



3-D Large Eddy Simulation of Turbulent Flow based on One-Dimensional Turbulence Modeling

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Turbulence modeling, even without the complications of atmospheric physics, remains a very challenging problem.

The accurate simulation of turbulent flow is a classic, longstanding multi-scale problem that has vexed scientists and engineers for many years.

- * Non-linear terms in the governing NS equations
- * Enormous cost of resolving the length and time-scales present in high Reynolds number flows



*“I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is the **turbulent motion of fluids**. And about the former I am rather optimistic.”*

~ Horace Lamb (1849 - 1934)

“. . . turbulence needs spirited inventors just as badly as dedicated analysts.”

H. Tennekes and J. L. Lumley, A First Course in Turbulence, pg. 4, 1972



Two Conceptual Approaches to the Multi-scale Nature of Turbulent Flow

- (1) Using one set of equations, resolve as much of the large scale (*time, space*) range as you can afford. Parameterize the smaller, unresolved-scale quantities as functions of your resolved scale quantities.

RANS and LES are both variations of this approach for turbulent flow

- (2) Solve different sets of equations for different space and time scale regions but couple the equation sets through appropriate constraints to enforce consistency. Balance the computational effort among these different space/time domains.

ODTLES (and LESODT) described here follow this approach

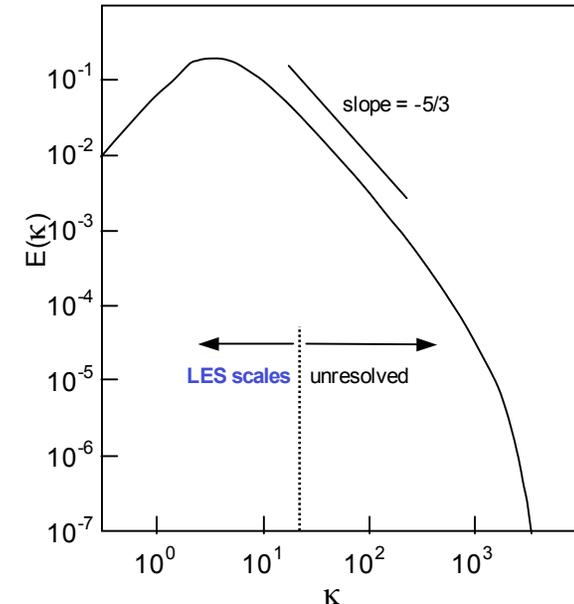


Problems with traditional LES closure models

Traditional LES begins by casting the problem in terms of only the large-scale “resolved” physics.

For solutions to be accurate:

- * “Unresolved” physics must be dependent on the “resolved” quantities
- * “Resolved” physics must be independent of the unresolved physics



This “top-down” approach to the closure problem is problematic in near-wall regions, where the eddy-sizes of importance scale with distance to the wall, and more generally in any situation where important small-scale physical processes are uncorrelated to the large-scale flow.

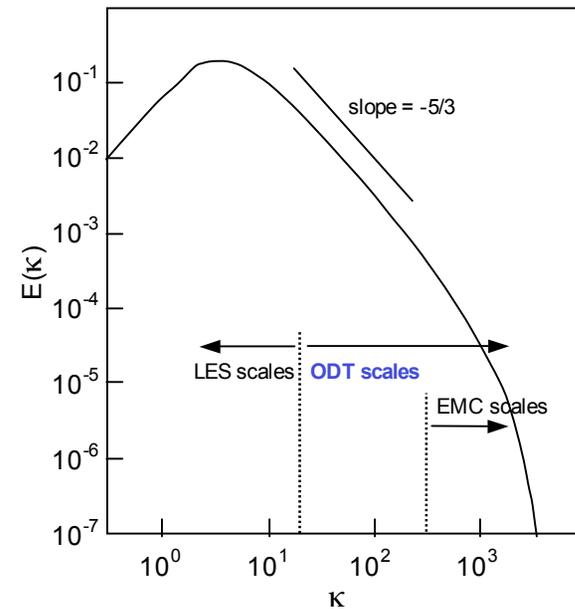


A non-traditional “bottom-up” alternative

Begins with the small-scale dynamics - modeled on one-dimensional domains using a modified form of the ODT model of Kerstein.

Large-scale (LES-like) dynamics obtained by coupling the one-dimensional domains in some manner that enforce 3D large-scale consistency constraints.

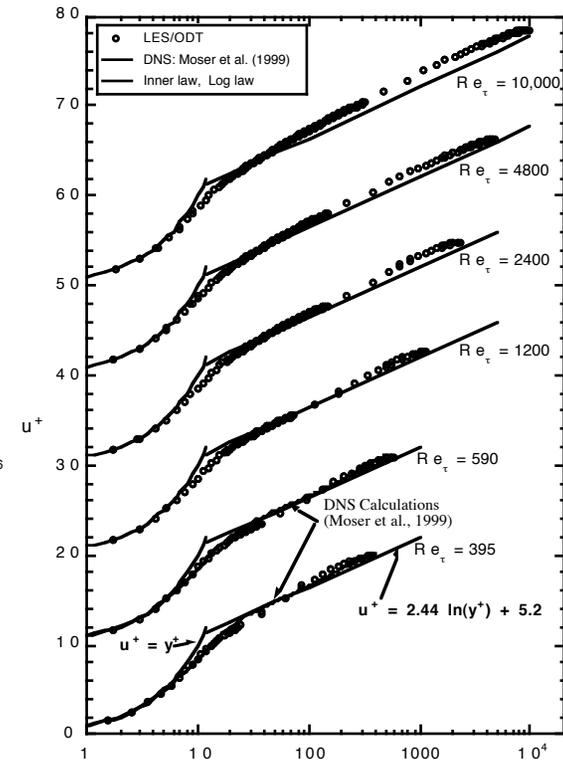
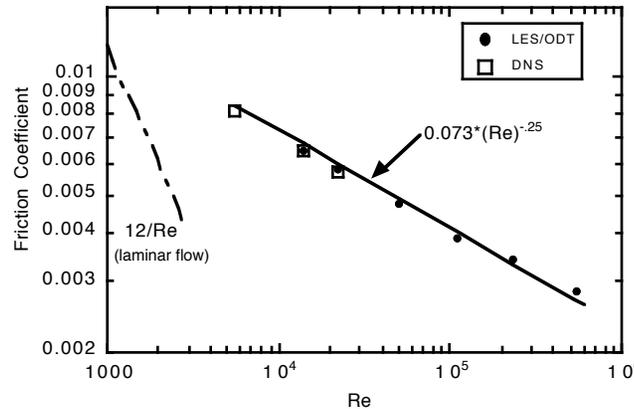
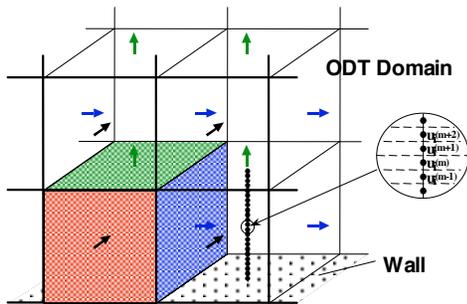
When the smallest scales (e.g. Kolmogorov scales) are not important, we use the “EMC” eddy viscosity model to represent the physics at the smallest scales (i.e. viscous dissipation).



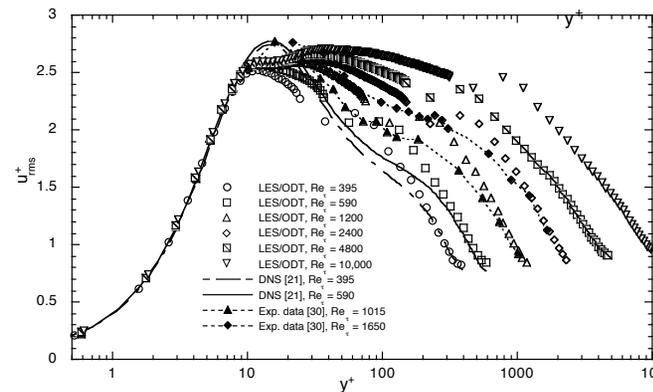
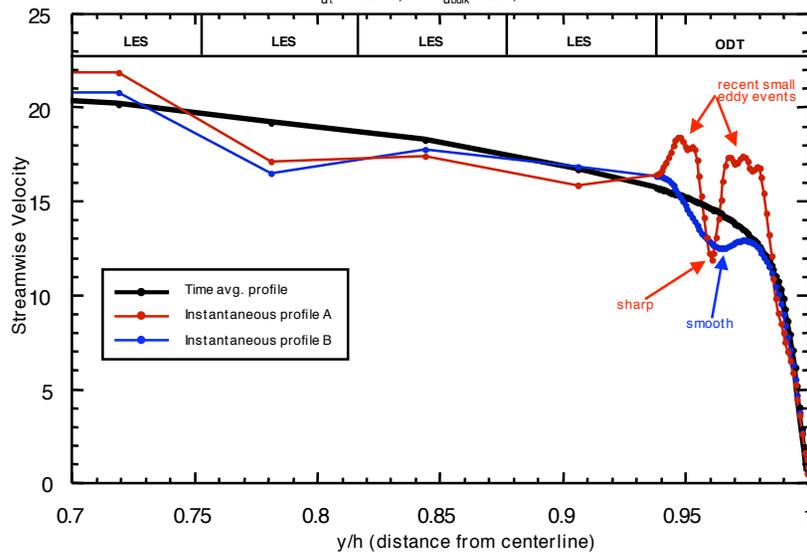


A previously developed ODT-based LES near-wall closure model LES provided useful insight into developing a more general model

Schmidt, Kerstein, Wunsch, Nilsen, "Near-wall LES closure based on one-dimensional turbulence modeling," JCP, 186:317, 2003

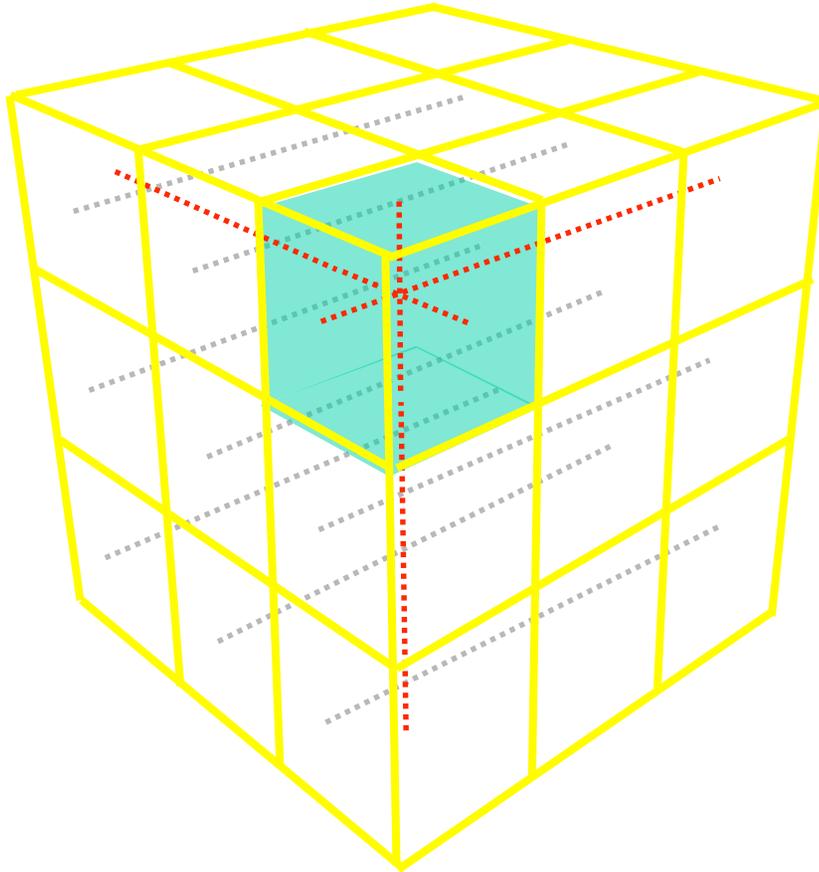


LES/ODT Simulation of Turbulent Channel Flow
 $Re_{U_t} = 1200, Re_{U_{bulk}} = 25,000$





Building a 3D model out of 1D components



“Stand-alone” ODT is solved on a single line.

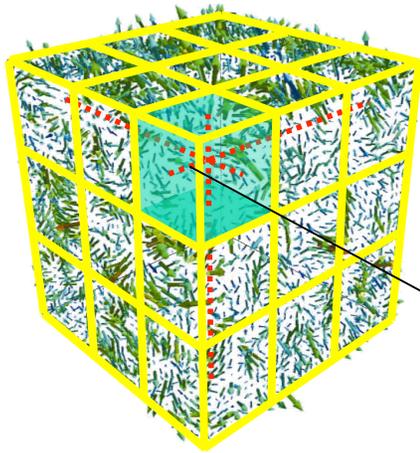
$$\frac{\partial v_i}{\partial t} = \nu \frac{\partial^2 v_i}{\partial x^2} + \text{eddies}$$

Three orthogonal ODT line sets embedded in a 3D domain discretized by a standard type of rectangular LES-scale control volumes

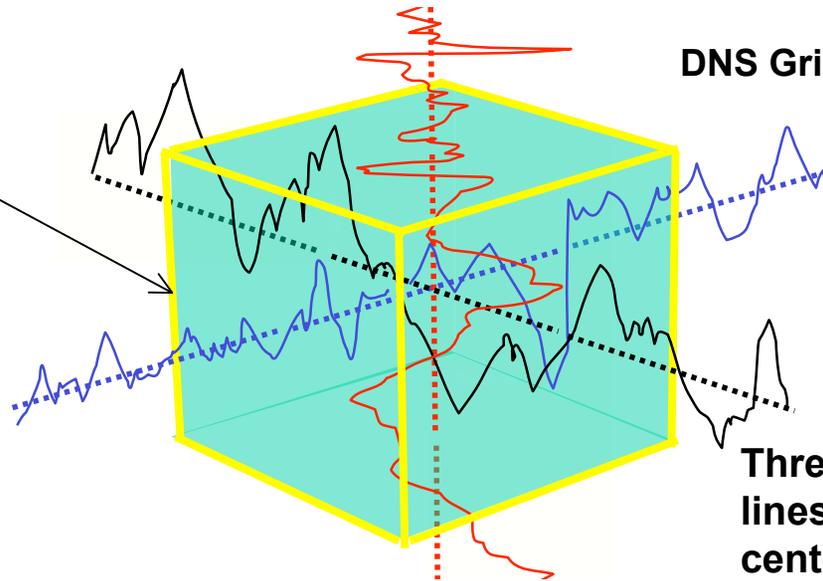


Conceptual illustration of the geometric framework for an ODT based modeling strategy for 3D turbulent flow

Domain discretized in two distinct but interdependent ways



$3N^2$ ODT lines
where, N = number of
LES cells in 1-D



Three orthogonal ODT
lines intersect at the
center of each LES-
scale control volume

Example Reduction in Grid pts:

Model Grid Points = $3 * 16 = 48$
vrs.
DNS Grid Points = $16^3 = 4096$

How can one couple the separate ODT domains in such a way that momentum and mass conservation balances are enforced on the 3D domain?



Strategy 1: “LESODT”

Close the LES equations with a standard ODT subgrid model

(Randy McDermott, DOE CSGF, U. of Utah)

LES Equations

$$\frac{\delta \bar{u}_i}{\delta t} + \frac{\delta}{\delta x_j} (\bar{u}_i \bar{u}_j) = -\frac{\delta \bar{p}}{\delta x_j} + \frac{\delta}{\delta x_j} (\overbrace{\bar{\tau}_{ij}^{visc} + \tau_{ij}^{sgs}})$$

$$\frac{\delta \bar{u}_i}{\delta x_j} = 0$$

Computed directly from a sub-time step evolution of 3-component ODT on 3 orthogonal ODT lines. No eddy Viscosity is introduced!

ODT Equations

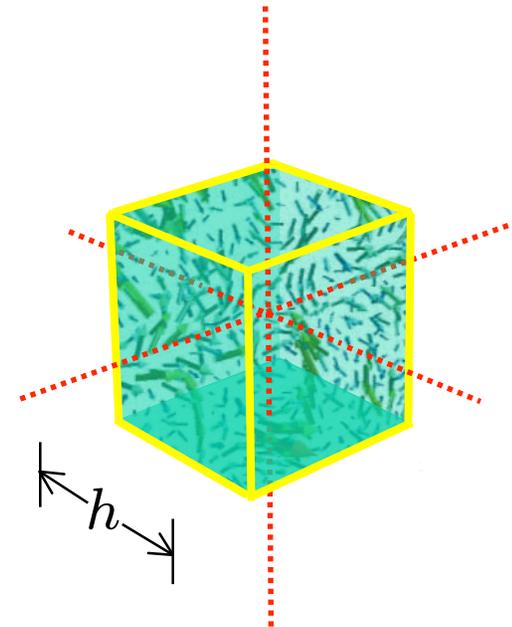
$$\frac{\partial v_i}{\partial t} = \nu \frac{\partial^2 v_i}{\partial x_i^2} + \text{eddies}$$

Solved simultaneously on $3N^2$ ODT lines. “DNS” scale time steps for LES-scale time intervals

Imposed Constraint

$$\frac{1}{N} \sum_{n=1}^N v_{i,n} = \bar{u}_i$$

Imposed once each LES time step through an adjustment procedure.





Strategy 2: ODTLES

Include “LES-scale” terms in modified ODT equations

(R. Schmidt, SNL)

ODT Equations

$$\frac{\partial v_{ki}}{\partial t} - \nu \frac{\partial^2 v_{ki}}{\partial x^2} = (LES_Pres.)_i - (LES_Conv.)_{k,i} + (3D_Visc.)_{k,i} + eddies$$

$$= \frac{\delta \bar{P}}{\delta x_i} \quad \text{3D LES-scale pressure-grad}$$

$$- \frac{\delta}{\delta x_i} (\bar{u}_{k,i} v_{k,i}) - \frac{\delta}{\delta x_j} (\bar{u}_{k,j} v_{k,i}) - \frac{\partial}{\partial x_k} (\bar{u}_{k,k} v_{k,i}) \quad \text{LES-scale advection}$$

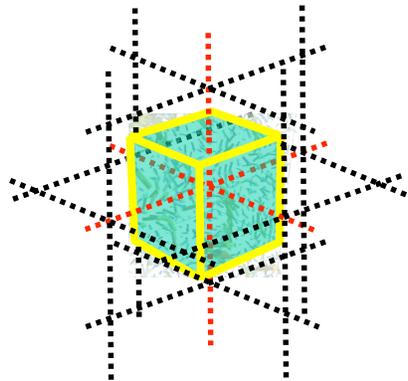
$$+ \frac{\partial}{\partial x_j} \left(\nu \frac{\partial v_{j,i}}{\partial x_j} \right) |_{jk\text{-interp}} + \frac{\delta}{\delta x_i} \left(\nu \frac{\delta v_{k,i}}{\delta x_i} \right) \quad \text{3D ODT-scale diffusion}$$

+ eddies

where

$$\bar{u}_{k,i} = \frac{1}{\Delta T_{les}} \int_{t-\Delta T_{les}}^t v_{k,i} dt \quad (1) \quad \text{Time-filtered ODT-scale velocities used for advection}$$

$$\bar{u}_{k,k}(x_k) = \bar{u}_{k,k}(0) - \int_0^{x_k} \left(\frac{\delta \bar{u}_{k,i}}{\delta x_i} + \frac{\delta \bar{u}_{k,j}}{\delta x_j} \right) dx_k \quad \text{ODT-scale continuity constraint}$$





ODTLES (continued)

“LES” Equations

$$\frac{\delta \bar{U}_1}{\delta x_1} + \frac{\delta \bar{U}_2}{\delta x_2} + \frac{\delta \bar{U}_3}{\delta x_3} = 0$$

where

$$\bar{U}_i = \frac{0.5}{\Delta X_k} \int_{-\frac{\Delta X_k}{2}}^{+\frac{\Delta X_k}{2}} \bar{u}_{k,i} dx_k + \frac{0.5}{\Delta X_l} \int_{-\frac{\Delta X_l}{2}}^{+\frac{\Delta X_l}{2}} \bar{u}_{l,i} dx_l \quad (2)$$

Note: Spatial/time-filtered LES-scale continuity Eq. requires solution of a Poisson Eq. for an LES pressure field each LES time step.

No LES-scale momentum equation need be solved as this is satisfied implicitly, by construction.

The ODT equations reduce to 2 copies of the NS equations in the limit of $\Delta X_{les} \rightarrow \Delta X_{odt}$.

Imposed Constraints

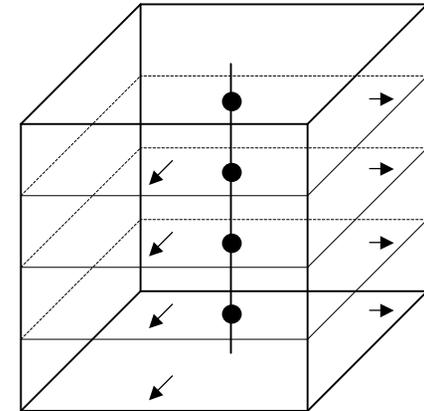
Before pressure projection, (1) and (2) are definitions.

After pressure projection, (1) and (2) are constraints, imposed through an adjustment procedure that preserves small-scale structure.

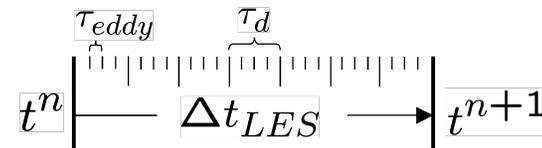


ODTLES: Additional Details

1. A two-velocity-component ODT model is used in ODTLES
2. ODT-scale velocities are located on control volume faces. This facilitates continuity preserving advection and means the corresponding LES-scale velocity field forms a standard staggered mesh.



3. ODT time steps, which are much smaller than LES time steps, are generally controlled by limits required in the ODT eddy-sampling procedure. The LES time step is controlled by CFL stability criteria.



4. If desired, an eddy viscosity closure in the ODT equations can be activated, e.g.

$$\nu_S = CC_{emc}(l_{max})^2 \left(\left| \frac{\partial v_i}{\partial x_k} \right| + \left| \frac{\partial v_j}{\partial x_k} \right| \right)$$



ODTLES: Additional Details (continued . . .)

5. The overall time integration scheme has the following 4 key parts:

i. Evolve the ODT equations in time on each individual ODT line over a time period equal to the LES time step.

ii. Compute “intermediate” values of $\hat{u}_{k,i}^{n+1}$ and $\hat{U}_{k,i}^{n+1}$ from given definitions.

iii. Solve the following discrete Poisson equation for the pressure correction ϕ , and update the LES scale pressure and velocity fields.

$$\frac{\delta^2 \phi}{\delta x_i \delta x_i} = \left(\frac{1}{\Delta T} \right) \frac{\delta \hat{U}_i^{n+1}}{\delta x_i}$$

$$\bar{P}^{n+1} = \bar{P}^n + \phi \quad \bar{U}_i^{n+1} = \hat{U}_i^{n+1} - \Delta T \left(\frac{\delta \phi}{\delta x_i} \right)$$

iv. Compute “corrected” values for $\bar{u}_{k,i}^{n+1}$ and $v_{k,i}$ through an adjustment procedure that makes these values consistent with \bar{U}_i^{n+1} .

Note: Parts iii and iv are a consequence of solving the incompressible form of the governing equations.



ODTLES: Additional Details (continued)

6. Characteristics of the ODT adjustment algorithm:
 - i. The small-scale, high wave number content of the ODT velocity field is unaltered, only the large-scale, low wave number content is affected so that $\bar{u}_{k,i}^{n+1}$ are constrained to be consistent with the updated values of \bar{U}_i^{n+1} .
 - ii. The algorithm is explicit, fast, and robust. Details are given elsewhere.

7. The ODT model requires the specification of three coefficients:
 - i. The overall rate constant, C .
 - ii. The largest eddy size, L_{\max} . In ODTLES, L_{\max} corresponds to largest eddy-size modeled with “eddy events”, which also equals the smallest length scale captured by the LES grid. We typically set $L_{\max}/\Delta X = 4$.
 - iii. Either the viscous cutoff parameter Z (if fully resolving the velocity field), or the eddy viscosity coefficient C_{emc} .



Initial Testing of the ODTLES Model: Simulations of Decaying Isotropic Turbulent Flow

- Low Re data of Comte-Bellot and Corrsin ($Re_\lambda = 72$)
- High Re data of Kang, Chester and Mineveau ($Re_\lambda = 720$)
- Periodic BC in all directions with $L_{\text{box}} = 2\pi$
- Four baseline calculations of Kang et al.:

Time step 

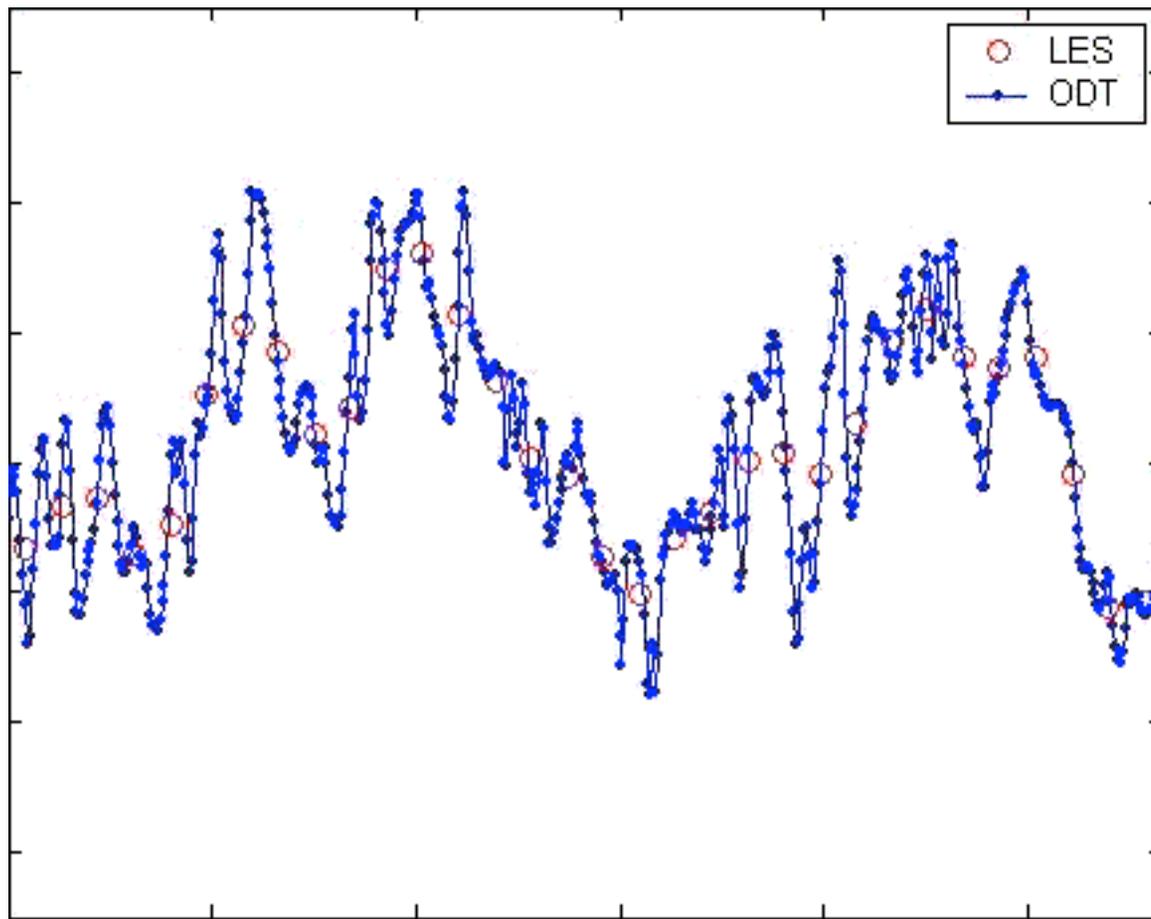
Run	N_{les}	N_{odt}	N_{cell}	$L_{max}/\Delta X$	$\Delta T/\Delta T_{cfl}$	$C/\sqrt{54}$	C_{emc}
1	32	128	4	4	0.1	1.0	.002
2	32	256	8	4	0.1	1.0	.002
3	32	512	16	4	0.1	1.0	.002
4	32	1024	32	4	0.1	1.0	.002

- 10 additional runs tested model parameter sensitivities.
- Additional details (e.g. initial condition specification) found in Schmidt et. al., SAND2005-0206, 2005)



Animated example of dynamics obtained on a single ODT line in a 3D ODTLES simulation

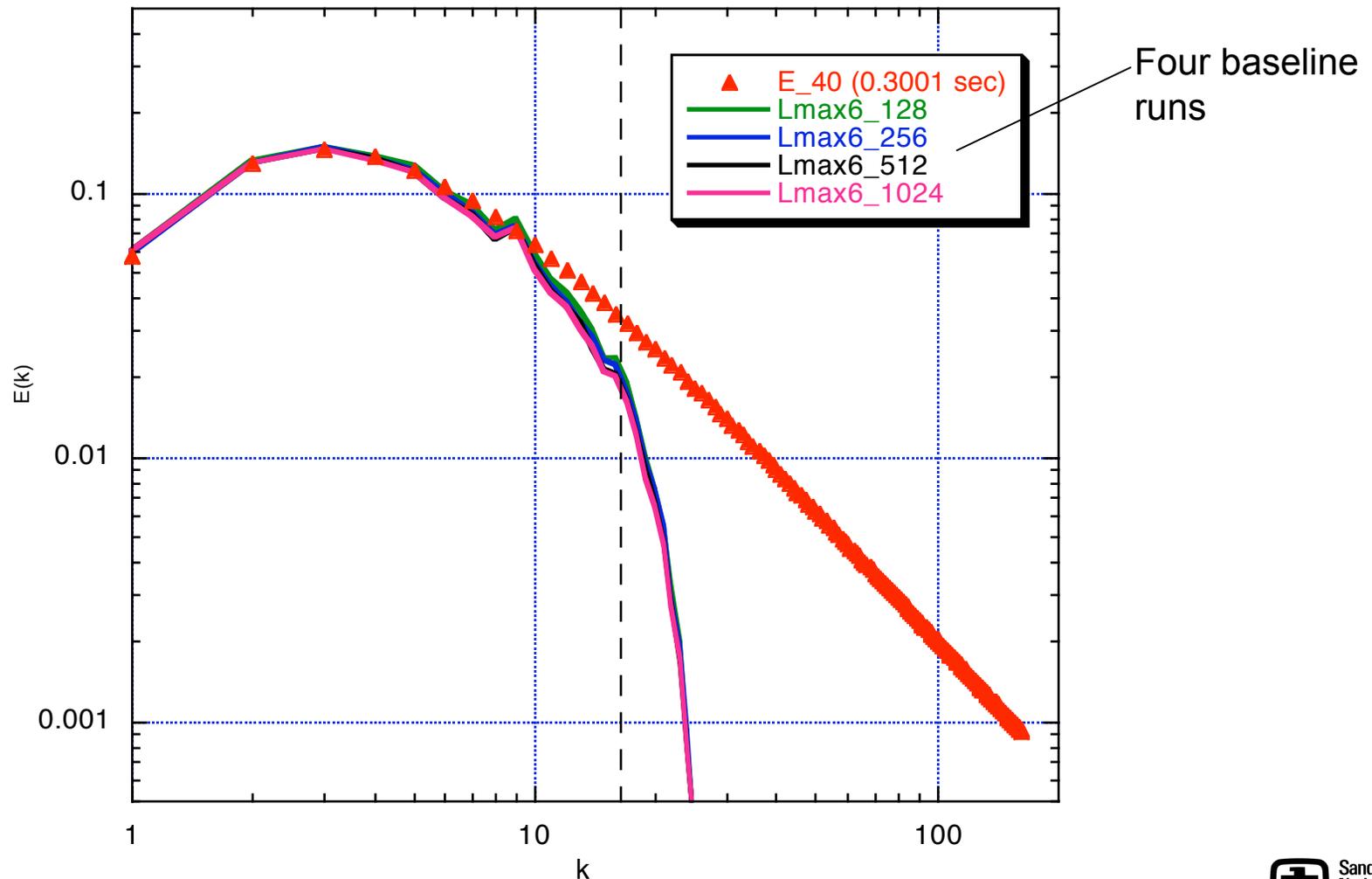
Decaying Isotropic Turbulence, $Re_\lambda = 72$, 32^3 LES / 512 ODT
(Exp. conditions from Comte-Bellot and Corrsin)





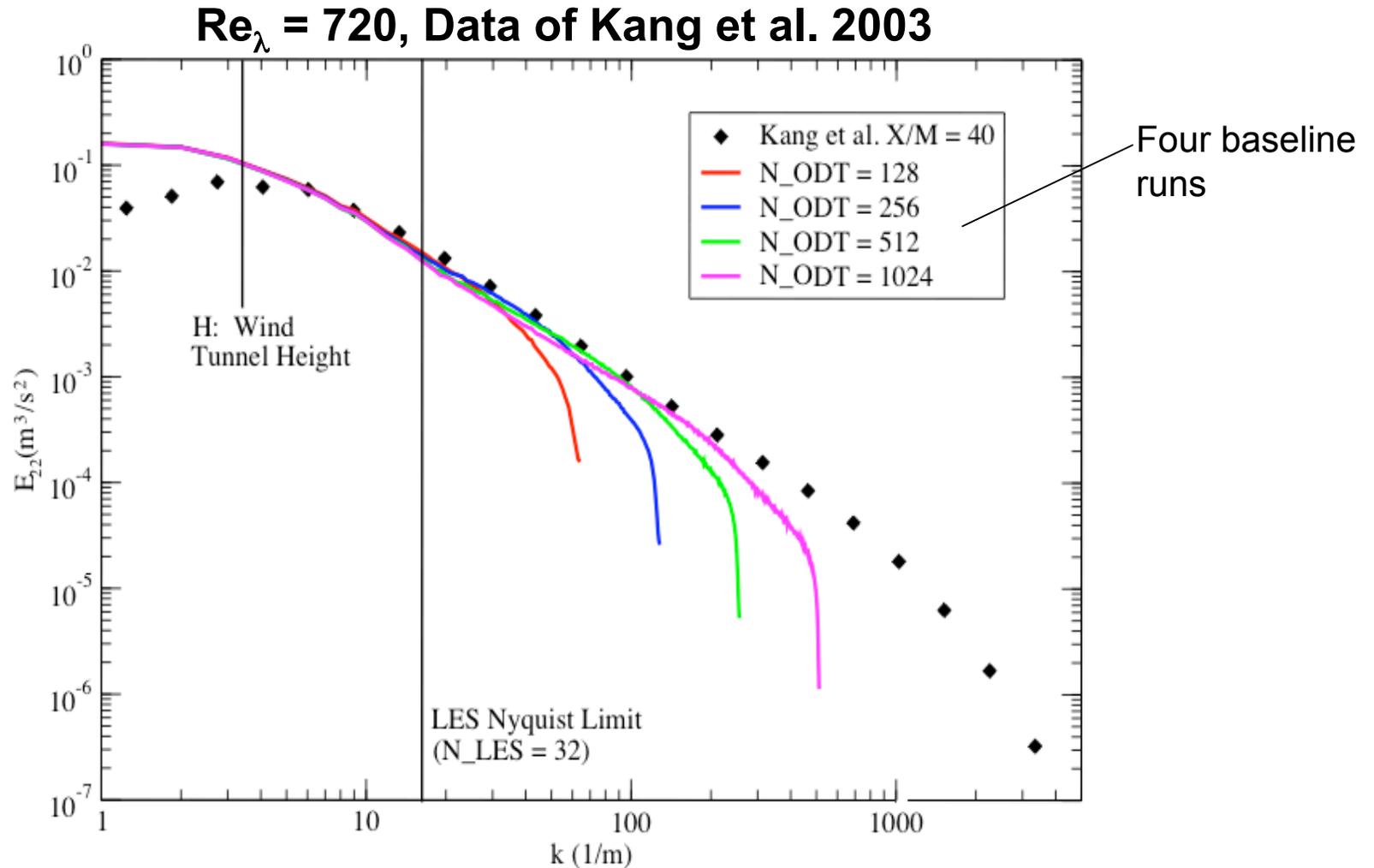
Simulation of High Re, Decaying Isotropic Turbulence, 3D Energy Spectrum: Sensitivity to ODT resolution

$Re_\lambda = 720$, Data of Kang et al. 2003





Simulation of High Re, Decaying Isotropic Turbulence, 1D Energy Spectrum: Sensitivity to ODT Resolution

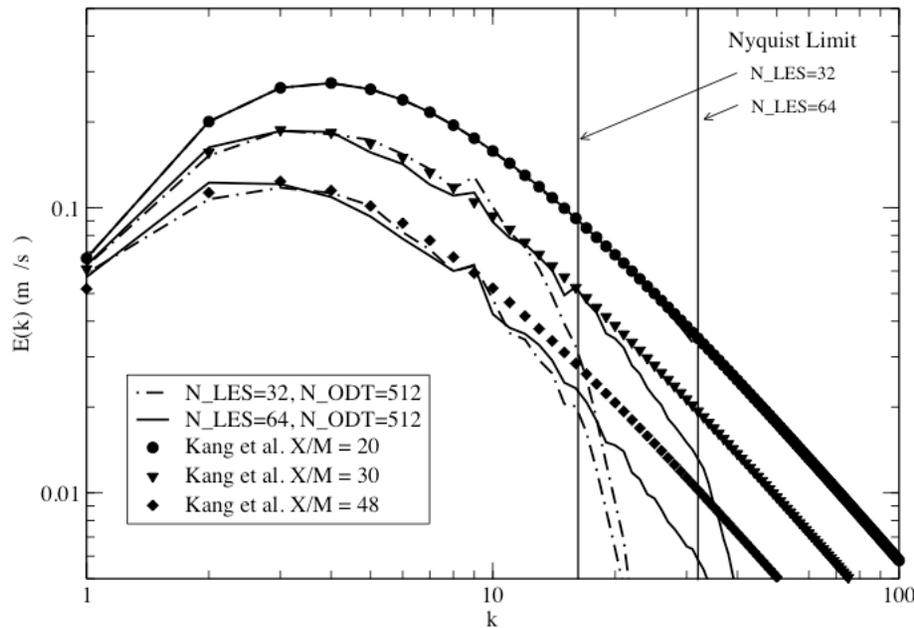


Note: Closing the 1D equations with a compatible eddy viscosity model (EMC) enables the model to resolve the dynamics to whatever length/time scales desired.

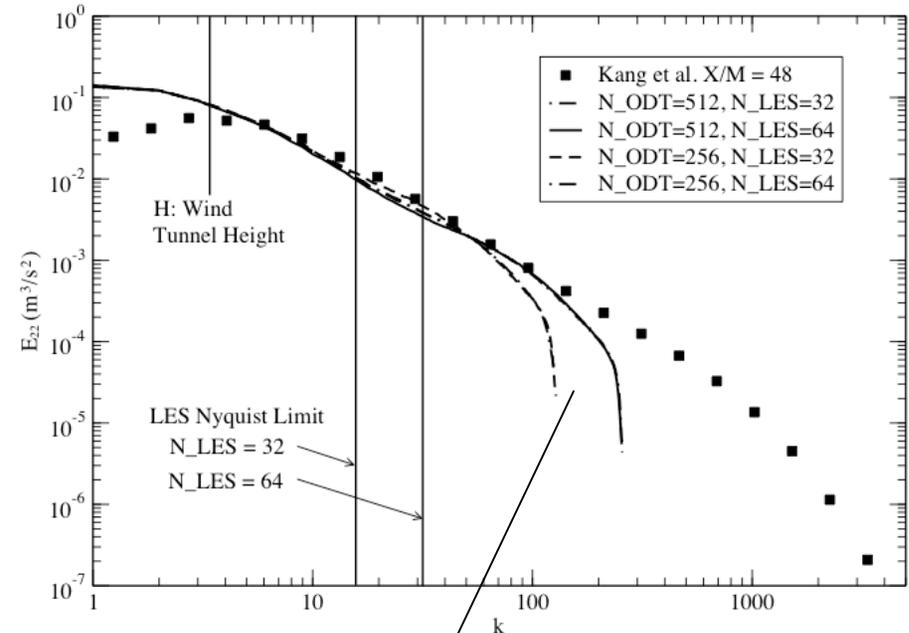


Sensitivity to LES-scale mesh size

32^3 and 64^3 LES grids, 256 and 512 pt ODT grids



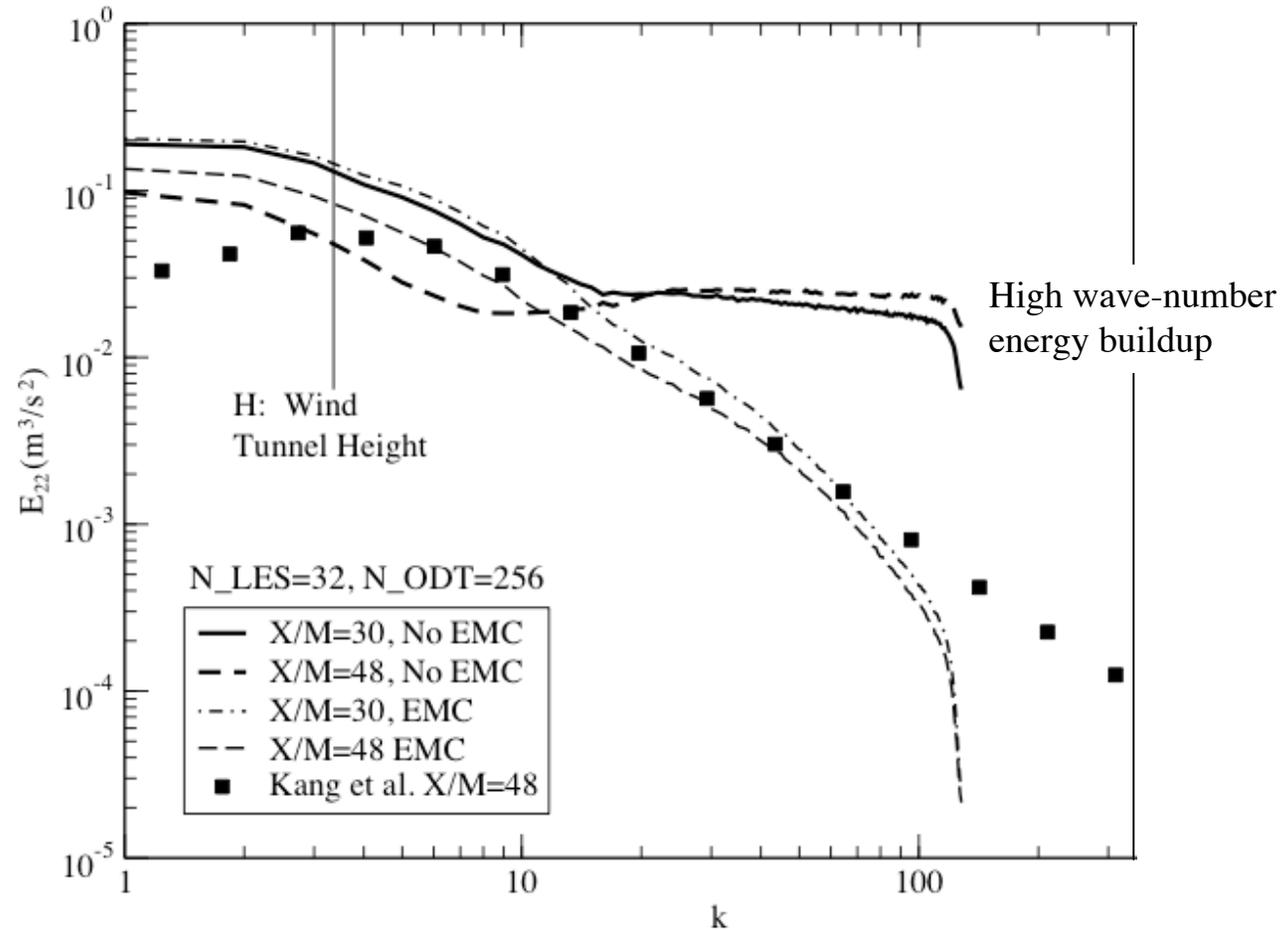
The expected differences in $E(k)$ for runs with different LES mesh sizes are clearly distinguishable.



The differences in E_{22} for runs with different LES mesh sizes are essentially indistinguishable.



Illustration of high wave-number energy build-up for under-resolved ODT without eddy-viscosity closure

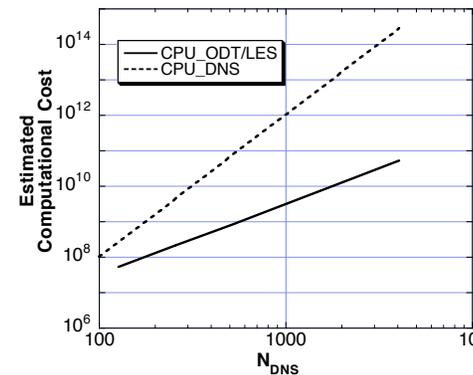




Closing Summary

- A novel multi-scale approach to turbulent flow simulations, called ODTLES, has been developed and tested that couples physical models at different length/time scales into an overall simulation approach.

- Major computational cost savings (as compared to DNS) are obtained by applying reduced dimensional modeling at the small scales



- Initial testing of the ODTLES approach on isotropic turbulent decay problem has yielded excellent results.

Schmidt, McDermott, Kerstein, "ODTLES: A Model for 3D Turbulent Flow Based on One-Dimensional Turbulence Modeling Concepts," Sandia National Labs, SAND2005-0206, 2005

- Techniques developed here for coupling 1-D model simulations at the small scales to 3-D model simulations at the large scale may be useful in suggesting strategies for super parameterization approaches being developed in the atmospheric sciences arena.





Models for Simulating Turbulent Flow

Navier-Stokes Equations (DNS)

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k} (\rho u_k) = 0 \quad \rho \frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_k} (\rho u_j u_k) = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_i} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + \rho f_j$$

Time Averaged (RANS)

$$\frac{\partial}{\partial x_k} (\rho \bar{u}_k) = 0$$

$$\frac{\partial}{\partial x_k} (\rho \bar{u}_j \bar{u}_k) = -\frac{\partial \bar{p}}{\partial x_j} + \frac{\partial}{\partial x_i} \left[\mu \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \rho \overline{u'_i u'_j} \right] + \bar{\rho} \bar{f}_j$$

where the overbar denotes a Reynolds averaged quantity, e.g.

$$\bar{\phi} = \lim_{\Delta t \rightarrow \infty} \frac{1}{\Delta T} \int_{t_0}^{t_0 + \Delta t} \phi(t) dt$$

and the prime denotes the instantaneous difference between the average and the mean, e.g.

$$\phi' = \phi - \bar{\phi}$$

Spatially “Filtered” (LES)

$$\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial}{\partial x_k} (\tilde{\rho} \tilde{u}_k) = 0$$

$$\tilde{\rho} \frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_k} (\tilde{\rho} \tilde{u}_j \tilde{u}_k) = -\frac{\partial \tilde{p}}{\partial x_j} + \frac{\partial}{\partial x_i} \left[\mu \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \right] + \tilde{\rho} \tilde{f}_j$$

Where $\tilde{\cdot}$ denotes a spatially filtered quantity, defined as

$$\tilde{\phi} = \int_D \phi(z,t) G(x-z, \Delta) dz$$

Here, G is the filter kernel, D is the domain of the flow, and Δ is the filter width in each spatial direction.

Note that $\tilde{\tilde{\phi}} \neq \tilde{\phi}$, and that the LES equations are derived under the assumption that the filtering operation commutes.

ODT Equations

$$\rho \frac{\partial u_i}{\partial t} = \frac{\partial}{\partial x_i} \left[\mu \left(\frac{\partial u_i}{\partial x_i} \right) \right] + \rho f_j + \text{eddy events}$$

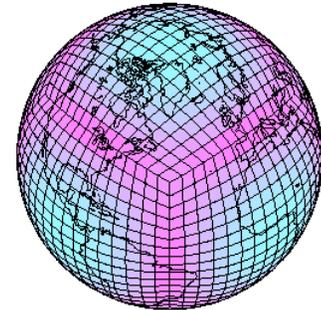


Introductory Comments 1: Why a novice like me is attending and giving a talk at a workshop like this.

- * SNL LDRD project called “MP Scalable Atmospheric Model”.
 - Bill Spotz, Mark Taylor, . . .

- * The **overall project goal** is to help develop a highly efficient, MP, global atmospheric model (SEAM) and demonstrate capability on Sandia’s new MP platforms
 - spectral element approach
 - local adaptive mesh refinement capability.

- * I was invited to look at the compatibility of current physics parameterizations with the higher resolution simulations that may soon be possible using adaptive mesh refinement and next generation computational software and hardware. This led to looking at how ODT modeling work may be applicable in this context.





The “Traditional” Large Eddy Simulation (LES) Approach

Based on the concept of “spatial filtering”

$$\bar{\phi}(\mathbf{x}, t) = \int_D \phi(\mathbf{x}, t) G(\mathbf{x} - \mathbf{z}, \Delta) d\mathbf{z},$$

For a filter that commutes with differentiation, direct application of the filtering operation to the incompressible NS equations yields

$$\rho \frac{\partial \bar{u}_i}{\partial t} + \rho \frac{\partial}{\partial x_j} (\overline{u_i u_j}) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial \bar{u}_i}{\partial x_j} \right) \right] + \rho \bar{f}_i$$

Defining a “sub-grid scale” stress tensor $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$, we can write

$$\rho \frac{\partial \bar{u}_i}{\partial t} + \rho \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial \bar{u}_i}{\partial x_j} \right) + \rho \tau_{ij} \right].$$

Parameterize τ_{ij} as a function of the filtered velocity field, e.g.

$$\tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = \frac{\mu_S}{\rho} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

Solve a **discretized** form of the equations on a finite mesh.



An early alternative LES approach: The discrete “Volume Balance method” of Schumann (1975)

Based on simple control-volume theory

Direct application of the control volume approach on a finite grid to the NS equations yields

Recast the equations in terms of a “sub-grid scale” surface flux tensor τ_{ij}

Parameterize τ_{ij} as a function of the volume averaged velocity field