LES Fundamentals, Equations, SGS-Models

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The Role of Turbulence (I)

- **Most flows in nature & technical applications are turbulent**
- **Significance of turbulence**
  - Meteorology / Oceanography: Transport processes of momentum, heat, water vapor as well as other scalars
  - Health care: Air pollution
  - Aviation, Engineering: Wind impact on airplanes, buildings, power output of windfarms
- **Characteristics of turbulence**
  - non-periodical, 3D stochastic movements
  - mixes air and its properties on scales between large-scale advection and molecular diffusion
  - non-linear → energy is distributed smoothly with wavelength
  - wide range of spatial and temporal scales

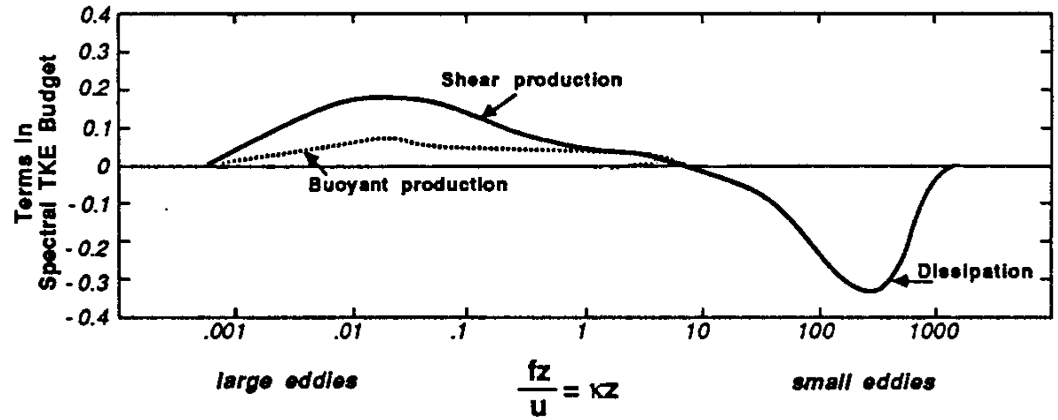
LES Fundamentals
The Role of Turbulence (II)

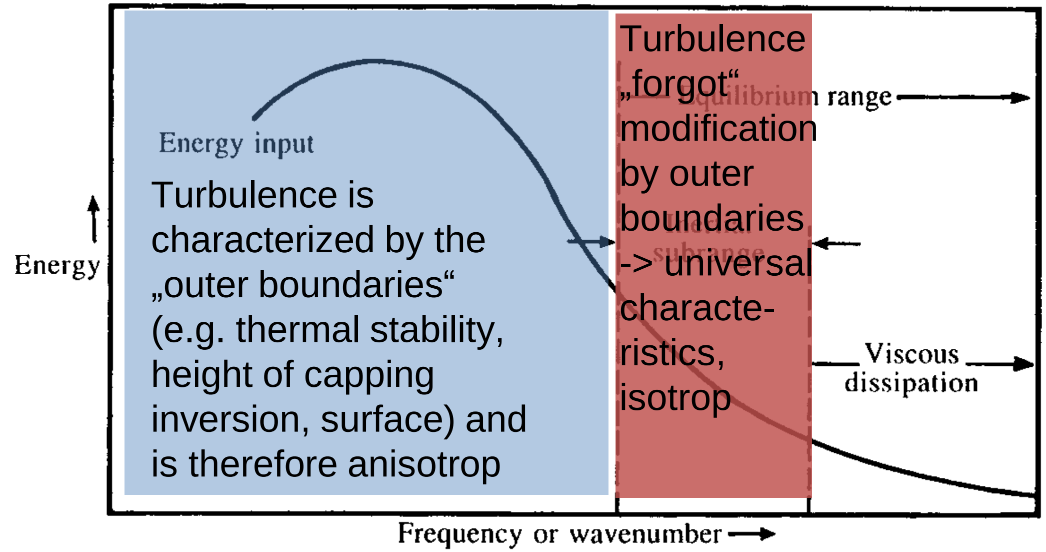
- **Large eddies:** 10^3 m (**L**), 1 h
  Small eddies: 10^{-3} m (η), 0.1 s

- **Energy production and dissipation on different scales**
  - Large scales: shear and buoyant production
  - Small scales: viscous dissipation

- **Large eddies contain most energy**

- **Energy-cascade**
  Large eddies are broken up by instabilities and their energy is handled down to smaller scales.





Stull (1988); Garratt (1992)

Resource requirements for Turbulence Simulation

$$\frac{L}{\eta} \approx Re^{\frac{3}{4}} \approx 10^6$$ (in the atmosphere)

$$Re = \frac{|\mathbf{u} \cdot \nabla \mathbf{u}|}{|\nu \nabla^2 \mathbf{u}|} \hat{=} \frac{LU}{\nu}$$

$\frac{\text{inertia forces}}{\text{viscous forces}}$

- $\mathbf{u}$ 3D wind vector
- υ kinematic molecular viscosity
- L outer scale of turbulence
- U characteristic velocity scale
- η inner scale of turbulence (Kolmogorov dissipation length)

➡ Number of gridpoints for a 3D simulation of the turbulent atmospheric boundary layer:

$$\left(\frac{L}{\eta}\right)^3 \approx Re^{\frac{9}{4}} \approx 10^{18}$$ (in the atmosphere)

Classes of Turbulence Models (I)

- **Direct numerical simulation (DNS)**
  - **Most straight-forward approach:**
    - Resolve all scales of turbulent flow explicitly.
  - **Advantage:**
    - (In principle) a very accurate turbulence representation.
  - **Problem:**
    - Limited computer resources (1996: ~10^8, today: ~ 10^{12} gridpoints, but ~ 10^{18} gridpoints needed, see prior slide).
    - 1 h simulation of 10^{10} (2150^3) gridpoints on 12288 cores (512 nodes) a Cray-XC40 needs about 10 h wallclock time .
  - **Consequences:**
    - DNS is restricted to moderately turbulent flows (low Reynolds-number flows).
    - Highly turbulent atmospheric turbulent flows cannot be simulated.

Classes of Turbulence Models (II)

- **Reynolds averaged (Navier-Stokes) simulation (RANS)**
  - **Opposite strategy:**
    - Applications that only require average statistics of the flow (i.e. the mean flow).
    - Integrate merely the ensemble-averaged equations.
    - Parameterize turbulence over the whole eddy spectrum.
  - **Advantage:**
    - Computationally inexpensive, fast.
  - **Problems:**
    - Turbulent fluctuations not explicitly captured.
    - Parameterizations are very sensitive to large-eddy structure that depends on environmental conditions such as geometry and stratification → Parameterizations are not valid for a wide range of different flows.
  - **Consequence:**
    - Not suitable for studies of turbulence (because it is parameterized).

Classes of Turbulence Models (III)

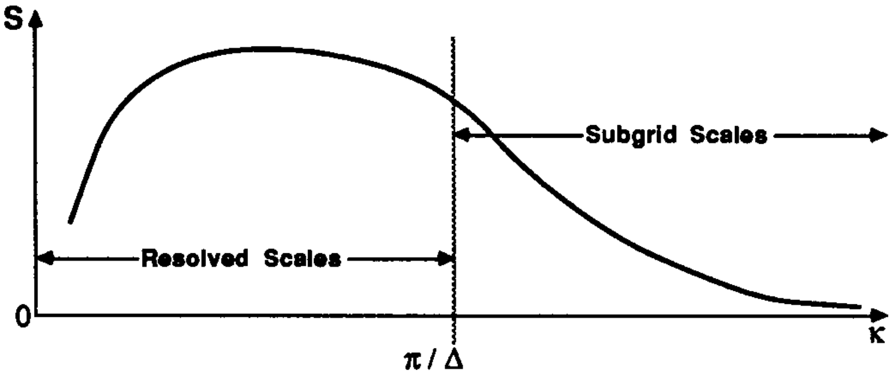
- **Large eddy simulation (LES)**
  - Seeks to combine advantages and avoid disadvantages of DNS and RANS by treating large scales and small scales separately, based on Kolmogorov's (1941) similarity theory of turbulence.
  - Large eddies are explicitly resolved.
  - The impact of small eddies on the large-scale flow is parameterized.
- **Advantages:**
  - Highly turbulent flows can be simulated.
  - Local homogeneity and isotropy at large Re (Kolmogorov's 1st hypothesis) leaves parameterizations uniformly valid for a wide range of different flows.

Concept of Large-eddy simulation (I)

Filtering:

- Spectral cut at wavelength Δ
- Structures larger than Δ are explicitly calculated (resolved scales).
- Structures smaller than Δ must be filtered out (subgrid scales), formally known as low-pass filtering.
- Like for Reynolds averaging: split variables in mean part and fluctuation, spatially average the model equations, e.g.:

$$w = \overline{w} + w', \;\; \theta = \overline{\theta} + \theta'$$



Stull (1988)

Concept of Large-eddy simulation (II)

- **Parameterization**
  - The filter procedure removes the small scales from the model equations, but it produces new unknowns, mainly averages of fluctuation products.
    - e.g., $\overline{w'\theta'}$
  - These unknowns describe the effect of the unresolved, small scales on the resolved, large scales; therefore it is important to include them in the model.
  - We do not have information about the variables (e.g., vertical wind component and potential temperature) on these small scales of their fluctuations.
  - Therefore, these unknowns have to be parameterized using information from the resolved scales.
    - A typical example is the flux-gradient relationship, e.g.,

$$\overline{w'\theta'} = -\nu_h \cdot \frac{\partial \overline{\theta}}{\partial z}$$

- Navier-Stokes equations

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_k u_i}{\partial x_k} = -\frac{1}{\rho_0}\frac{\partial p^*}{\partial x_i} - \varepsilon_{ijk} f_j u_k + \varepsilon_{i3k} f_3 u_{k_\mathrm{g}} + g\frac{T - T_0}{T_0}\delta_{i3} + \nu \frac{\partial^2 u_i}{\partial x_k^2}$$

- First principle of thermodynamics

$$\frac{\partial T}{\partial t} + u_k \frac{\partial T}{\partial x_k} = \nu_\mathrm{h} \frac{\partial^2 T}{\partial x_k^2} + Q$$

This set of equations is valid for almost all kind of CFD models!

- Equation for passive scalar

$$\frac{\partial \psi}{\partial t} + u_k \frac{\partial \psi}{\partial x_k} = \nu_\psi \frac{\partial^2 \psi}{\partial x_k^2} + Q_\psi$$

- Continuity equation

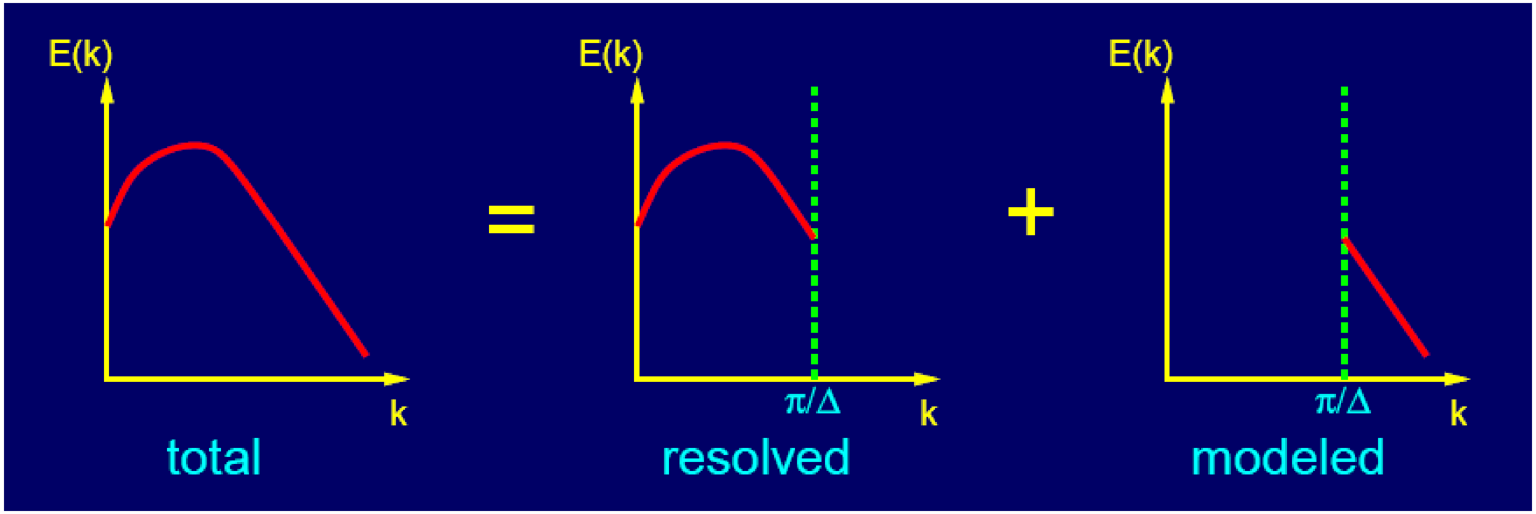
$$\frac{\partial u_k}{\partial x_k} = 0$$

$$\frac{\partial \rho_0(z)\, u_k}{\partial x_k} = 0$$ anelastic approximation

LES – Scale separation by spatial filtering (I)

$$\Psi(x_i, t) = \overline{\Psi}(x_i, t) + \Psi'(x_i, t)$$

- LES technique is based on scale separation, in order to reduce the number of degrees of freedom of the solution.
- Large (low-frequency) modes $\overline{\Psi}$ are calculated directly (resolved scales).
- Small (high-frequency) modes Ψ‘ are parameterized using a statistical model (subgrid / subfilter scales, SGS model).
- These two categories of scales are separated by defining a cutoff length Δ.



LES – Scale separation by spatial filtering (II)

- The filter applied is a spatial filter:

$$\overline{\Psi}(x_i) = \int_D G(x_i - x_i')\Psi(x_i')dx_i'$$

Filterfunction e.g. Boxfilter:

$$G(x_i - x_i') = \begin{cases} \frac{1}{\Delta} & ; |x_i - x_i'| \leq \frac{\Delta}{2} \\ 0 & ; \text{else} \end{cases}$$

$$\overline{\Psi'}(x_i) = 0 \quad but \quad \overline{\overline{\Psi}} \neq \overline{\Psi}(x_i)$$

compare: →

Ensemble average:

$$\overline{\overline{\Psi}}(x_i) = \overline{\Psi}(x_i)$$

$$\overline{u_k u_i} = \overline{u_k}\,\overline{u_i} + \overline{u_k' u_i'}$$

- Filter applied to the nonlinear advection term:

$$\overline{u_k u_i} = \overline{(\overline{u_k} + u_k')(\overline{u_i} + u_i')} = \overline{\overline{u_k}\,\overline{u_i}} + \underbrace{\overline{\overline{u_k} u_i'} + \overline{u_k' \overline{u_i}}}_{C_{ki}} + \underbrace{\overline{u_k' u_i'}}_{R_{ki}}$$

Filter would need to be applied a second time. To avoid this,

- Leonard proposes a further decomposition:

$$\overline{\overline{u_k}\,\overline{u_i}} = \overline{u_k}\,\overline{u_i} + \underbrace{\left(\overline{\overline{u_k}\,\overline{u_i}} - \overline{u_k}\,\overline{u_i}\right)}_{L_{ki}}$$

R_{ki}: **Reynolds-stress**
C_{ki}: **cross-stress**
L_{ki}: **Leonard-stress**
τ_{ki}: **total stress-tensor generalized Reynolds stress**

➡ $$\overline{u_k u_i} = \overline{u_k}\,\overline{u_i} + \underbrace{L_{ki} + C_{ki} + R_{ki}}_{\text{To be parameterized}} = \overline{u_k}\,\overline{u_i} + \tau_{ki}$$

To be parameterized

LES – Scale separation by spatial filtering (III)

- Volume-balance approach (Schumann, 1975)
  advantage: numerical discretization acts as a Reynolds operator

$$\Psi(V,t) = \frac{1}{\Delta x \cdot \Delta y \cdot \Delta z} \int\int\int_V \Psi(V',t)\,dV'$$

$$\overline{\Psi'}(x_i) = 0 \quad \text{and} \quad \overline{\overline{\Psi}} = \overline{\Psi}$$

Ensemble average:

$$\overline{\overline{\Psi}}(x_i) = \overline{\Psi}(x_i)$$

$$\overline{u_k u_i} = \overline{u_k}\,\overline{u_i} + \overline{u_k' u_i'}$$

$$V = \left[x - \frac{\Delta x}{2}, x + \frac{\Delta x}{2}\right] \times \left[y - \frac{\Delta y}{2}, y + \frac{\Delta y}{2}\right] \times \left[z - \frac{\Delta z}{2}, z + \frac{\Delta z}{2}\right]$$

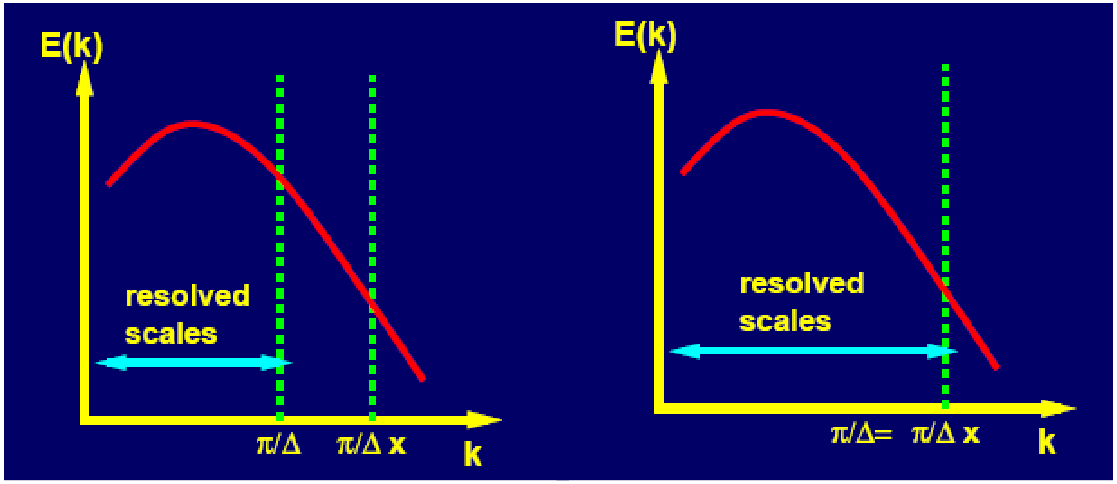
- Filter applied to the nonlinear advection term:

$$\overline{u_k u_i} = \overline{(\overline{u_k} + u_k')(\overline{u_i} + u_i')} = \overline{u_k}\,\overline{u_i} + \overline{u_k' u_i'}$$

The filtered equations

$$\frac{\partial \overline{u_i}}{\partial t} + \frac{\partial \overline{u_k}\,\overline{u_i}}{\partial x_k} = -\frac{1}{\rho_0}\frac{\partial \overline{p}^*}{\partial x_i} - \varepsilon_{ijk} f_j \overline{u_k} + \varepsilon_{i3k} f_3 \overline{u}_{k_g} + g\frac{\overline{T} - T_0}{T_0}\delta_{i3} + \nu \frac{\partial^2 \overline{u_i}}{\partial x_k^2} - \frac{\partial \tau_{ki}}{\partial x_k}$$

- The computational grid introduces another spatial scale: the discretization step Δx_i.
- Δx_i has to be small enough to be able to apply the filtering process correctly: $\Delta x_i \leq \Delta$
- Two possibilities:
  - Pre-filtering technique ($\Delta x < \Delta$, explicit filtering)
  - Linking the analytical filter to the computational grid ($\Delta x = \Delta$, implicit filtering)



Explicit versus implicit filtering

- **Explicit filtering:**
  - Requires that the analytical filter is applied explicitly.
  - Filter characteristics are known exactly.
  - Rarely used in practice, due to additional computational costs.
- **Implicit filtering:**
  - The analytical cutoff length is associated with the grid spacing.
  - This method does not require the use of an analytical filter.
  - The filter characteristic cannot really be controlled.
  - Because of its simplicity, this method is used by nearly all LES models.

Literature:

Sagaut, P., 2001: Large eddy simulation for incompressible flows: An introduction. Springer Verlag, Berlin/Heidelberg/New York, 319 pp.

Schumann, U., 1975: Subgrid scale model for finite difference simulations of turbulent flows in plane channels and annuli. J. Comp. Phys., 18, 376-404.

Wyngaard, J.C., 2010: Turbulence in the Atmosphere. Cambridge University Press, New York, 393 pp.

LES Fundamentals

The final set of equations (PALM)

- Navier-Stokes equations:

$$\frac{\partial \overline{u_i}}{\partial t} = -\frac{\partial \overline{u_k}\,\overline{u_i}}{\partial x_k} - \frac{1}{\rho_0}\frac{\partial \overline{\pi}^*}{\partial x_i} - \varepsilon_{ijk} f_j \overline{u_k} + \varepsilon_{i3k} f_3 \overline{u}_{k_g} + g\frac{\overline{\theta}_v - \theta_0}{\theta_0}\delta_{i3} - \frac{\partial \tau^r_{ki}}{\partial x_k}$$

- First principle (using virtual potential temperature)

$$\theta_v = \theta\,(1 + 0.61q - q_L)$$

$$\frac{\partial \overline{\theta}_v}{\partial t} = -\frac{\partial \overline{u_k}\,\overline{\theta}}{\partial x_k} - \frac{\partial H_k}{\partial x_k} + Q_\theta$$

normal stresses included in the stress tensor are now included in a modified dynamic pressure:

$$\tau^r_{ki} = \tau_{ki} - \frac{1}{3}\tau_{jj}\delta_{ki}$$

$$\overline{\pi}^* = \overline{p}^* + \frac{1}{3}\tau_{jj}\delta_{ki}$$

- Equation for specific humidity (passive scalar q = s)

$$\frac{\partial \overline{q}}{\partial t} = -\frac{\partial \overline{u_k}\,\overline{q}}{\partial x_k} - \frac{\partial W_k}{\partial x_k} + Q_w$$

subgrid-scale stresses (fluxes) to be parameterized in the SGS model:

$$\tau_{ki} = \overline{u_k u_i} - \overline{u_k}\,\overline{u_i} \quad = \overline{u'_k u'_i}$$

$$H_k = \overline{u_k \theta} - \overline{u_k}\,\overline{\theta} \quad = \overline{u'_k \theta'}$$

$$W_k = \overline{u_k q} - \overline{u_k}\,\overline{q} \quad = \overline{u'_k q'}$$

In case of Schumann-filtering

- Continuity equation

$$\frac{\partial \overline{u_k}}{\partial x_k} = 0 \qquad \frac{\partial \overline{\rho}_0(z)\,\overline{u}_k}{\partial x_k} = 0$$

SGS Models (I)

- The SGS model has to parameterize the effect of the SGS motions (small-scale turbulence) on the large eddies (resolved-scale turbulence).

- Features of small-scale turbulence (within the inertial subrange): **local, isotropic, dissipative**

- SGS stresses should depend on:
  - local resolved-scale field and / or
  - past history of the local fluid (via a PDE)

- Importance of the model depends on how much energy is contained in the subgrid-scales:
  - $E_{SGS} / E < 50\%$: results relatively insensitive to the model, (but sensitive to the numerics, e.g. in case of upwind scheme)
  - $E_{SGS} / E = 1$: SGS-model is more important
  - **If the large-scale eddies are not resolved, the SGS model and the LES will fail at all!**

SGS Models (II)

- **Requirements that a good SGS model must fulfill:**
  - Represent interactions with small scales.
  - Provide adequate dissipation (transport of energy from the resolved grid scales to the unresolved grid scales; the rate of dissipation ε in this context is the flux of energy through the inertial subrange).
  - Dissipation rate must depend on the large scales of the flow rather than being imposed arbitrarily by the model. The SGS model must depend on the large-scale statistics and must be sufficiently flexible to adjust to changes in these statistics.
  - In energy conserving codes (ideal for LES) the only way for TKE to leave the resolved modes is by the dissipation provided by the SGS model.
  - **The primary goal of an SGS model is to obtain correct statistics of the energy containing scales of motion.**

SGS Models (III)

All the above observations suggest the use of an eddy viscosity type SGS model:

- Take idea from RANS modeling, introduce eddy viscosity ν_T:

$$\tau_{ki} = -\nu_T \left(\frac{\partial \overline{u_k}}{\partial x_i} + \frac{\partial \overline{u_i}}{\partial x_k} \right) = -2\nu_T \overline{S}_{ki} \qquad \text{with} \quad \overline{S}_{ki} = \frac{1}{2} \left(\frac{\partial \overline{u_k}}{\partial x_i} + \frac{\partial \overline{u_i}}{\partial x_k} \right)$$

filtered strain rate tensor

Now we need a model for the **eddy viscosity**:

- Dimensionality of ν_T is l^2/t [m²/s]
- Obvious choice: $\nu_T = Cql$ (q, l : characteristic velocity / length scale)
- Turbulence length scale is easy to define: largest size of the unresolved scales is Δ:

$$l = \Delta$$

- Velocity scale not as obvious (smallest resolved scales, their size is of the order of the variation of velocity over one grid element)

$$q = l \frac{\partial \overline{u}}{\partial x} = l\overline{S} \qquad \text{for 3D: } \overline{S} = \sqrt{2\overline{S}_{ki}\,\overline{S}_{ki}}$$

characteristic filtered rate of strain

The Smagorinsky model

- Combine previous expressions to obtain:

$$\nu_T = C\Delta^2\overline{S} = (C_S\Delta)^2\overline{S}$$

- Model due to Smagorinsky (1963):
  - Originally designed at NCAR for global weather modeling.
  - Can be derived in several ways: heuristically (above), from inertial range arguments (Lilly), from turbulence theories.
  - Constant predicted by all methods (based on theory, decay of isotropic turbulence):

$$C_S = \sqrt{C} \approx 0.2$$

The Smagorinsky model: Performance

- Predicts many flows reasonably well
- **Problems:**
  - Optimum parameter value varies with flow type:
    - Isotropic turbulence: $C_S \approx 0.2$
    - Shear (channel) flows: $C_S \approx 0.065$
  - Length scale uncertain with anisotropic filter:

$$(\Delta_x \Delta_y \Delta_z)^{1/3} \qquad (\Delta_x + \Delta_y + \Delta_z)/3$$

  - Needs modification to account for:
    - stratification: $C_S = F(Ri,\ldots)$, Ri: Richardson number
    - near-wall region: $C_S = F(z+)$, z+: distance from wall

Deardorff (1980) modification used in PALM (I)

$$\nu_T = Cql = C_M \Lambda \sqrt{\bar{e}} \quad \text{with} \quad \bar{e} = \frac{\overline{u_i' u_i'}}{2} \quad \text{SGS-turbulent kinetic energy}$$

see also Moeng and Wyngaard (1988), Saiki et al. (2000)

- The SGS-TKE allows a much better estimation of the velocity scale for the SGS fluctuations and also contains information about the past history of the local fluid.

$$C_M = const. = 0.1$$

$$\Lambda = \begin{cases} min\left(0.7 \cdot z, \Delta\right), & \textbf{unstable or neutral stratification} \\ min\left(0.7 \cdot z, \Delta, 0.76\sqrt{\bar{e}}\left[\frac{g}{\Theta_0}\frac{\partial\bar{\Theta}}{\partial z}\right]^{-1/2}\right), & \textbf{stable stratification} \end{cases}$$

$$\Delta = (\Delta x \Delta y \Delta z)^{1/3}$$

Deardorff (1980) modification used in PALM (II)

- SGS-TKE from prognostic equation

$$\frac{\partial \bar{e}}{\partial t} = -\bar{u}_k \frac{\partial \bar{e}}{\partial x_k} - \tau_{ki} \frac{\partial \bar{u}_i}{\partial x_k} + \frac{g}{\Theta_0} \overline{u_3' \Theta'} - \frac{\partial}{\partial x_k} \left\{ \overline{u_k' \left(e' + \frac{\pi'}{\rho_0} \right)} \right\} - \varepsilon$$

$$\tau_{ki} = -\nu_T \left(\frac{\partial \bar{u}_i}{\partial x_k} + \frac{\partial \bar{u}_k}{\partial x_i} \right) + \frac{2}{3} \delta_{ik} \bar{e} \qquad \text{with} \qquad \nu_T = 0.1 \cdot \Lambda \sqrt{\bar{e}}$$

$$H_k = \overline{u_k' \Theta'} = -\nu_h \frac{\partial \bar{\Theta}}{\partial x_k} \qquad \text{with} \qquad \nu_h = \left(1 + 2 \frac{\Lambda}{\Delta} \right)$$

$$\frac{\partial}{\partial x_k} \left[\overline{u_k' \left(e' + \frac{\pi'}{\rho_0} \right)} \right] = -\frac{\partial}{\partial x_k} \nu_e \frac{\partial \bar{e}}{\partial x_k}$$

$$\nu_e = 2 \nu_T$$

$$\epsilon = C_\epsilon \frac{\bar{e}^{3/2}}{\Lambda} \qquad C_\epsilon = 0.19 + 0.74 \frac{\Lambda}{\Delta}$$

Deardorff (1980) modification used in PALM (III)

- There are still problems with this parameterization:
  - The model overestimates the velocity shear near the wall.
  - C_M is still a constant but actually varies for different types of flows.
  - Backscatter of energy from the SGS-turbulence to the resolved-scale flow can not be considered.
- Several other SGS models have been developed:
  - Two part eddy viscosity model (Sullivan, et al.)
  - Scale similarity model, dynamic SGS (Bardina et al.)
  - Backscatter model (Mason)
  - PALM optionally offers a dynamic SGS model (Mokhtarpoor et al.)
- For fine grid resolutions ($E_{SGS} << E$) LES results become less and less dependent from the different models.
- However, SGS models still show significant dependence on grid spacing under stable stratification (no convergence of results).
  - A modified Deardorff SGS-model from Dai et al. (2020), which is implemented in PALM, too, shows less dependence.