PETASCALE COMPUTING AND THE TERRA INCOGNITA

John C. Wyngaard

Penn State University

Funded by the National Science Foundation and the Army Research Office

OUTLINE

- What is the Terra Incognita?
- Are we now there?
- Turbulence modeling: Strong views from engineering.
- An echo from the atmospheric side.
- An approach to subgrid modeling in the Terra Incognita.
- A revised “first order theory” for subgrid stress.
- The “array technique” for measuring subgrid fluxes.
- Improved modeling of subgrid stress.
- The maintenance of subgrid scalar flux.
- Improved modeling of subgrid scalar flux.
- *Context*, *Tasks*, and *Concluding Thoughts* from the 2004 Board on Atmospheric Sciences Workshop.

WHAT IS THE TERRA INCOGNITA?

In high-Reynolds-number turbulent flows we must first average the fluid equations — say over a region of space of linear scale Δ — before solving them numerically. The averaged forms of the constant-density Navier-Stokes and continuity equations are

$$\overline{u}_{i,t} + (\overline{u}_i \overline{u}_j)_{,j} = -\frac{1}{\rho}\overline{p}_{,i} + \frac{1}{\rho}\tau_{ij,j}, \quad \text{where } \frac{\tau_{ij}}{\rho} = \overline{u}_i \overline{u}_j - \overline{u_i u_j} \ ;$$

$$\overline{u}_{i,i} = 0.$$

One needs a *subgrid model* for the unresolved stress τ_{ij}.

THE LES AND MESOSCALE LIMITS

If the (integral) scale of the turbulence is ℓ, then in the *LES limit*, i.e., $\Delta \ll \ell$, the numerical grid resolves all of the energy-containing turbulence. The subgrid model is responsible only for energy transfer from the resolved scales. The standard (Smagorinsky) subgrid model produces this transfer at the correct mean rate.

In the *mesoscale limit*, $\Delta \gg \ell$, no turbulence is resolved. Turbulence effects are represented through a subgrid model, typically of the ensemble-mean type. In principle the subgrid model can be adjusted to perform well in this limit.

Between these two limits lies the *Terra Incognita* where the subgrid model carries significant fluxes and transfers energy. In principle neither ensemble-mean nor the traditional LES closures are appropriate there.

THE LES AND MESOSCALE LIMITS

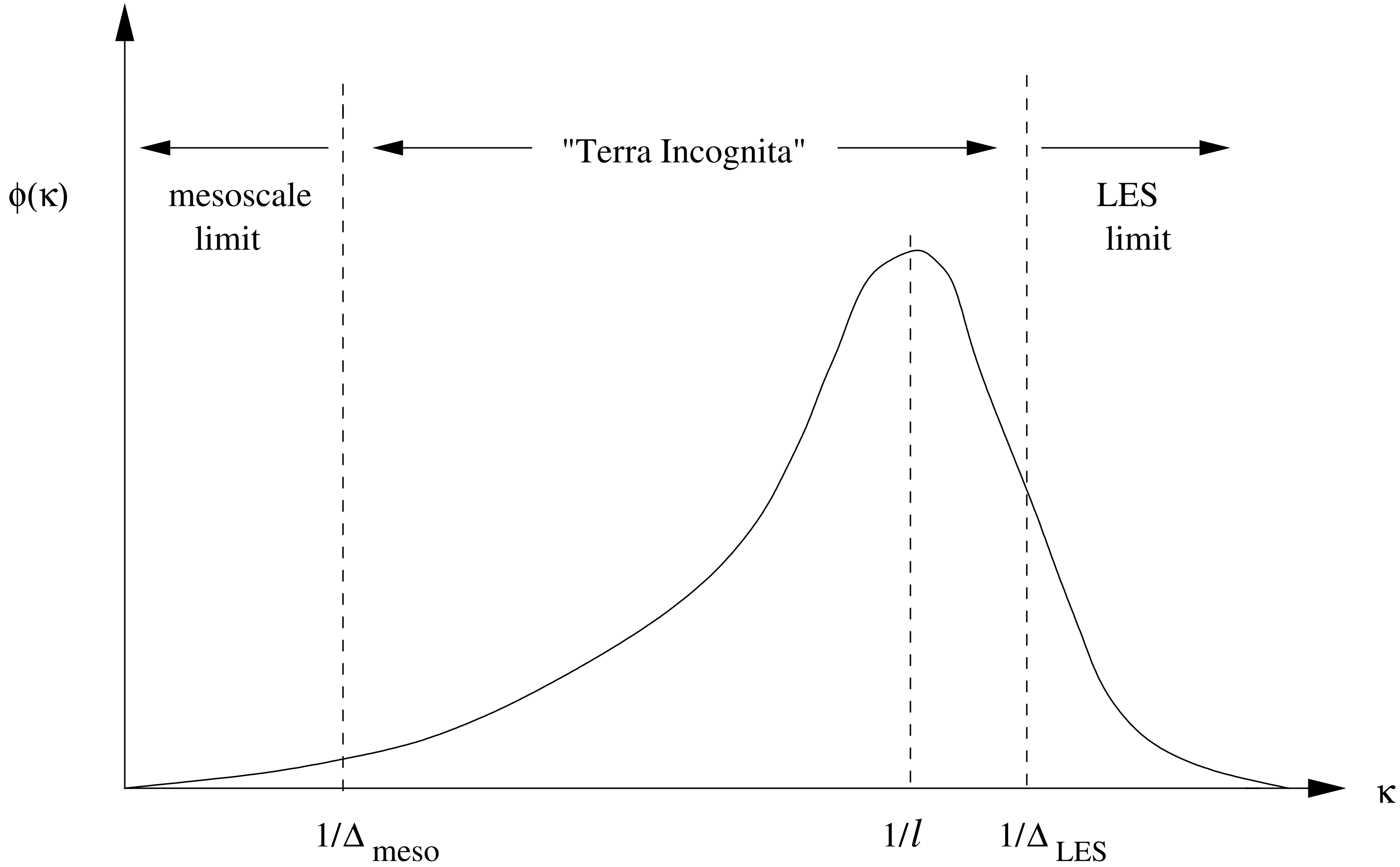

Figure 1: The wave number spectrum of turbulence and the Terra Incognita. Δ_{meso} is the scale of a mesoscale model grid, ℓ is the scale of the energy-containing turbulence, and Δ_{LES} is the scale of the LES grid.

ARE WE NOW THERE?

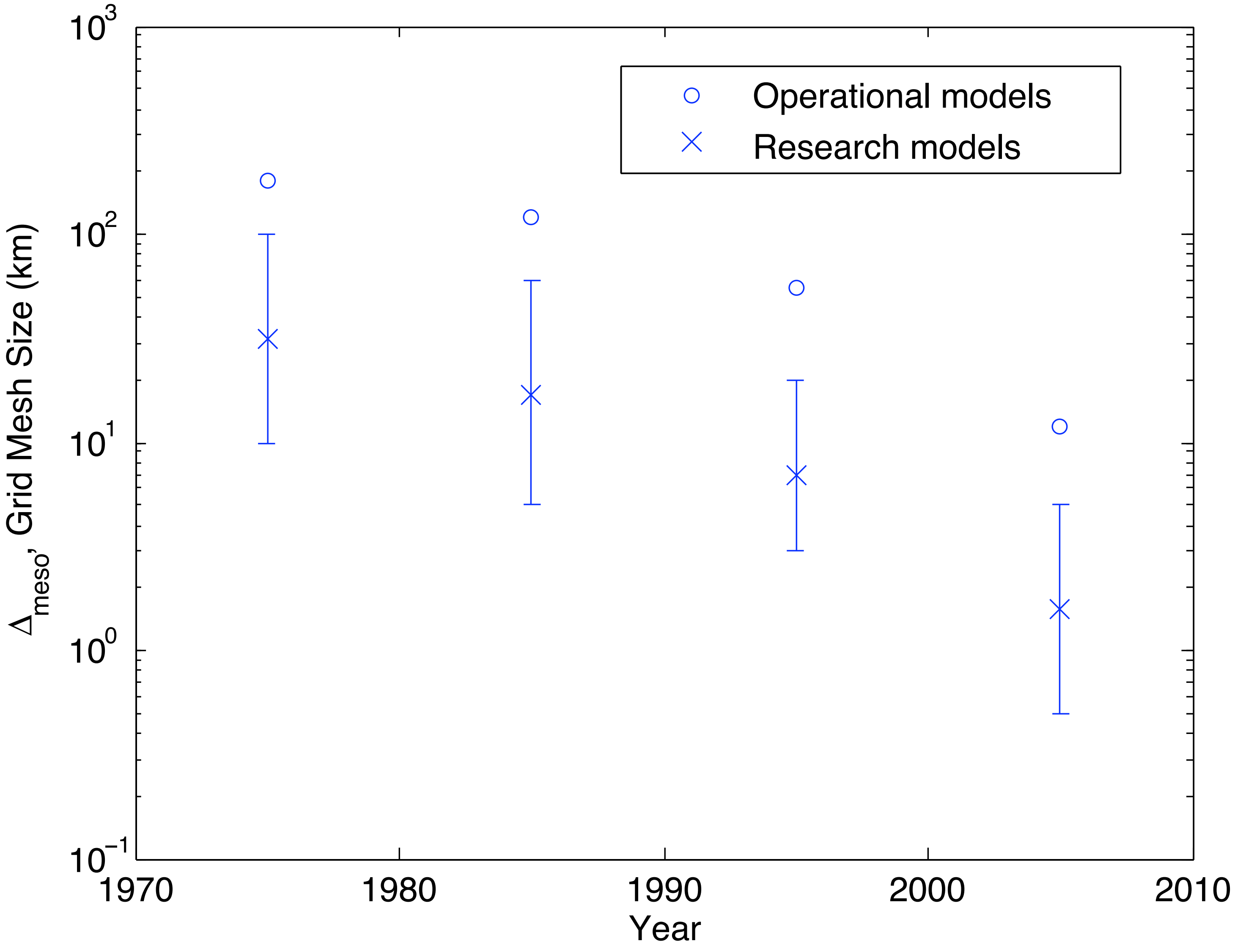

Figure 2: The evolution of Δ_{meso}, the grid-mesh size of typical mesoscale models, over the past 30 years.

TURBULENCE MODELING: STRONG VIEWS FROM ENGINEERING

Hans Liepmann, “The rise and fall of ideas in turbulence,” *Am. Scientist*, 1973:

> Problems of technological importance are always approached by approximate methods, and a large body of turbulence modeling has been established under prodding from industrial users. The Reynolds-averaged equations are almost always applied in such work, and the hierarchy of equations is closed by semi-empirical arguments which range from very simple guesses . . . to much more sophisticated hierarchies. . . .
>
> I am convinced that much of this huge effort will be of passing interest only. Except for rare critical appraisals such as the 1968 Stanford contest for computation of turbulent boundary layers, much of this work is never subjected to any kind of critical or comparative judgment. The only encouraging prospect is that current progress in understanding turbulence will . . . guide these efforts to a more reliable discipline.

John Lumley, "Atmospheric modelling," *Mech. Eng. Trans., Inst. of Eng. Australia*, 1983:

> One should not expect too much from these *"calibrated surrogates for turbulence."* (italics added). They should work satisfactorily in situations not too far removed geometrically, or in parameter values, from the benchmark situations used to calibrate them. Many of the initial successes of the models . . . have been in flows . . . where details of the models are irrelevant. Thus emboldened, the modelers have been over enthusiastic in promoting their models . . . often without considering in depth the difficult questions that arise. Consequently, there is some disillusionment with the models . . . . This reaction is probably justified, but it would be a shame if it resulted in a cessation of efforts to put a little more physics and mathematics into the models.

Peter Bradshaw, “Turbulence: the chief outstanding difficulty of our subject,” *Experiments in Fluids*, 1994:

> . . . even if one makes generous estimates of required engineering accuracy and requires predictions only of the Reynolds stresses, the likelihood is that a simplified model of turbulence will be significantly less accurate, or significantly less widely applicable, than the Navier-Stokes equations themselves—i.e., *it will not be ‘universal’*.. . . It is becoming more and more probable that really reliable turbulence models are likely to be so long in development that large eddy simulations (from which, of course, all required statistics can be derived) will arrive at their maturity first.

AN ECHO FROM THE ATMOSPHERIC SIDE

From *Improving the Scientific Foundation for Atmosphere-Land-Ocean Simulations*, NAS, 2005:

> Many workshop participants agreed that progress in model development is being impeded, and they identified several likely contributors to this situation, many of them cultural:
>
> - Widely available, easily run models and the current funding and academic environments may be turning both graduate students and their faculty advisors toward fast-turnaround research in numerical simulation and away from the traditional but much slower path of theory and observation.
> - Progress in parameterization, which often requires interactions across traditional disciplinary boundaries, could now be inhibited by the compartmentalization of educational, research, and funding institutions.
> - The rigidity of long-existing models and the lack of efforts to remove inferior or flawed physical representations hinder progress by preventing opportunities for new, fresh thinking.

The authors felt these trends “could cloud the future” of the atmospheric sciences, climate, and oceanography.

SUBGRID MODELING IN THE TERRA INCOGNITA

Lilly's (1967) evolution equation for the *deviatoric subgrid stress*, $\tau_{ij} = \overline{u}_i\overline{u}_j - \overline{u_i u_j} + \frac{2}{3}\delta_{ij}e$, is

$$
\begin{aligned}
\frac{\partial \tau_{ij}}{\partial t} + \overline{u}_k \frac{\partial \tau_{ij}}{\partial x_k} = \frac{\partial}{\partial x_k}\Bigg[& \overline{u_i u_j u_k} - \overline{u}_i \overline{u_j u_k} - \overline{u}_j \overline{u_i u_k} - \overline{u}_k \overline{u_i u_j} + 2\overline{u}_i \overline{u}_j \overline{u}_k \\
& - \frac{\delta_{ij}}{3}\left(\overline{u_l^2 u_k} - 2\overline{u}_l \overline{u_l u_k} - \overline{u}_k \overline{u_l^2} + 2\overline{u_l}^2 \overline{u_k}\right)\Bigg] \quad \text{(transport)} \\
& + \frac{2e}{3}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) \quad \text{(isotropic production)} \\
& - \left[\tau_{ik}\frac{\partial \overline{u}_j}{\partial x_k} + \tau_{jk}\frac{\partial \overline{u}_i}{\partial x_k} - \frac{1}{3}\delta_{ij}\tau_{kl}\left(\frac{\partial \overline{u}_k}{\partial x_l} + \frac{\partial \overline{u}_l}{\partial x_k}\right)\right] \quad \text{(deviatoric production)} \\
& - \overline{\left[\frac{p}{\rho}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right]} + \overline{p}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) \quad \text{(pressure destruction)} \\
& + \frac{1}{\rho}\frac{\partial}{\partial x_k}\left(\delta_{ik}\left[\overline{u_j p} - \overline{u}_j \overline{p}\right] + \delta_{jk}\left[\overline{u_i p} - \overline{u}_i \overline{p}\right] - \frac{2}{3}\delta_{ij}\left[\overline{u_k p} - \overline{u}_k \overline{p}\right]\right). \quad \text{(pressure trans.)}
\end{aligned}
$$

- When $\overline{(\ )}$ is the ensemble average this is the basis of RANS.

- When $\overline{(\ )}$ is a local volume average this is the basis of LES.

A REVISED "FIRST ORDER THEORY" FOR SUBGRID STRESS

Lilly's (1967) "first order theory" ignores all but isotropic production and pressure destruction in the evolution equation for τ_{ij}, giving

$$\frac{\partial \tau_{ij}}{\partial t} = \frac{2e}{3}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) - \frac{\tau_{ij}}{T},$$

with $T \sim \Delta / e^{1/2}$ a time scale of pressure destruction. The steady result is the standard (Smagorinsky) subgrid model in LES:

$$\tau_{ij} = \frac{2eT}{3}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right), \qquad T \sim \Delta / e^{1/2}.$$

However, the deviatoric production term, being of the same order as isotropic production, should appear here as well, so the revised first order theory is

$$\frac{\partial \tau_{ij}}{\partial t} = \frac{2e}{3}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) - \left[\tau_{ik}\frac{\partial \overline{u}_j}{\partial x_k} + \tau_{jk}\frac{\partial \overline{u}_i}{\partial x_k} - \frac{1}{3}\delta_{ij}\tau_{kl}\left(\frac{\partial \overline{u}_k}{\partial x_l} + \frac{\partial \overline{u}_l}{\partial x_k}\right)\right] - \frac{\tau_{ij}}{T}.$$

THE “ARRAY TECHNIQUE” FOR MEASURING SUBGRID FLUXES

In the mid-90s we conceived the notion of doing the averaging (or, more generally, the filtering) involved in the subgrid fluxes by using the time-filtered outputs from a lateral array of velocity and scalar sensors. Key developments were

- Chenning Tong used LES fields to show that two-dimensional filtering in the horizontal plane is a good surrogate for three dimensional filtering.
- We did the first field measurements of subgrid fluxes at Penn State in 1996.
- Chenning presented the first results in a seminar at NCAR in 1997.
- NCAR carried out the HATS experiment in 2000.
- Then came OHATS (2005) and CHATS (2007); AHATS is scheduled for 2008.

Figure 3: A view of our field site and Chenning Tong at Rock Spring, Pa., where we carried out the first array experiment in 1996.

HORIZONTAL ARRAY TURBULENCE STUDY

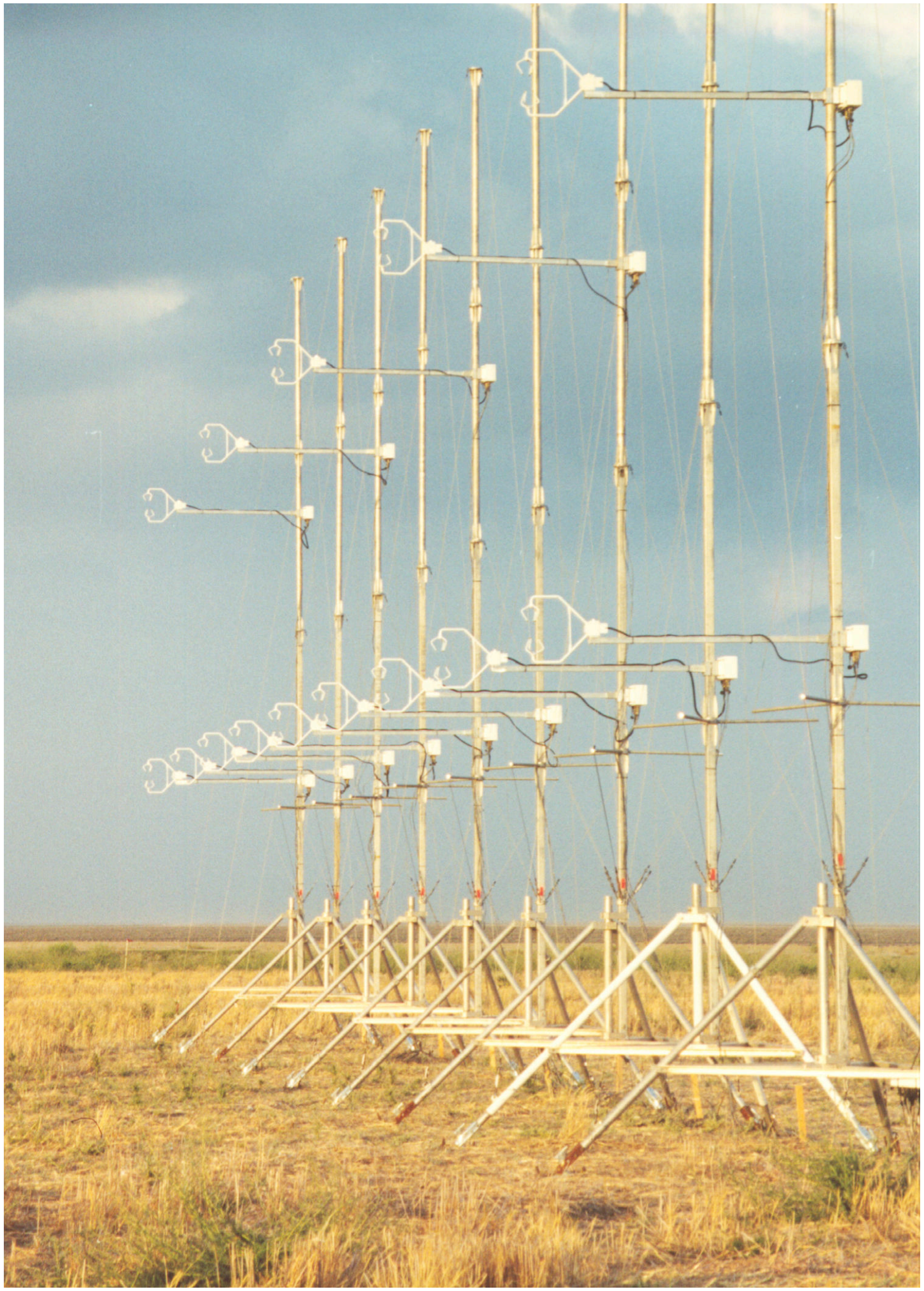

Figure 4: The sonic-anemometer array used in the HATS experiment carried out in 2000 by NCAR near Kettleman City, Ca.

IMPROVED MODELING OF SUBGRID STRESS

The array experiments confirm that the lowest-order subgrid stress model is, in rate-equation form,

$$\frac{\partial \tau_{ij}}{\partial t} = \frac{2e}{3}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) - \left[\tau_{ik}\frac{\partial \overline{u}_j}{\partial x_k} + \tau_{jk}\frac{\partial \overline{u}_i}{\partial x_k} - \frac{1}{3}\delta_{ij}\tau_{kl}\left(\frac{\partial \overline{u}_k}{\partial x_l} + \frac{\partial \overline{u}_l}{\partial x_k}\right)\right] - \frac{\tau_{ij}}{T}.$$

The terms on the right represent isotropic production, deviatoric (anisotropic) production, and pressure destruction.
Hatlee and Wyngaard (2007) showed that this revised model performed much better than the standard Smagorinsky model in HATS.

IMPROVED MODELING OF SUBGRID STRESS

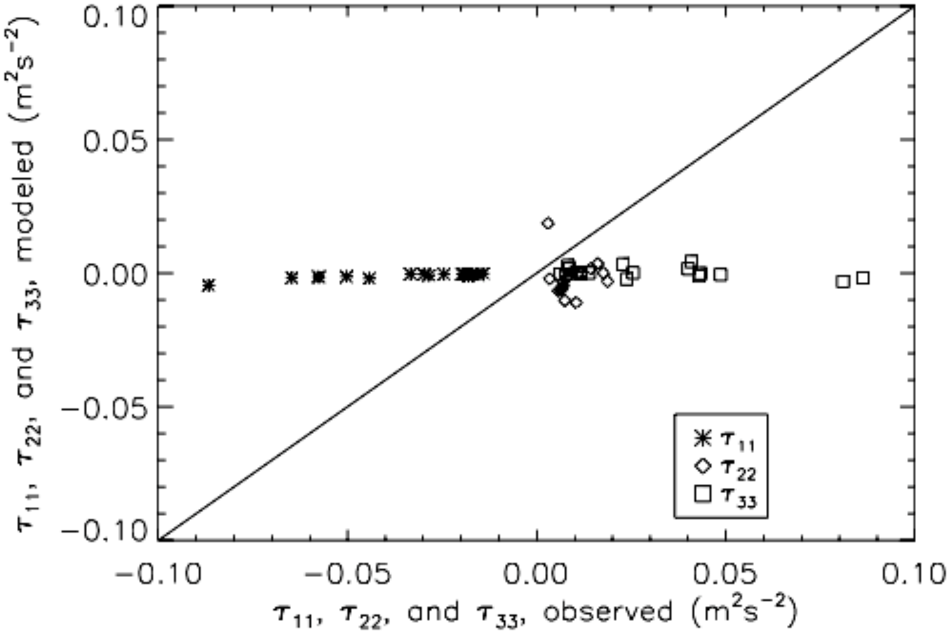

Figure 5: The performance of the standard subgrid stress model in the HATS experiment.

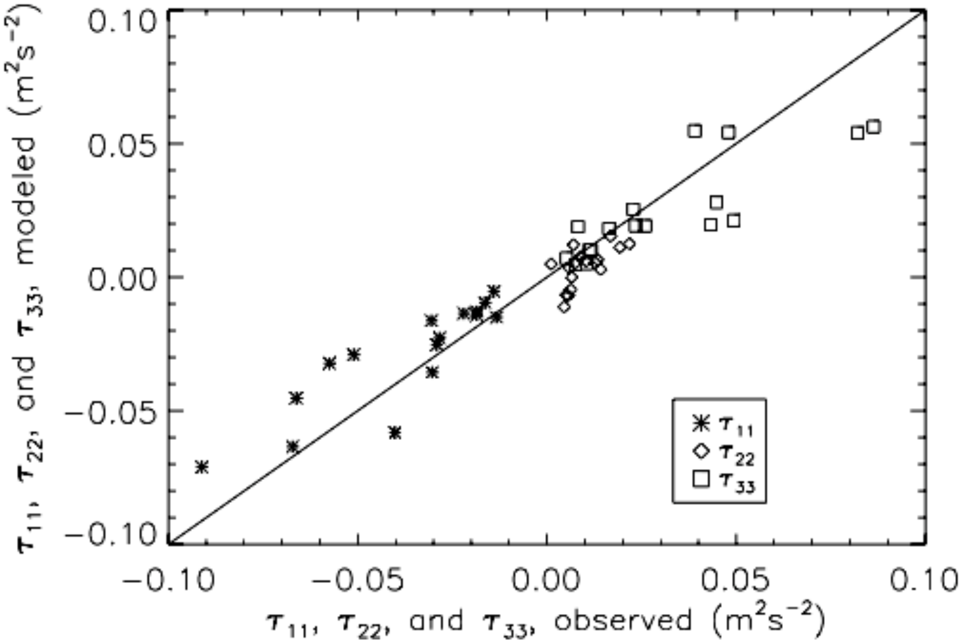

Figure 6: The performance of the revised subgrid stress model in the HATS experiment.

THE MAINTENANCE OF SUBGRID SCALAR FLUX

Early LES appears not to have used the corresponding conservation equation for the subgrid flux f_i of a conserved scalar. It reads

$$\frac{\partial f_i}{\partial t}+\overline{u}_j\frac{\partial f_i}{\partial x_j}=-\frac{\partial}{\partial x_j}\left(\overline{cu_iu_j}-\overline{cu_i}\;\overline{u}_j-\overline{c}\;\overline{u_iu_j}+\overline{u}_i\;\overline{cu_j}+2\overline{c}\,\overline{u}_i\overline{u}_j\right)\quad\text{(transport)}$$

$$-\frac{1}{\rho}\frac{\partial}{\partial x_i}\left(\overline{pc}-\overline{p}\;\overline{c}\right)\quad\text{(pressure transport)}$$

$$-f_j\frac{\partial\overline{u}_i}{\partial x_j}-R_{ij}\frac{\partial\overline{c}}{\partial x_j}\quad\text{(tilting production, gradient production)}$$

$$+\frac{1}{\rho}\left(\overline{p\frac{\partial c}{\partial x_i}}-\overline{p}\frac{\partial\overline{c}}{\partial x_i}\right).\quad\text{(pressure destruction)}$$

$$R_{ij}=\overline{u_iu_j}-\overline{u}_i\,\overline{u}_j$$

Since it ignores tilting production and the tensor nature of the diffusivity associated with the scalar gradient, the standard LES closure

$$f_i=-K\frac{\partial\overline{c}}{\partial x_i}$$

is not a plausible model of this equation in the Terra Incognita.

IMPROVED MODELING OF SUBGRID SCALAR FLUX

The array experiments confirm that the lowest-order subgrid scalar flux model is, in rate-equation form,

$$\frac{\partial f_i}{\partial t} = -f_j \frac{\partial \overline{u}_i}{\partial x_j} - R_{ij} \frac{\partial \overline{c}}{\partial x_j} - \frac{f_i}{T}.$$

This expresses a balance among tilting production, gradient production, and pressure destruction.
Hatlee and Wyngaard (2007) showed that this revised model performed much better than the standard model in HATS.

IMPROVED MODELING OF SUBGRID SCALAR FLUX

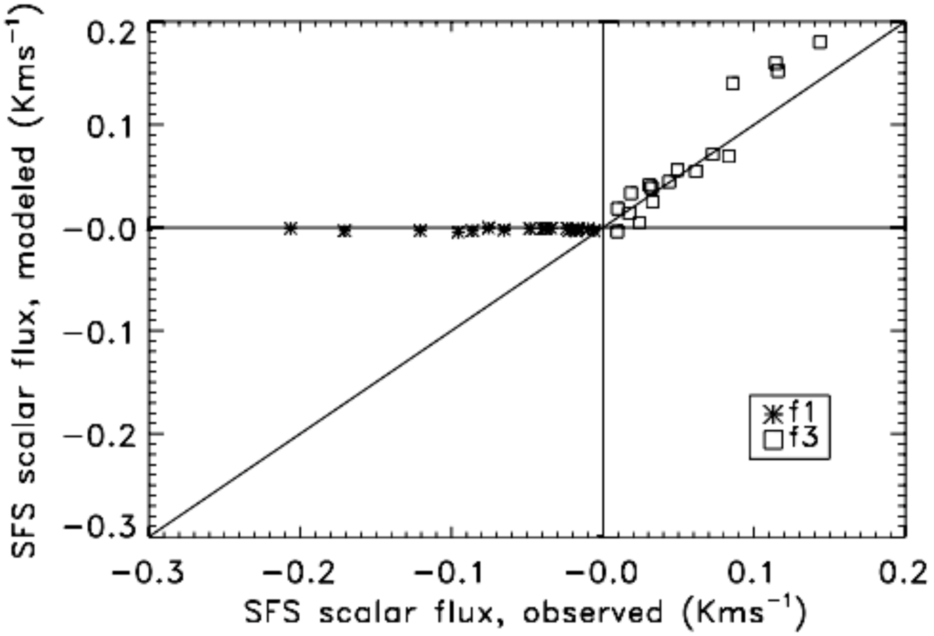

Figure 7: The performance of the standard subgrid scalar flux model in the HATS experiment.

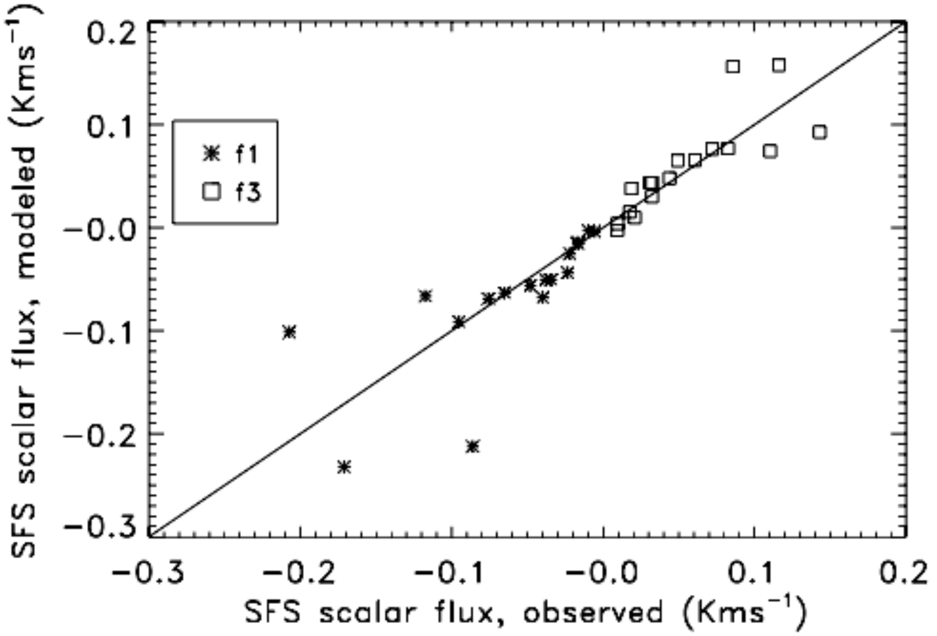

Figure 8: The performance of the revised subgrid scalar flux model in the HATS experiment.

THE 2004 BOARD ON ATMOSPHERIC SCIENCES WORKSHOP:

“IMPROVING THE SCIENTIFIC FOUNDATION FOR ATMOSPHERIC-LAND-OCEAN SIMULATIONS”

Workshop Context (p. 3)

At the dawning of the age of numerical simulation in the 1960s, few imagined the influence it would have on the atmospheric and oceanic sciences. . . . Yet. . . the models tend not to adequately represent our knowledge of the underlying physics. . . . there is evidence that further progress in numerical simulations is being impeded by the slow pace of improvement in the representation of certain key processes in the models.

There is an emerging perception that the physics . . . of geophysical flow models is not receiving the continuing attention needed . . . . Some of the problem seems cultural: today’s modelers and users of model output seem less engaged with improving model physics than with . . . the numerics, graphics, and architecture of the model system and with using models rather than observations to study geophysical flows.

Statement of Task (p. 33)

- What is the status of and what are the major errors associated with the parameterization of physical processes in A-L-O models?

- How can model parameterizations be improved to represent the essential physics in A-L-O models? How can these parameterizations be tested rigorously, and what supporting infrastructure is needed to do so?

- What is the appropriate balance between improving physical parameterizations and other model development and application activities?

THE 2004 BOARD ON ATMOSPHERIC SCIENCES WORKSHOP

Concluding Thoughts (p. 28)

- An important field of parameterization science has emerged over the past 40 years. . . . Workshop participants believe that our educational, research, and funding institutions need to recognize, accommodate, and foster this new field.

- More extensive and rigorous comparisons of models with observations and field experiments designed to support such comparisons are needed.

- The cultural issues thought by the workshop participants to be limiting progress in model development might not be self-correcting; they could require the institutional adjustments that are occasionally but necessarily made as society and the atmospheric and oceanic sciences respond to changing conditions.