE RATE EQUATIONS FOR LES

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LARGE-EDDY SIMULATIONS AND OBSERVATIONS

Why LES of the PBL:
- Outdoor 4-D measurements are challenging
- Unsteady nature of the atmosphere and ocean
- Systematic investigation of the parameter space
- Advances in parallel computing

Validating/Improving LES with observations:
- Test the output
- Test the input subgrid-scale parameterizations
LES APPLICATIONS AND THE PBL

- Turbulence dynamics, stratification, entrainment
- Surface-atmosphere interactions
- Dispersion, chemistry
- Clouds
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Stable boundary layers $z_i/L \sim 1.2$
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Non-equilibrium winds and waves
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Plumes and dust-devils in a convective PBL $1024^3$ simulation on 4096 cpus

Stable boundary layers $z_i/L \sim 1.2$

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LES EQUATIONS FOR DRY ATMOSPHERIC PBL

Momentum
\[
\frac{D\overline{u}}{Dt} = -f \times \overline{u} - \nabla \pi + \frac{\dot{\theta}}{\theta_*} - \nabla \cdot T
\]

Scalar
\[
\frac{D\overline{b}}{Dt} = -\nabla \cdot B
\]

TKE
\[
\frac{D\overline{e}}{Dt} = -T : S + B \cdot \hat{z} - \mathcal{E} + \nabla \cdot (2\nu_t \nabla e)
\]

Subgrid-scale momentum and scalar fluxes

\[
\begin{align*}
T &= \overline{u_i u_j} - \overline{u_i} \overline{u_j} \\
B &= \overline{u_i b} - \overline{u_i} \overline{b}
\end{align*}
\]

Random variables, require a parameterization
SIMPLE (CHEAP) FILTERING
EXAMPLE ...

\[ \tau_{11} = \overline{u_1 u_1} - \overline{u_1} \overline{u_1} \]
What happens to $\bar{u}_i$ and $T_{ij}$ as we vary the filter cutoff $k_c$?
MOVING BETWEEN DNS ↔ LES ↔ RANS

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HIGH REYNOLDS NUMBER OBSERVATIONS AND LES

- **SINGLE-POINT MEASUREMENTS**
  - Cannot be used directly to improve LES

- **MULTI-POINT MEASUREMENTS**
  - Span a range of filter widths, e.g., \( O(\text{m}) \) to \( O(100\text{m}) \)
  - Ideally 3-D, time varying “volume” of turbulence and scalars in canonical flows with shear, stratification, near boundaries, ...
HATS CONFIGURATIONS

- 36 cases
- \(-1.2 < \frac{z}{L} < 1.6\)
- \(0.15 < \frac{\Lambda_w}{\Delta f} < 15\)
OHATS FIELD CAMPAIGN

Laser altimeters
18 CSATS
275 hours "12 days of data" analyzed
CANOPY HORIZONTAL ARRAY TURBULENCE STUDY
AN EXAMPLE OF LATERAL (Y) FILTERING

$\delta_{yd}$

$f(y, t)$

$\bar{f}(y, t)$

$U$

$y$

``2D plane of turbulence''
AN EXAMPLE OF LATERAL (Y) FILTERING
AN EXAMPLE OF LATERAL (Y) FILTERING
SFS VELOCITY VARIANCES

$3\tau_{11}/2E_{\text{sfs}}$

$3\tau_{22}/2E_{\text{sfs}}$

$3\tau_{33}/2E_{\text{sfs}}$

$\Lambda_w/\Delta_f$
RATE EQUATIONS FOR SUBGRID DEVIATORIC STRESS

- What are the parent equations for the Smagorinsky model?
RATE EQUATIONS FOR SUBGRID DEViatoric STRESS

- What are the parent equations for the Smagorinsky model?

\[
\frac{D\tau_{ij}}{Dt} = \frac{2}{3} \epsilon \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \\
- \left[ \tau_{ik} \frac{\partial \bar{u}_j}{\partial x_k} + \tau_{jk} \frac{\partial \bar{u}_i}{\partial x_k} - \frac{1}{3} \delta_{ij} \tau_{kl} \left( \frac{\partial \bar{u}_k}{\partial x_l} + \frac{\partial \bar{u}_l}{\partial x_k} \right) \right] \\
- \frac{1}{\rho} \left[ p \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \bar{p} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right] \\
+ \text{transport} + \text{buoyancy production}
\]
**RATE EQUATIONS FOR SUBGRID DEVIATORIC STRESS**

- What are the parent equations for the Smagorinsky model?

\[
\frac{D\tau_{ij}}{Dt} = 0 = \frac{2}{3} e \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \\
- \left[ \tau_{ik} \frac{\partial u_j}{\partial x_k} + \tau_{jk} \frac{\partial u_i}{\partial x_k} - \frac{1}{3} \delta_{ij} \tau_{kl} \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \right] \\
- \frac{1}{\rho} \left[ \bar{p} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \bar{p} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \\
+ \text{transport} + \text{buoyancy production}
\]

\[
\frac{\tau_{ij}}{T} = \frac{2}{3} e \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

\[
T = c \frac{\Delta f}{\sqrt{e}}
\]
PRODUCTION OF SUBFILTER SCALE FLUX $\tau_{11}$

$$- \left[ \tau_{ik} \frac{\partial u_j}{\partial x_k} + \tau_{jk} \frac{\partial u_i}{\partial x_k} - \frac{1}{3} \delta_{ij} \tau_{kl} \left( \frac{\partial u_k}{\partial x_i} + \frac{\partial u_i}{\partial x_k} \right) \right]$$

$$\frac{2}{3} e \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$
PRODUCTION OF SUBFILTER SCALE FLUX $\tau_{33}$

$$- \left[ \tau_{ik} \frac{\partial \bar{u}_k}{\partial x_k} + \tau_{jk} \frac{\partial \bar{u}_i}{\partial x_k} - \frac{1}{3} \delta_{ij} \tau_{kl} \left( \frac{\partial \bar{u}_k}{\partial x_l} + \frac{\partial \bar{u}_l}{\partial x_k} \right) \right]$$

$$\frac{2}{3} e \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$
PRODUCTION OF SUBFILTER SCALE FLUX $\tau_{13}$

$$- \left[ \tau_{ik} \frac{\partial \bar{\mu}_j}{\partial x_k} + \tau_{jk} \frac{\partial \bar{\mu}_i}{\partial x_k} - \frac{1}{3} \delta_{ij} \tau_{kl} \left( \frac{\partial \bar{\mu}_k}{\partial x_l} + \frac{\partial \bar{\mu}_l}{\partial x_k} \right) \right]$$

$$\frac{2}{3} \epsilon \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

![Graphs showing aniso, iso, and total production of subfilter scale flux with respect to $\Lambda_w / \Delta_t$.]
PRODUCTION OF SUBFILTER SCALE FLUX $\tau_{22}$

\[ -\left[ \tau_{ik} \frac{\partial \tilde{u}_j}{\partial x_k} + \tau_{jk} \frac{\partial \tilde{u}_i}{\partial x_k} - \frac{1}{3} \delta_{ij} \tau_{kl} \left( \frac{\partial \tilde{u}_k}{\partial x_1} + \frac{\partial \tilde{u}_l}{\partial x_k} \right) \right] \]

\[ \frac{2}{3} \varepsilon \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \]

Aniso (2,2)

Iso (2,2)

$\Lambda_w / \Delta_f$
VARIATION OF DEVIATORIC STRESS IN LIMIT $\Lambda_w/\Delta_f \to 0$

\[
\begin{align*}
\langle \tau_{11} \rangle &= T \left( -2\langle \tau_{13} \rangle \frac{\partial U}{\partial z} + \frac{2}{3} \epsilon \right) \\
\langle \tau_{22} \rangle &= T \left( \frac{2}{3} \epsilon \right) \\
\langle \tau_{33} \rangle &= T \left( \frac{2}{3} \epsilon \right) \\
\langle \tau_{13} \rangle &= T \left( \frac{2}{3} \epsilon \frac{\partial U}{\partial z} - \langle \tau_{33} \rangle \frac{\partial U}{\partial z} \right)
\end{align*}
\]

\[
\begin{align*}
\langle \tau_{11} \rangle &= 0 \\
\langle \tau_{22} \rangle &= 0 \\
\langle \tau_{33} \rangle &= 0 \\
\langle \tau_{13} \rangle &= T \left( \frac{2}{3} \epsilon \frac{\partial U}{\partial z} \right)
\end{align*}
\]

Steady-state rate equations
Smagorinsky model
WHAT ABOUT SCALARS?
RATE EQUATIONS FOR SUBGRID SCALAR FLUX

- What are the parent equations for subgrid-scale scalar flux?

\[ f_i = \overline{u_i c} - \bar{u}_i \bar{c} \]

\[ \frac{Df_i}{Dt} = \frac{2}{3} \rho \frac{\partial \bar{c}}{\partial x_i} - f_j \frac{\partial \bar{u}_i}{\partial x_j} + \tau_{ij} \frac{\partial \bar{c}}{\partial x_j} \]

\[ + \frac{1}{\rho} \left( \overline{p \frac{\partial c}{\partial x_i}} - \bar{p} \frac{\partial \bar{c}}{\partial x_i} \right) \]

+ transport + buoyancy

Isotropic production

Pressure destruction

Anisotropic production
RATE EQUATIONS FOR SUBGRID SCALAR FLUX

- What are the parent equations for subgrid-scale scalar flux?

\[
\begin{align*}
    f_i &= \bar{u}_i \bar{c} - \bar{u}_i \bar{c} \\
    \frac{D f_i}{Dt} &= -\frac{2}{3} e \frac{\partial \bar{c}}{\partial x_i} \\
    &\quad - f_j \frac{\partial \bar{u}_i}{\partial x_j} + \tau_{ij} \frac{\partial \bar{c}}{\partial x_j} \\
    &\quad + \frac{1}{\rho} \left( \bar{p} \frac{\partial \bar{c}}{\partial x_i} - \bar{c} \frac{\partial \bar{c}}{\partial x_i} \right) \\
    &\quad + \text{transport} + \text{buoyancy}
\end{align*}
\]

Eddy viscosity model

\[
\begin{align*}
    f_i &= -\nu_h \frac{\partial \bar{c}}{\partial x_i} \\
    \nu_h &= \frac{2c_h \Lambda_f \sqrt{\epsilon}}{3}
\end{align*}
\]
PRODUCTION OF SUBFILTER SCALE SCALAR FLUX $f_1$

![Diagram showing Prod Dev (1) and Prod Iso (1) against $\Lambda_w / \Delta_t$ for black stable and red unstable cases.](image)
PRODUCTION OF SUBFILTER SCALE SCALAR FLUX $f_3$

![Graphs showing production deviation, production iso, total production vs. ratio $\Lambda_w / \Lambda_f$.]

- **Prod Dev (3)**: Black stable, red unstable
- **Prod Iso (3)**
- **Total Prod (3)**

Graphs with data points illustrating the relationship between production and the ratio $\Lambda_w / \Lambda_f$. 

$\Lambda_w / \Lambda_f$ ranges from $10^0$ to $10^1$. The graphs show distinct behaviors for stable (black) and unstable (red) conditions.
SUBGRID-SCALE SCALAR FLUX

Comments:

• Net horizontal scalar flux $f_1 = \langle \overline{u'c'} - \overline{u_c} \rangle \neq 0$ even horizontally homogeneous PBLs, i.e., $\frac{\partial}{\partial x} \langle C \rangle = 0$

• Tilting of vertical flux by vertical shear is important
  $f_1 \sim -f_3 \frac{\partial \overline{u}}{\partial z} T$

• No eddy viscosity model, including the “dynamic approach”, can capture anisotropic production
SUBFILTER-SCALE PRESSURE DESTRUCTION

\[
-\frac{1}{\rho} \left[ p \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \bar{p} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] = -\frac{\tau_{ij} \sqrt{e}}{C_m \Delta_f}
\]

\[
+ \frac{1}{\rho} \left( p \frac{\partial c}{\partial x_i} - \bar{p} \frac{\partial \bar{c}}{\partial x_i} \right) = -\frac{f_i \sqrt{e}}{C_s \Delta_f}
\]

CHATS PRESSURE SENSOR (Steven Oncley)
AHATS (2008) “HORIZONTAL ARRAY” OF PRESSURE SENSORS
VALIDATION OF ROTTA MODEL FOR MOMENTUM AND SCALARS

Production ≈ Destruction
SUMMARY

- LES is being applied to a richer set of boundary layer flows because of advances in parallel computing

- Subgrid-scale parameterizations in LES need to be validated/improved for geophysical applications

- Multi-point measurements from the HATS field campaigns compliment our ability to compute
  - Evaluation of subgrid scale models with high $Re$ data
  - Rate equations provide insight into SGS dynamics
  - Importance of anisotropic production for stress and scalar especially for $\Lambda_w/\Delta_f \sim O(1)$ or less
  - Data highlights the shortcomings of an eddy viscosity approach